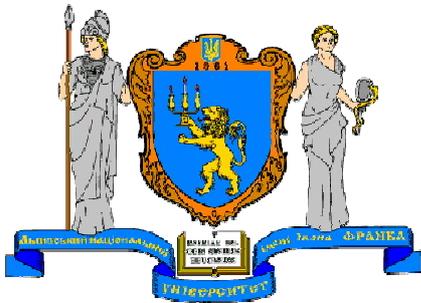


Міністерство освіти і науки України  
Львівський національний університет імені Івана Франка  
Фізичний факультет



**МАТЕРІАЛИ**  
**VI Міжнародної наукової конференції**  
**“Фізика неупорядкованих систем”,**  
*присвяченої 80-річчю від дня народження*  
*професора Ярослава Дутчака*

*14-16 жовтня 2013р.*

**ЛЬВІВ, УКРАЇНА**

**Фізика неупорядкованих систем.** Збірник тез, Львів, Україна, 14-16 жовтня 2013, Львівський національний університет імені Івана Франка, 172с.

Опубліковано матеріали VI Міжнародної конференції з фізики неупорядкованих систем, присвяченої 80-річчю з дня народження професора Я.Й.Дутчака. Відображено результати теоретичних та експериментальних досліджень рідин, аморфних сплавів та інших структурно неупорядкованих систем.

Розглянуто структурні особливості цих систем та закономірності зміни ближнього порядку від температури та складу. Значна кількість доповідей присвячена структурі та властивостям наноструктурованих матеріалів. Описано результати модельних досліджень фізичних процесів, пов'язаних з явищами релаксації в аморфних сплавах, нанокристалізацією та іншими фазовими перетвореннями.

Матеріали надруковано в авторській редакції

Відповідальний за випуск професор Мудрий С.І.  
Макетування асистент Присяжнюк В.І.

Фізичний факультет, кафедра фізики металів,  
вул. Кирила і Мефодія, 8, Львів, 79005, Україна  
**Тел.:** 8-(0322) 72-70-64  
**E-mail:** pds2013@ukr.net  
**Web:** <http://physics.lnu.edu.ua/pds2013/>

(С) Львівський національний університет імені Івана Франка, 2013



## ДУТЧАК Ярослав Йосипович

(14.X.1933, село Гаї Смоленські Бродівського району, Львівської області – 8.II.1988, місто Львів) – видатний фізик, кандидат фізико-математичних наук (*К вопросу о структуре и физических свойствах некоторых металлических жидкостей*, 1962), доцент (1963), доктор. фізико-математичних наук (*Некоторые результаты исследований по физике жидких металлов и тонких пленок*, 1967), професор (1968). Закінчив фізичний факультет Львівського університету

(1956). У 1956-62р. асистент, 1962-63р. доцент, 1963-88 завідував кафедрою рентгенометалофізики Львівського університету, ініціатор її створення. Наукові інтереси: дослідження структури рідких кристалів та фізика тонких плівок. Був ініціатором і брав участь у розвитку експериментальної бази і наукових досліджень на кафедрі; започаткував наукові напрями з рентгенівської спектроскопії, дослідження структури і фізичних властивостей рідких металів, динаміки кристалічної ґратки, електрофізичних властивостей, розробив методики рентгенографії, електронної і растрової мікроскопії. Керівник 2 докторських, 50 кандидатських дисертацій. Автор близько 400 наукових праць, зокрема, *Рентгенография жидких металлов* (Львів, 1977); *Методология исследования развития сложных систем: Естественнаучный подход* (1974; с соавт.); *Стабильность превращения и фазовые равновесия в металлических системах* (Белград, 1988; с соавт.); *Молекулярна фізика* (Львів, 1973); *Молекулярна фізика* (1990; зі співат.); *Фізика металів* (1993; зі співат.).

Член координаційних рад при АН УРСР і Мінвузі України з фізики рідкого стану, фізики твердого тіла, організаційних комітетів з проведення наукових конференцій, неодноразово очолював їх, упродовж 10 років очолював спеціалізовану раду з захисту докторських і кандидатських дисертацій, відповідальний редактор Вісника Львівського університету. Серія фізична. За видатні досягнення в науковій діяльності отримав Державну премію України в галузі науки і техніки (1983).

# **Fundamental importance of the Ya. Dutchak works in study of melts for modern nanophysics and nanotechnologies**

*S.Mudry*

*Ivan Franko National University of Lviv, Ukraine*

Most of structure studies carried out by prof. Ja Dutchak and co-workers by means of X-Ray diffraction and structure- sensitive properties measurements. Among numerous molten metallic and semi-conducting systems eutectic alloys were in centre of his interest and he was the first, who systematically have investigated the structure of liquid eutectics within some temperature range upon melting.among different kind alloys are systems with large terminal solubility, ones with envelope point in liquidus curve, eutectic systems with negative mixing enthalpy and degenerated eutectics.

Main conclusion, which followed from studies of liquid eutectic alloys, was the fact that these alloys reveal an inhomogeneous atomic distribution within temperature range near melting point. In other words the eutectic melts significantly transform their structure at heating and reveal the transition from cluster-cluster structure to structure, corresponding to random atomic distribution.

Many results, obtained by prof. Ja. Dutchak are cited in many publications over the world. Main feature of his studies is an attempt to combine the structure data, obtained by means of diffraction data with results of structure- sensitive properties measurements (density, viscosity, electroconductivity, surface tension etc.)

# Професор Дутчак Я.Й. – знання і рішучість

Романюк М.О.

*Львівський національний університет імені Івана Франка, Львів, Україна*

Винесені у заголовок слова – одні з важливих характеристик Ярослава Йосиповича як людини і вченого. Про нього знаю не тільки як колега по факультету, сусід по кафедрі, але й як очевидець відповідних ситуацій. Ось характерні з багатьох приклади.

1. Навальна робота Ярослава Йосиповича над докторською дисертацією та її захист на стороні (Баку) були викликані певною затримкою у присвоєнні йому вченого звання доцента. На це він реагував так: *«нічого, скоро присвоять звання професора»*.
2. На часто неочікувану і термінову інформацію про надходження документів для вступу в університет та характеристику абітурієнтів за школами, успішністю, соціальним походженням та ін., він, як відповідальний секретар Приймальної комісії, створив спеціальну групу працівників цієї комісії, а згодом *розпочав машинну обробку відповідних даних*. І хоч перфорування матеріалів гальмувало справу, цей підхід сьогодні є не замінимим.
3. Щоб не зірвати засідання Ради фізичного факультету по захисту дисертації через неявку «прикріпленої» до ради стенографістки, він, як голова Ради, порушує існуючі норми і *вирішує вести магнітофонний запис цього засідання*, чим по суті започатковує теперішню процедуру захисту.
4. При звіті нашої спеціалізованої Ради по захисту дисертацій про роботу у ВАК СРСР (Москва) на специфічне запитання члена комісії «Что ТЫ сделал для внедрения материалов защищенных в Совете работ?», яке ставило під сумнів успішність роботи Ради, *він відповів достойно хоч ризиковано лише кількома словами: «А какие полномочия ТЫ мне для этого дал? Більше питань не було. Після певної напруженої тиші професор Московського державного університету Ахманов С.А. запропонував схвалити звіт про роботу нашої Ради, що й було зроблено.*

Так знання та рішучість давали хороші результати, працювали на перспективу, що варто активно наслідувати.

## Секція 1

*Теорія неупорядкованих систем.*

*Міжчастинкові кореляції у квантових системах.*

*Моделювання і симуляція структури та фізичних*

*властивостей.*

# Effect of ion polarization on transverse excitations in molten salts

<sup>1</sup>Markiv B., <sup>1</sup>Vasylenko A., <sup>1,2</sup>Tokarchuk M.

<sup>1</sup>*Institute for Condensed Matter Physics, Lviv, Ukraine*

<sup>2</sup>*National University "Lviv Polytechnic", Lviv, Ukraine*

The study of equilibrium and nonequilibrium properties of molten salts remains an active area of research from the viewpoint of experimental, theoretical as well as computer simulation approaches. The study of collective modes in such systems is of a great interest. In earlier researches of collective dynamics in molten salts the rigid-ion model was used according to which ions are supposed to have a rigid form without any polarization. However, in real melts, outer electron shells can deform and ions can be polarized. In Ref. [1] based on both the rigid-ion and ab initio molecular dynamics simulations it was shown that, in the domain of small wavenumbers, the rigid-ion model yields higher values of optic modes frequencies compared to ab initio calculations that take into account the polarization processes. This is the evidence that polarization effects in NaCl (in this case caused mainly by the Cl<sup>-</sup> ions due to their higher polarizability) can not be neglected. In Ref. [2] the effect of ion polarization on longitudinal excitations in molten salt in hydrodynamic limit was studied theoretically.

In the present work a spectrum of transverse collective excitations in molten salt is investigated theoretically with taking into account polarization effects. Within the model only negatively charged ions are considered to be polarized. By means of the perturbation theory the cross-correlations between optic-like modes and dipole one are taken into account. Based on the obtained analytical expressions the effect of ion polarization on transverse excitations in molten salt is analyzed.

1. Bryk T., Mryglod I., Ab initio study of dispersion of optic-like modes in a molten salt: Effect of ion polarization // Chem. Phys. Lett., 2008, Vol. 466, 56-60.
2. Markiv B., Vasylenko A., Tokarchuk M., Statistical description of hydrodynamic processes in ionic melts while taking into account polarization effects // J. Chem. Phys., 2012, Vol. 136, 234502.

## Kinetics of spinodal decomposition in amorphous alloys

Terekhova Yu.V., Stefanovich L.I., Yurchenko V.M.  
*Galkin Institute for Physics & Engineering, Donetsk, Ukraine*

It is known that spinodal decomposition takes place in the cases when we succeed to transfer a system into a region characterized by an absolute instability of a homogeneous state, i.e. under the spinodal curve. If the such transfer to realize by a rapid quenching, then it needs very high quenching rates that phase separation did not occurs in the binodal region yet. It follows that spinodal decomposition is actual first of all for metallic amorphous alloys which are formed over the very short times  $10^{-9} - 10^{-3}$  s.

For a description of spinodal decomposition in these systems we are used a phenomenological approach, in the framework of which a generalized, nonlinear diffusion Cahn-Hilliard equation has been received. The analysis of this equation showed that if the system is in the average outside the spinodal, the effective diffusion coefficient is positive and the system behaves itself as in the ordinary diffusion. If an average composition of alloy is within the spinodal region, the effective diffusion coefficient turns out a negative one, resulting in the "uphill" diffusion and the modulated structures [1, 2]. To this equation it should be attached the initial condition connected with a presence of concentration fluctuations immediately after quenching. Considering that a function appearing in the initial condition is a random function of the coordinates, so thereafter a statistical approach was used to describe the evolution of the amorphous alloy. As a result the system of evolution equations for the correlators of second and third orders was obtained. In distinction to [1-3] in the present work the "gradient" terms were included, result in a system equations of fourth order.

The solution of this system enables to obtain a quite total information about a process of concentration separation, in particular, to search for the average spatial scale of concentration inhomogeneities, their dispersion (i.e. the root-mean-square amplitude of inhomogeneities) and the asymmetry parameter (which allows to estimate the concentration in precipitates of new phase and a volume of precipitates also).

1. E.P. Feldman, L.I. Stefanovich. Evolution of "frozen" concentration fluctuations during decomposition of glasses with near-spinodal compositions// *Zh. Eksp. Teor. Fiz.* – 1989. – V. 96. – P. 1513 – 1521.
2. E.P. Feldman, L.I. Stefanovich. Kinetics of the spinodal decomposition of glasses // *Zh. Eksp. Teor. Fiz.* – 1990. – V. 98. – P. 1695 – 1704.
3. L.I. Stefanovich, Yu.V. Terekhova, Yurchenko V.M. The influence of concentration dependence of mobility on the spinodal decomposition of glasses// *Physics and technology of high pressures.* – 2010. – V. 20. – P. 63 – 73. (in Russian).

# **Statistical theory of reaction-diffusion processes lithium ions in the system “electrolyte – electrode”**

Kostrobij P. P.<sup>1</sup>, Markovycn B. M.<sup>1</sup>, Tokarchuk R. M.<sup>1</sup>,  
Chornomorets Yu.<sup>2</sup>, Tokarchuk M. V.<sup>1,2</sup>

<sup>1</sup>*Lviv Polytechnic National University, Lviv, Ukraine*

<sup>2</sup>*Institute for Condensed Matter Physics, Lviv, Ukraine*

Statistical consistent description of the system “electrolyte – electrode” with account to reaction–diffusion and electromagnetic processes is formulated. For the first time, the self-consistent system of generalized reaction-diffusion kinetic transport equations agreed with the averaged Maxwell equations for electromagnetic fields of the system “electrolyte – electrode” is obtained with use the Zubarev’s method of nonequilibrium statistical operator .

# Узгоджений опис кінетики та гідродинаміки слабонерівноважних процесів у простих рідинах

Токарчук М., Марків Б., Омелян І.

*Інститут фізики конденсованих систем НАН України, Львів, Україна*

Проблема побудови узгодженого опису кінетичних та гідродинамічних процесів у густих газах, рідинах та плазмі залишається актуальною в наш час. В даній роботі досліджено систему рівнянь переносу узгодженого опису кінетики та гідродинаміки слабонерівноважних процесів, отриману в рамках методу нерівноважного статистичного оператора Д.Зубарєва. Розкрито структуру функцій пам'яті, що входять у рівняння. Показано, що інтеграл зіткнень кінетичного рівняння для нерівноважної одночастинкової функції розподілу має структуру типу Фоккера-Планка з узагальненим коефіцієнтом тертя в імпульсному просторі. Він також містить внески від узагальненого коефіцієнта дифузії в імпульсному просторі. Методом проектування такої системи рівнянь переносу на перші моменти нерівноважної одночастинкової функції розподілу отримано систему рівнянь розширеної гідродинаміки та виконано перехід до рівнянь молекулярної гідродинаміки.

Цікавим є випадок, коли потенціал взаємодії в системі можна представити у вигляді суми потенціалу взаємодії твердих сфер та деякого далекосяжного потенціалу. Тоді, враховуючи особливості динаміки моделі твердих сфер, у кінетичному рівнянні можна виділити інтеграл зіткнення Енскога-Больцмана. Проектуючи таку систему рівнянь на моменти нерівноважної одночастинкової функції розподілу, отримано систему рівнянь переносу з виділеним вкладом моделі твердих сфер. На її основі отримано спектр колективних збуджень системи у гідродинамічній границі. Показано, що, окрім вкладу від потенціалу взаємодії твердих сфер, усі гідродинамічні модах містять вклади від далекосяжної частини потенціалу.

1. B. Markiv, I. Omelyan, M. Tokarchuk, Consistent description of kinetics and hydrodynamics of weakly nonequilibrium processes in simple liquids // Preprint arXiv:1308.3627, 2013.

# Coupling of longitudinal and transverse collective excitations in collective dynamics of liquid metals

Bryk T.<sup>1</sup>, Ruocco G.<sup>2</sup>, Scopigno T.<sup>2</sup>

<sup>1</sup> *Institute for Condensed Matter Physics, NASU, Lviv, Ukraine*

<sup>2</sup> *Dipartimento di Fisica, Universita' di Roma "La Sapienza", Roma, Italy*

An issue of visibility of transverse collective excitations in dynamic structure factors of metallic liquids has emerged after a report by Hosokawa *et al* [1] on a combined experimental (with inelastic X-ray scattering) and simulation study of liquid Ga. Since the linearized hydrodynamic theory gives an evidence of decoupled longitudinal (L) and transverse (T) dynamics in liquids on macroscopic scale it was believed that even beyond the hydrodynamic regime transverse collective modes cannot contribute to the dynamic structure factors of liquids.

We will report a generalized hydrodynamic scheme for description of possible L-T coupling in liquid metals, which is based on extended slow dynamic variables recently successfully used in a study of slow collective modes in metallic glasses [2]. The issue of sum rules will be discussed. The proposed theoretical approach will be combined with *ab initio* simulations for a few molten alkali metals [3] in order to estimate the effect of L-T coupling on current spectral functions  $C^{L,T}(k,\omega)$ .

1. S.Hosokawa, M.Inui, Y.Kajihara *et al.* Transverse acoustic excitations in liquid Ga// Phys. Rev. Lett. -2009. -Vol.102. -P.105502.
2. T.Bryk, I.Mryglod. Concentration fluctuations and boson peak in a binary metallic glass: A generalized collective modes study // Phys. Rev. B. -2010. -Vol.82. -P.174205.
3. T.Bryk, S.De Panfilis, F.A.Gorelli *et al.* Dynamical crossover at the liquid-liquid transformation of a compressed molten alkali metal// Phys. Rev. Lett. -2013. -Vol.111. -P.077801.

# **Characteristic features of the temperature and composition dependencies of the thermodynamic properties of liquid alloys of binary and ternary glass forming systems**

Agraval P.G., Dreval' L.O., Turchanin M.A.

*Donbass State Engineering Academy, Ukraine*

At this report will be considered the characteristic features of temperature and composition dependencies of the thermodynamic properties of liquid multicomponent alloys with a tendency to amorphisation. This will be done on example of binary and ternary alloys of Fe, Co, Ni and Cu with Ti, Zr and Hf. All experimental data on excess thermodynamic properties of liquid binary alloys show strong negative deviations from ideality. The mixing enthalpies of these alloys are negative and temperature dependent. These peculiarities of thermodynamic properties of liquid alloys indicate the possibility of strong chemical interaction, localization of chemical bonds in the liquid alloy and as result the formation of associates by the type of chemical compound in it. This allows us to use the associated solution model to describe the temperature and composition dependence of the thermodynamic properties of the liquid alloys.

This model was used to calculate the temperature and composition dependences of the thermodynamic properties of glass-forming binary liquid alloys in the whole range of compositions and a wide range of temperatures. The analysis of these properties shows that they are characterized by the following features: the mixing enthalpy is exothermic and becomes more exothermal with decreasing of temperature; the excess heat capacity is positive and passes through a maximum; this function decreases to zero near the glass transition temperature; the excess contribution to the thermodynamic stability of liquid phase increases with decreasing of temperature, which, obviously, is the main cause of the high tendency to amorphization at supercooling.

The mixing enthalpies of glass-forming ternary liquid alloys are negative in the most part of the concentration triangle. Usually coordinates of minimum mixing enthalpy associated with corresponding minimum of this function in one of a binary system. In all studied ternary systems a pair interaction of components plays a predominant role in the absolute values and composition dependence of the mixing enthalpy and other thermodynamic functions of mixing. In all cases, the contribution of the ternary interaction does not exceed 10% of the absolute total value of mixing enthalpy. The analysis of the temperature dependence of the excess thermodynamic properties of ternary liquid alloys indicates on increasing of negative deviations from ideality with decreasing of temperature.

# Experimental investigation and modeling of the mixing enthalpies of liquid Co–Cu–Zr and Cu–Fe–Zr alloys

Agraval P.G., Dreval L.A., Turchanin M.A.  
Donbass State Engineering Academy, Ukraine

The Co–Cu–Zr and Cu–Fe–Zr systems are promising candidates for the creation of multicomponent crystalline/amorphous composites through liquid immiscibility. The thermodynamic properties of liquid phase have to be studied in order to facilitate the development of such materials.

The partial mixing enthalpies of zirconium,  $\Delta\bar{H}_{Zr}$ , in liquid Co–Cu–Zr and Cu–Fe–Zr alloys were measured by high-temperature isoperibolic calorimeter. The following materials were used: electrolytic cobalt and copper (99.99 wt.%); carbonyl iron A-2 (99.95 wt.%); iodide zirconium (99.98 wt.%). All calorimetric investigations were carried out in a protective atmosphere of spectral-grade argon (99.997 vol.%). The crucibles for melts were fabricated from a stabilized zirconia. The measurements were carried out for alloys with  $x_{Zr} = 0-0.55$  at 1873 K along the sections  $x_{Co}/x_{Cu} = 3, 1, 1/3$  (the Co–Cu–Zr system) and  $x_{Cu}/x_{Fe} = 3, 1, 1/3$  (the Cu–Fe–Zr system).

According to our experimental results, the thermodynamic function  $\Delta\bar{H}_{Zr}$  is characterized by negative values in the investigated composition range for both systems. Furthermore, the integral mixing enthalpies,  $\Delta H$ , of liquid Co–Cu–Zr and Cu–Fe–Zr alloys along the investigated sections were calculated by integrating the Gibbs–Duhem equation. The function  $\Delta H$  is sign-changing for both systems.

The integral mixing enthalpies of ternary Co–Cu–Zr and Cu–Fe–Zr liquid alloys were described over the entire composition range using the Muggianu–Redlich–Kister equation. It is noted that a common feature of this excess thermodynamic property is the predominant influence of the pair interactions of components on the character of the composition dependence of the function. These are the Cu–Zr and Co–Zr interactions for the Co–Cu–Zr system as well as the Cu–Zr and Fe–Zr interactions for the Cu–Fe–Zr system. The ternary interaction contribution,  $\Delta H^{ter}$ , is sign-changing for the Co–Cu–Zr system and mainly negative for the Cu–Fe–Zr system. The calculated maximum and minimum values of the  $\Delta H$  and  $\Delta H^{ter}$  functions are given in Table 1.

Table 1. The coordinates of the critical points of the  $\Delta H$  and  $\Delta H^{ter}$  functions

Function	Co–Cu–Zr system		Cu–Fe–Zr system	
	Composition	Value	Composition	Value
$\Delta H_{min}$	$x_{Co}=0.36, x_{Zr} = 0.64$	–38.0	$x_{Fe}=0.55, x_{Zr} = 0.45$	–19.3
$\Delta H_{max}$	$x_{Co}=0.49, x_{Zr} = 0.51$	9.0	$x_{Fe} = 0.45, x_{Zr}=0.55$	11.0
$\Delta H_{min}^{ter}$	$x_{Co}=0.45, x_{Zr} = 0.15$	–3.4	$x_{Fe}=0.55, x_{Zr} = 0.07$	–0.7
$\Delta H_{max}^{ter}$	$x_{Co}=0.20, x_{Zr} = 0.62$	3.1	$x_{Fe} = 0.20, x_{Zr}=0.55$	4.5

## Chemical short-range order and composition range of amorphization of liquid Ni–Ti–Zr alloys

Agraval P.G., Dreval' L.O., Turchanin M.A.<sup>1</sup>, Storchak-Fedyuk A.M.<sup>2</sup>

<sup>1</sup>*Donbass State Engineering Academy, Ukraine*

<sup>2</sup>*Frantsevich Institute for Problems of Materials Science of NASU, Ukraine*

Glass-forming systems demonstrate a strong interaction of components of liquid alloys. The excess thermodynamic functions of such melts show significant negative deviations from ideality. For thermodynamic properties of liquid alloys of glass-forming systems negative enthalpies of formation are typical. Thermodynamic activities of components in such alloys show strong negative deviations from ideality. The thermodynamic properties of these alloys can be described in the frameworks of the associate solution model.

The temperature and composition dependencies of the thermodynamic properties of liquid Ni–Ti–Zr alloys were described using our experimental data on mixing enthalpies. The mixing enthalpy of these alloys was investigated using high-temperature calorimeter, created in the Laboratory of Physicochemical Properties of Metallic Liquid Alloys. Investigations of partial mixing enthalpies of zirconium and titanium were carried out at the temperature of 1873 K along sections with a constant ratio  $x_{\text{Ni}}/x_{\text{Ti}} = 1/4$  ( $x_{\text{Zr}} = 0-0.5$ ) and  $x_{\text{Ni}}/x_{\text{Zr}} = 1/4, 13/7$  ( $x_{\text{Ti}} = 0-0.5$ ), respectively. The values of the partial enthalpies are negative over the investigated composition region. The values of the integral mixing enthalpy of alloys along the studied sections were calculated by integration of the Gibbs–Duhem equation.

Excess thermodynamic properties of liquid Ni–Ti–Zr alloys were described using the ideal associated solution model with the set of associates  $\text{Ni}_3\text{Ti}$ ,  $\text{NiTi}$ ,  $\text{Ni}_3\text{Zr}$ ,  $\text{NiZr}$ . As follows from results of calculations the mixing enthalpy and excess mixing Gibbs energy decreased with decreasing of temperature down to glass-formation temperatures. The excess specific heat demonstrated complex temperature dependence. For alloy of every composition this function increased with decreasing of temperature, reached maximum value near glass-transition temperature and decreased sharply to zero with further lowering of temperature. The sharp maxima and the brake points on the  $\Delta H$ ,  $\Delta C_p^{\text{ex}}$ ,  $\Delta G^{\text{ex}}$  isotherms indicated the strong chemical short range order in the supercooled liquid alloys.

Previously for the number binary and ternary glass-forming systems an empirical rule was formulated that amorphization takes place in the composition range where the total mole fraction of associates in liquid alloys,  $\Sigma x_{\text{as}}$ , at the temperature near the glass transition temperature is more than 0.3. Accordingly, the composition of associated solution of Ni–Ti–Zr liquid alloys was calculated, and the  $\Sigma x_{\text{as}}$  was estimated. The composition range of amorphization of the ternary liquid alloys estimated using the above mentioned rule agrees satisfactory with the literature data on compositions of amorphous alloys. It is obvious that the proposed empirical rule is valid for the Ni–Ti–Zr system.

## Узагальнені кінетичні рівняння для густих газів та рідин у статистиці Рені

<sup>1</sup>Візнович О., <sup>1</sup>Костробій П., <sup>2</sup>Марків Б., <sup>2,1</sup>Токарчук М.

<sup>1</sup>Національний університет "Львівська політехніка", Львів, Україна

<sup>2</sup>Інститут фізики конденсованих систем НАН України, Львів, Україна

Для опису нерівноважних процесів у густих газах та рідинах пропонується використовувати ентропію Рені, яка залежить від параметра  $q$  ( $0 < q \leq 1$ ) і співпадає з ентропією Гіббса-Шеннона при  $q = 1$ . На основі методу нерівноважного статистичного оператора Зубарева та принципу максимуму ентропії Рені отримано нерівноважний статистичний оператор та узагальнені рівняння переносу для параметрів скороченого опису нерівноважних процесів в екстенсивній статистичній механіці [1]. Даний підхід застосовано до опису кінетичних процесів у газах та рідинах, коли параметрами скороченого опиу є нерівноважні одно- та двочастинкова функції розподілу.

1. Markiv B., Tokarchuk R., Kostrobij P., Tokarchuk M., Nonequilibrium statistical operator method in Renyi statistics. // Physica A, 2011, vol. 390, p.785-791.

# Effective Proton–Proton Interaction and Metallization of Hydrogen

Shvets V. T.

*Odesa National Academy of Foods Technology, Odesa, Ukraine*

The effective proton–proton interaction in metallic hydrogen has been calculated for various densities. In the potential of this interaction, which can be represented in the form of a series of perturbation theory in the electron–proton interaction, the second and third order terms are taken into account. The second order term gives a comparatively shallow potential well with one minimum. The position of the minimum corresponds to the equilibrium mutual position of protons in metallic hydrogen. When the third order term is additionally taken into account, the potential has two characteristic minima; the position of one of them corresponds to the distance between the protons in a hydrogen molecule. The depths of these potential wells depend on the density of the system. At fairly high densities, only the potential well corresponding to the equilibrium position of protons in the metallic phase holds in the proton–proton potential. Owing to the presence of two minima in the effective proton–proton potential, the density of hydrogen at the point of transition to the metallic state can be estimated. Analysis of the effective proton–proton interaction makes it also possible to estimate the possibility of the existence of metallic hydrogen in a stable state at quite low temperatures.

1. V.T. Shvets. Effective proton-proton interaction and metallization of hydrogen. *JETP Letters*. 2012. - Vol. 95, No. 1. - P. 29–32.
2. V. T. Shvets\*, A. S. Vlasenko, and A. D. Bukhanenko. Metallization Degree of Hydrogen at a Pressure of 1.4 Mbar and a Temperature a 3000 K. *JETP Letters*. - 2007, - Vol. 86, No. 8. - P. 552–555.

# Equation of State of Liquid Metallic Helium

Shvets V. T.

*Odesa National Academy of Foods Technology, Odesa, Ukraine*

The effective ion–ion interaction, free energy, pressure, and electric resistance of metallic liquid helium have been calculated in wide density and temperature ranges using perturbation theory in the electron–ion interaction potential. In the case of conduction electrons, the exchange interaction has been taken into account in the random\_phase approximation and correlations have been taken into account in the local field approximation. The solid\_sphere model has been used for the nuclear subsystem. The diameter of these spheres is the only parameter of this theory. The diameter and density of the system at which the transition of helium from the singly ionized to doubly ionized state occurs have been estimated by analyzing the pair effective interaction between helium atoms. The case of doubly ionized helium atoms has been considered. Terms up to the third order of perturbation theory have been taken into account in the numerical calculations. The contribution of the third\_order term is significant in all cases. The electric resistance and its temperature dependence for metallic helium are characteristic of simple divalent metals in the liquid state. The thermodynamic parameters—temperature and pressure densities—are within the ranges characteristic of the central regions of giant planets. This makes it possible to assume the existence of helium in the metallic state within the solar system.

1. V.T. Shvets. Equation of state of metallic Hydrogen. *Journal of Experimental and Theoretical Physics*. - 2013. - Vol. 116, No. 1. - P. 159–165.
2. V.T. Shvets. Pair\_Effective Interionic Interaction and Metallization of Helium. *The Physics of Metals and Metallography*. - 2012. - Vol. 113, No. 10. - P. 927–931.

## Higher Order Perturbation Theory Effects in the Resistance of Simple Disordered Metals

Shvets V. T.

*Odesa National Academy of Foods Technology, Odesa, Ukraine*

Based on the variational principle, an expression has been obtained for the coefficient of electrical resistance of simple disordered metals. The parameters of decoupling of higher\_order Green's functions that arise when deriving the quantum kinetic equation have been chosen based on the condition of the coincidence of the Boltzmann equation and the quantum kinetic equation in the lower\_order perturbation theory. For the first time, the contribution of cross scattering to the resistance of disordered metals in the limiting case of low temperatures has been calculated. It has been shown that with allowance for the terms of fourth and higher orders the resistivity can be expressed through both the relaxation time and the density of states of the electron gas interacting with ions. All the effects considered are on the order of  $\frac{\tau}{\hbar} \epsilon F$  where  $\epsilon F$  is the Fermi energy and  $\tau$  is the relaxation time, and are significant for the majority of simple disordered metals.

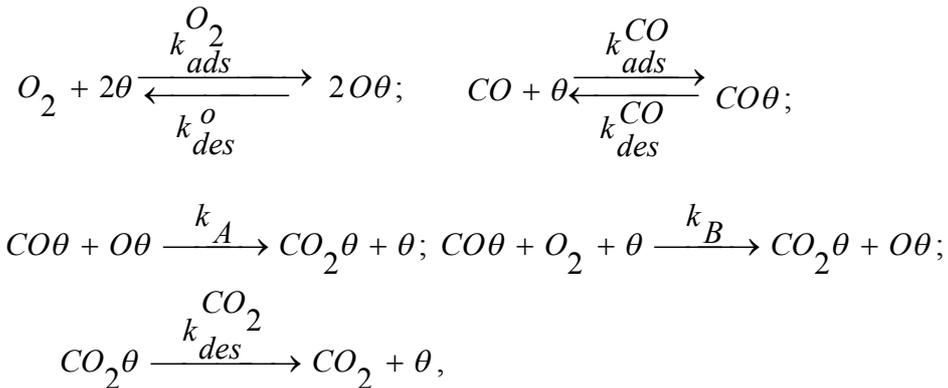
1. T.V. Shvets, V.T. Shvets. Higher order perturbation theory effects in the resistance of simple disordered metals. *The Physics of Metals and Metallography*. - 2011. - Vol. 111, No. 4. - P. 339–352.
2. T.V. Shvets, V.T. Shvets. Variational approach for studying the resistance of simple disordered metals. *Theoretical and Mathematical Physics*. - 2011. - Vol. 166, № 2. - P. 243 - 257.

# Stabilization of temperature in models of catalytic CO oxidation on the surface

P.Kostrobij, B.Hnativ, I.Penyak, I.Ryzha

*National University "Lviv Polytechnic", Lviv, Ukraine*

For classical oxidation reaction of carbon dioxide  $2CO+O_2 \rightarrow 2CO_2$  built diagram of the process

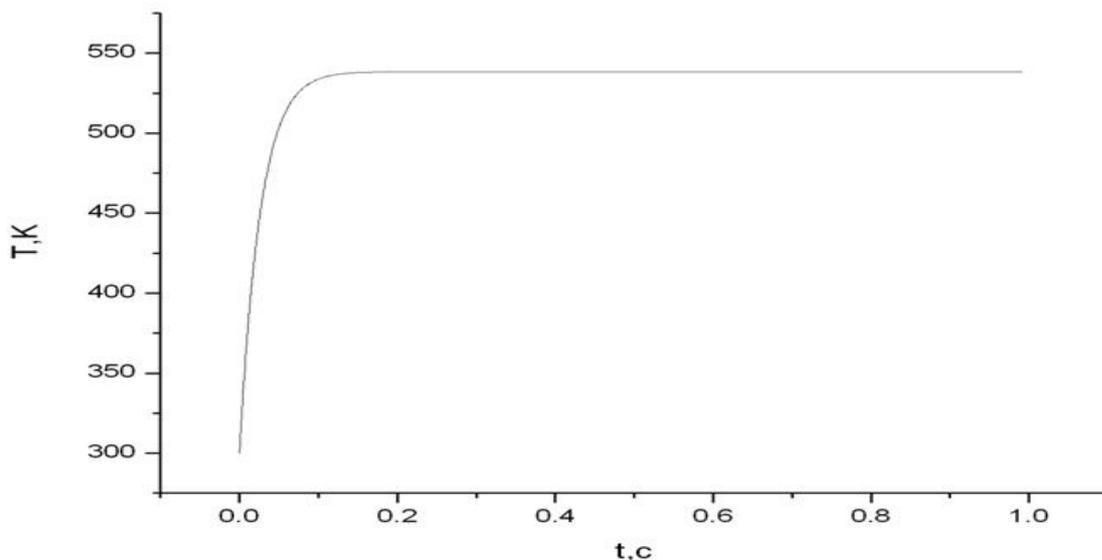


based on the equation of thermal balance reactions

$$\frac{dT}{dt} = -\frac{c_1}{A}(T(t) - T_{sup}) - \frac{c_2}{h}(T^4(t) - T_{env}^4) + \frac{c_3}{h}(38 \times CO \text{ ads. rate} + 54 \times O_2 \text{ ads. rate} - 38 \times CO \text{ des. rate} - 27.34 \times \text{reaction rate})$$

which is essential for the conversion rate constants of reactions.

The results of numerical experiments confirm the stabilization of the surface temperature



# Influence of the memory function for diffusion dynamics of low-dimensional systems

Kostrobij P.P., Uchanska O.M.

*National University "Lviv Polytechnic", Lviv, Ukraine*

The problem of influence as a function of memory on the diffusion dynamics of one-dimensional systems modeled by equation

$$\frac{\partial}{\partial t} \delta n(\vec{R}, t) = \int_{-\infty}^t K(t-t') \hat{L}^M \delta n(\vec{R}, t') dt',$$

where the  $K(t-t')$  – memory function,  $\hat{L}^M$  – Markov diffusion operator.

Using the method of [1] constructed solutions of one-dimensional diffusion problem with memory and the influence of the structure of the memory function for diffusion dynamics. It is shown that the memory function  $K(t-t') = re^{-r(t-t')}$  solution always exists, and the function of memory type  $K(t-t') = (t-t')^{-\alpha}$ ,  $0 < \alpha < 1$  physical solution exists only for those values  $\alpha$  for which  $\frac{1}{2-\alpha} = \frac{m_1}{m_2}$  is an irreducible fraction, and  $m_1, m_2$  – odd positive integers.

1. I.M.Sokolov. Solutions of a class of non-Markovian Fokker-Plank equations / Physical Review, E 66, 041101, 2002.

# **A method for describing the phase behaviour of many-body systems**

Kozlovskii M.P., Romanik R.V.

*Institute for Condensed Matter Physics of NASU, Lviv, Ukraina*

The behavior of many-particle system in both gaseous and liquid phases has been attracting attention of scientists for over a century. The task of microscopic description of such a behavior is topical even today. Especially urgent is the problem of describing fluid in the vicinity of and below the critical temperature  $T_c$ .

When a many-body interacting system considered, the pair interaction potential is usually chosen in the form of a function that does not possess the Fourier transform. The hard-spheres potential is itself such a function, as well as widely considered Lenard-Jones potential. However, the results can be found for a many-particle system interacting via a pair potential possessing the Fourier transform. For instance, the Morse fluid is indeed such a system.

The goal of this work is to propose a new method for calculating the grand partition function with interacting potential possessing the Fourier transform. In particular, the grand partition function is calculated for the Morse fluid. First, the equation of state and the phase diagram are calculated in the mean-field approximation. Then, by renormalization-group calculation, a sequence of effective Hamiltonians is obtained and the behaviour of coupling constants is investigated. The recurrence relations between coupling constants are found as well as their fixed-point solution. In a higher approximation  $\square$  the so-called  $\rho^4$ -model,  $\square$  the coordinates of the critical point are found in terms of temperature and activity.

# Функції розсіяння кінетичної теорії для густих газових сумішей з багатосходинковою взаємодією між частинками

Гуменюк Й.А.<sup>1</sup>, Токарчук М.В.<sup>1,2</sup>

<sup>1</sup>*Інститут фізики конденсованих систем НАН України, Львів*

<sup>2</sup>*Національний університет “Львівська політехніка”, Львів*

Важлива проблема у теорії коефіцієнтів переносу густих газів та газових сумішей — це відтворення їхніх залежностей від температури. Кінетичні теорії для густих систем з розривними потенціалами дають змогу явно врахувати вплив далекосяжної частини взаємодії на коефіцієнти переносу і частково з'ясувати її роль у формуванні температурних залежностей цих величин.

Недавно одержані вирази для коефіцієнтів переносу густої газової суміші з багатосходинковим потенціалом [1] мають перевагу над попередніми для одностороннього випадку [2,3], оскільки виведені з дотриманням закону збереження енергії, а для парної функції розподілу використано наближення неоднорідної рівноваги, яке помітно краще. Однак ці результати потрібно доповнити формулами для інтегральних дужок і відповідних функцій розсіяння — транспортних перерізів та омега-інтегралів. Ми розглядаємо проблему розрахунку цих величин.

У найнижчих наближеннях отримано вирази для матричних елементів лінеаризованого оператора зіткнень. Одержано аналітичні вирази для функцій розсіяння від процесів опускання, підйому та відбиття на відштовхувальних і притягальних сходинках. Головні відмінності пов'язані з першими двома процесами, для яких дещо змінюється означення транспортних перерізів і, крім того, з'являються внески нового типу, пов'язані зі зміною модуля відносної швидкості пари частинок. Отримані аналітичні вирази для омега-інтегралів містять складні залежності від температури, які проявляються у коефіцієнтах переносу.

1. Гуменюк Й.А., Токарчук М.В. / Препринт ІФКС НАН України, ІСМР-11-06U, Львів, 2011, 126 с.
2. Токарчук М.В., Омелян І.П. // Укр. фіз. журн., 1990, **35**, 1255.
3. Tokarchuk M.V., Omelyan I.P., Kobryn A.E. // Phys. Rev. E, 2000, **62**, 8021.

# Correlation analysis of giant optical fluctuations of 2D electrons

A.L. Parakhonsky<sup>1</sup>, M.V. Lebedev<sup>1</sup>, A.A. Dremin<sup>1</sup>, and I.V. Kukushkin<sup>1, 2</sup>

<sup>1</sup>*Institute of Solid State Physics / Russian Academy of Sciences, Chernogolovka, Russia*

<sup>2</sup>*Max-Planck-Institute für Festkörperforschung, Stuttgart, Germany*

The methods of the theory of open dissipative dynamic systems (ODDS) is known to be a powerful tool for determination of a degree of correlation and the character of fluctuating signals [1]. In particular, that includes the study of correlation functions for time signals in ODDS. These methods were applied to a wide range of dynamic systems. In our experiments, a 2D electron system (a single GaAs/AlGaAs quantum well) under the quantum Hall Effect (QHE) conditions is also an open dissipative system being far from equilibrium (the giant optical fluctuations (GOF) of 2D electrons [2]). Using the method of correlation functions, we have analyzed uniform and non-uniform 2D states in the GOF regime and its vicinity.

Coincidence of autocorrelation and cross-correlation functions of 2D electron photoluminescence in a filling factor 2 (a point of uniformity of an electronic density) was investigated. It was revealed that in a 2D system there is switching between the uniform and non-uniform states. Uniform state formation occurs due to an exchange of electrons between the neighboring regions of 2D layer. As a magnetic field increases, the photoexcited 2D system disintegrates into local regions and the correlations are of considerably more complex character.

1. H.G. Schuster and W. Just, *Deterministic Chaos: an introduction*, Physik Verlag, Weinheim, 248 p, 1984.
2. O.V. Volkov, I.V. Kukushkin, M.V. Lebedev, G.B. Lesovik, K. von Klitzing, and K. Eberl, *JETP Lett.* 71, 383 (2000).

# Energies of affinity for metastable triplet states of the negative ion of hydrogen isotopes in a one-dimensional space in hyperspherical adiabatic approach

<sup>1</sup>Haysak M.I., <sup>2</sup>Haysak I.I., <sup>1</sup>Klenivskyi M.S.

<sup>1</sup>*Institute of Electron Physics, Uzhgorod, Ukraine*

<sup>2</sup>*Uzhgorod National University, Uzhgorod, Ukraine*

The three-body problem is relevant in view of the fact that it has all the features of the many-body problem, so it is the basis for the development of a many-body theory. The main feature of this problem is that for real physical potentials it has no solutions in the analytical form.

Today, there are a number of methods (variation, configuration interaction, etc.) enabling one to carry out calculations of spectroscopic parameters and calculations for the scattering problem. Here we use the method of hyperspherical coordinates [1] which has certain advantages among the methods mentioned above. It allows one to perform a natural classification of quantum states by series described by adiabatic potentials and to consider the isotopic composition of the system.

In the simpler case of a one-dimensional space, we start with the non-relativistic Schrödinger equation for the three-particle problem with Coulomb pair interaction between the particles. This enables the motion of the center of mass to be separated and correlation between the particles to be taken into account. The relative motion of the system is described in relative Jacobi coordinates. This approach enables the radial and angular motions of the system to be approximately separated [1] in an elliptical coordinate system. By solving a parametric boundary problem for the angular variables we obtain adiabatic potentials which describe the radial motion of the system. In order to determine the adiabatic potentials to eliminate differences in the matrix elements we use a scalable factor introduced by H. Nakatsuji [2]. The radial system of equations is solved numerically in the Born-Oppenheimer approximation.

The numerical calculations are performed for the isotopes of negative hydrogen ion and isotopes of helium atom. These two problems differ only in the charge of the nucleus. In the literature, there is the statement [3] that the negative hydrogen ion has only one bound state, while others are autoionizing. Our calculations revealed that the negative hydrogen ion, like the helium atom, in addition to the basic triplet state has a metastable triplet state, but the energy of affinity for such state is of the order of tens of meV. The fact is that series over Channel functions converge very slowly but applying the Richardson extrapolation formula to the results by the base dimension (50, 100, 200) enable the energy of metastable state  $1s2s H^-$  to be obtained.

1. J.H.Machek. // J. Phys. B. -1968. -Vol.1. -P.831-843.
2. H. Nakatsuji. // Phys. Rev. Lett. -2004. -Vol.93. -P.030403-4.
3. E.A. Hylleraas.// ApNr. -1964. -Vol.9. -P.345-349.

# Binding energy of ground states of negative hydrogen ion and helium isotopes in two-dimensional space

Haysak<sup>1</sup> M.I., Muchychka<sup>1</sup> Yu.Yu., Onysko<sup>2</sup> V.V.

<sup>1</sup>*Institute of Electron Physics, Uzhgorod, Ukraine*

<sup>2</sup>*Uzhgorod National University, Uzhgorod, Ukraine*

In the recent years the interest towards quantum mechanical problems associated with small size quantum systems and nanostructures is constantly growing. In this paper, we consider isotopes of the negative ion of hydrogen atom and helium atom in a two-dimensional space. The three-body problem is important in developing the N-particle theory because this problem has all the properties which are characteristic for few-body systems. A relative simplicity and a small number of independent variables distinguishes this problem among other problems of atomic, nuclear, solid state physics and elementary particle physics.

We consider a non-relativistic Schrödinger equation for a system of three charged particles with Coulomb pair interaction. In relative Jacobi coordinates such equation enables one to separate the motion of the center of mass. The relative motion equation is a differential equation of the second order in partial derivatives of four independent variables. Angular and radial motions are roughly separated in hyperspherical coordinates [1]. Boundary problem for the angular variables gives adiabatic potentials and channel functions that parametrically depend on the radial variable. At zero radial variable, this problem has an analytical solution while at other values of the radial variable the problem is solved only numerically.

The obtained adiabatic potentials and analytical channel functions are used for solving the radial motion of the system, which we solve in the Born–Oppenheimer approximation. To eliminate differences in the matrix elements of the potential energy operator a scalable factor proposed by H. Nakatsuyi [2] is applied, which depends on the angular variables. The values of energies for two triplet series of negative hydrogen isotopes and helium atoms were obtained and compared with calculations obtained in other approaches. These series are the solutions of boundary problems satisfying Dirichlet and Neumann conditions. The energy values for the series with the Neumann boundary conditions are by about four times higher in comparison with the energy value in the three-dimensional case. On the other hand, the values of other series almost coincide with the energy values for the three-dimensional case. The series describing the triplet states are divergent. The reason for the differences lies in the consistent consideration of confinement [3].

1. J.H.Macek. // J. Phys. B. -1968.-Vol.1. -P.831-843.
2. H. Nakatsuji // Phys. Rev. Lett. -2004. -Vol.93. -P.030403 -4.
3. N. Aquino // Adv. Quan. Chem. -2009. -Vol.57. -P.123-171.

# Binding energy of odd quantum states of negative exciton ions for CdSe and Si semiconductors in a one-dimensional space

Haysak<sup>1</sup> M.I., Yevych<sup>2</sup> M.J., Yevych<sup>2</sup> R.  
<sup>1</sup>*Institute of Electron Physics, Uzhgorod, Ukraine*  
<sup>2</sup>*Uzhgorod National University, Uzhgorod, Ukraine*

Calculations of the energy of affinity for negative exciton ions for CdSe and Si semiconductors were performed within hyperspherical adiabatic approach [1] in the Born-Oppenheimer approximation. The binding energy for negative excitons that was predicted by Lompert in 1956 can be obtained using different approaches, such as variational method, configuration interaction method, etc. [2]. However, these methods have both advantages and shortcomings.

This paper uses hyperspherical approach which is based on collective variables and enables one to carry out both calculations of spectroscopic parameters and classification of quantum states with respect to series of one- and two-particle excitations. To apply this method to the problems of few-body systems in solids the effective mass approximation is used. Non-relativistic Schrödinger equation for an *(ehē)* system accounting for the pair Coulomb interaction between the particles enables one to separate the motion of the center of mass in relative Jacobi variables.

The equation describing the motion of the center of mass is the Helmholtz equation, the solutions of which are well known. So, the solution of the Schrödinger equation is reduced to the solution of the equation of relative motion of the system. The number of independent unknown variables is smaller by the number of independent variables of the motion of the center of mass. The equation of relative motion can be conveniently solved in a polar coordinate system.

It turned out that using this approach one can approximately separate the radial part of the motion from the angular one. The equation of the angular part is solved in an analytical form only at zero value of the radial variable. For other values of the radial variable the angular equation can be solved only numerically.

The boundary problem for the radial equation is solved by the Bubnov-Galerkin method. We chose analytic functions obtained by solving the angular equation at zero value of radial variable as basis functions. To eliminate differences in the matrix elements of the potential energy operator a scalable factor proposed H. Nakatsuji [3] is used.

Our results are compared with the experimental data and results obtained in other approaches.

1. J.H.Macek. // J. Phys. B. -1968. -Vol.1. -P.831-843.
2. H. Munschy, B.Stebe. // Phys. Status Solidi. -1974. -Vol.64. -P.213-221.
3. H. Nakatsuji. // Phys. Rev. Lett. -2004. -Vol.93. -P.030403-4.

# Directed random walk on the eight–branching cayley tree

A.V. Nazarenko

*Bogolyubov Institute for Theoretical Physics, Kiev , Ukraine*

The object of the present investigation is an ensemble of self-avoiding and directed graphs belonging to eight-branching Cayley tree generated by the Fuchsian group  $\Gamma$  of a Riemann surface in genus two and embedded in the Pincare unit disk  $D$ .

We first formulate and study two-parametric model of an octagonal lattice  $D/\Gamma$ , fundamental domain (cell) of which can be interpreted as a “minimal” deformation of the regular hyperbolic octagon. Applying the methods of differential geometry of the Riemann surfaces, we find the symplectic Weil–Petersson two-form in two-dimensional space of the lattice parameters.

Our talk is mainly dedicated to consideration of directed random walk on the Cayley tree as dual lattice to  $D/\Gamma$ . Starting point is a partition function with Boltzmann weights for ensemble of lengths of tree graphs. We calculate the multifractal scaling exponents for the moments of the graph lengths distribution as functions of the lattice parameters. We compare the results of numerical simulations and statistical computations in the Markov chain approximation.

**Keywords:** directed random walk; Cayley tree; Fuchsian group.

# **On the role of correlations in systems of particles interacting with multiplying and capturing hydrodynamic media under external stochastic field**

Yu.V. Slyusarenko, S.O. Nikolayenko

*Akhiezer Institute for Theoretical Physics NSC KIPT, Kharkov, Ukraine*

Non-equilibrium long wave fluctuations generated by external stochastic field in systems of particles interacting with multiplying and capturing media have been studied. General dynamic equations for long wave fluctuations are obtained using the method of averaging over external random force. The case of additive Gaussian noise is considered in detail. It is shown that in the case of such an external random force there exists a time interval during which the description of the evolution of the system can be limited to considering only the dynamics of the hydrodynamic pair correlations. Linearised dynamic equations for pair correlations are obtained, and their solutions in case of small spatial inhomogeneity are considered. The formation of stationary states and the problem of their stability are studied. It has been shown that long wave fluctuations can be generated by external random force and dramatically influence on stability of stationary states in some cases.

## Дисперсія звуку в бозе-газі за наявності конденсату

Шигорін П.П., Дмитрук І.П., Головій В.М.

*Східноєвропейський національний університет імені Лесі Українки, Луцьк, Україна*

Розглянуто задачу про теоретичний опис акустичних хвиль у слабковзаємодіючому бозе-газі за наявності конденсату.

Для дослідження розріджених ультраохолоджених атомарних газів за наявності у них бозе-конденсату застосовують модель, у якій розглядається теплова хмара атомів на фоні бозе-айнштайнівського конденсату [1]. Теоретичний опис нерівноважних процесів у такій моделі заснований на системі двох рівнянь динаміки: рівняння Гросса-Пітаєвського для хвильової функції конденсату та квантового кінетичного рівняння Больцмана для функції розподілу атомів теплової хмарини (надконденсату).

У даній роботі на основі лінеаризованої форми рівнянь динаміки бозе-газу досліджено процес поширення звукової хвилі в просторово-однорідному слабковзаємодіючому газі за наявності у ньому бозе-айнштайнівського конденсату. Побудовано дисперсійне співвідношення між частотою та хвильовим числом звукових хвиль. Отримано вирази для швидкостей звуків у бозе-газі за наявності конденсату. Досліджено вплив теплопровідності та в'язкості на дисперсію звуку. Побудовано температурні залежності коефіцієнта затухання звуку.

1. Griffin, T. Nikuni, E. Zaremba. Bose-Condensed Gases at Finite Temperatures // Cambridge University Press (2009)

## **Electron-hole pair–phonon interaction in semiconductor quantum dots**

Boichuk V.I., Bilynskyi I.V., Shevchuk I.S.

*Drohobych Ivan Franko State Pedagogical University, Drohobych, Ukraine*

Electron-hole pair–phonon interaction is often referred to in order to treat the optical spectra of semiconductor quantum dots. In case of small quantum dots there is a number of experimental reports of Huang-Rhys factors being by two orders of magnitude larger than in the bulk crystals. We consider quantum dots of small radii where nonadiabatic effects can be neglected, so the adiabatic approach can be applied. We assume a Fröhlich-type interaction between electron-hole pair and longitudinal optical phonons. A model of spherical CdTe quantum dot (with dimensions smaller than its exciton Bohr radius) embedded in the HgTe matrix is chosen. A Coulomb term which describes the electron-hole interaction has the energy close to that of longitudinal optical phonons. We take finite confinement potentials for electron and hole, and assume the effective-mass approximation. As a result of choosing finite confinement potentials for both electron and hole, the electron-hole pair–phonon interaction cannot be neglected. Also in our calculations the complexity of valence band structure and the exchange interaction is taken into account.

We obtain the optical selection rules, the Huang-Rhys factors, and analyze the absorption and photoluminescence spectra. The obtained photoluminescence spectra are in good agreement with the experiment in [1], and testify to the fact of formation of the electron-hole pair–polaron [2]. In the adiabatic approach the calculated values of Huang-Rhys factors are larger by one to two orders of magnitude than those in the bulk. Increasing of Huang-Rhys factor with decreasing of quantum-dot radius is observed. The range of validity of the adiabatic approach is discussed.

1. M. Bissiri, G. Baldassarri, M. Capizzi, V.M.Fomin, V.N. Gladilin, J.T. Devreese. Polaron Interaction in InAs/GaAs Quantum Dots and Resonant Photoluminescence// *Phys. Stat. Sol.(b)*. -2001.-Vol.224. –P. 639–642.
2. O. Verzelen, R. Ferreira, and G. Bastard. Excitonic polarons in semiconductor quantum dots// *Phys. Rev. Lett.* -2002. –Vol.88.–P 146803.

# Preparation of a Quantum States of Two Spin-1/2

Kuzmak A. R.

*Ivan Franko National University of Lviv, Ukraine*

Quantum computation is based on qubits. A qubit is a quantum two-level system for instance a photon with the vertical and horizontal polarizations, or with two spin states a spin-1/2 particle such as electron, or a two-level atom. Computations are based by quantum algorithms which carried out on the qubits and measurement of these qubits determine the output results. The calculation which is based on photons are controlled and measured by means of beam splitters, polarisers, photo-detectors et al.. Quantum states of electrons and nuclear spins are controlled and measured by magnetic and electric fields.

We consider a system of two spins and their interaction is represented by isotropic Heisenberg Hamiltonian. Our aim is to create arbitrary quantum state of two spins having started with  $|\uparrow\downarrow\rangle$  state. We can easily prepare this state because it is an eigenvector of the system of two spins which is located in the magnetic field directed along the z-axis. The method which we suggest consist of two steps. At the first step, using the evolution operator with isotropic Heisenberg Hamiltonian we obtain the state which depends on time of evolution. At the second step, the spins are driven individually by magnetic pulse fields. The final state is defined by time of evolution and parameters which are determined strength and direction of magnetic fields.

We propose to realize this method on the physical system of a  $^{31}\text{P}$  donor in silicon because it is system with high degree of quantum coherence, and states of this system are measured with high fidelity [1]. The  $^{31}\text{P}$  donor in silicon has a nuclear spin  $I$  of 1/2, and at cryogen temperatures it can catch an electron (with spin  $S = 1/2$ ). Therefore, a single  $^{31}\text{P}$  donor can be considered as a two-qubit system. Factorized initial state  $|\uparrow\downarrow\rangle$  can be easily prepared for this system [1].

1. Pla J. J. et. al.. High-fidelity readout and control of a nuclear spin qubit in silicon// Nature. -2013. -Vol.496. -P.334-338.

# Fractional statistics in $D$ dimensions: Thermodynamics of the harmonic oscillator system

Andrij Rovenchak

*Ivan Franko National University of Lviv, Ukraine*

A system of isotropic harmonic oscillators obeying the Polychronakos fractional statistics [1] with a complex parameter [2] in a space having the dimension  $D > 1$  is studied. With the statistics parameter being a complex number on the unit circle  $\alpha = e^{i\pi\nu}$  the calculations are made for the “bosonic” side  $0 \leq \nu \leq 1/2$  with a special attention to the bosonic limit  $\nu \rightarrow 0$ .

Temperature dependences of the thermodynamic functions are analyzed in different temperature domains. At high temperatures, preliminary analysis of the virial expansion allows establishing approximate correspondence between the described statistics and some other types of fractional statistics, including anyonic, Haldane–Wu, and  $q$ -deformed bosons. Bose-like behavior is observed in the low-temperature limit. The nature of the observed phase transitions is clarified. Both numerical and analytical estimates for the critical temperature are made depending on the number of particles, space dimensionality, and statistics parameter.

The phenomena described in this work are related to several real physical systems with small dissipation. First of all, these are trapped bosons, for which the shape of the external potential determines the effective dimensionality  $D$ , and helium films, where the phonon branch of the excitation spectrum corresponds to the density of states  $g(\epsilon) \sim \epsilon^{D-1}$ , and  $2 \leq D \leq 3$  smoothly interpolates between planar and bulk geometries.

As previous estimations for 1D systems of harmonic oscillators show, experimental tests of the predicted phase transitions are in principle within accessible accuracies [3]. A properly prepared system to be effectively described by the Polychronakos fractional statistics with a complex parameter remains so far an open issue.

1. *P. Polychronakos*. Probabilities and path-integral realization of exclusion statistics // *Phys. Lett. B*. — 1996. — Vol. 365. — P. 202–206.
2. *Rovenchak*. Polychronakos fractional statistics with a complex-valued parameter // *J. Phys.: Conf. Ser.* — 2012. — Vol. 400. — 012064. — 4 p.
3. *Rovenchak*. Phase transition in a system of 1D harmonic oscillators obeying Polychronakos statistics with a complex parameter // *Fiz. Nizk. Temp.* — 2013. — Vol. 39. — P. 1141–1145.

# Quantum mechanical analogy and sypersymmetry of electromagnetic wave propagation in planar waveguides

H. P. Laba<sup>1</sup>, V. M Tkachuk<sup>2</sup>

<sup>1</sup>*Lviv Polytechnic National University, Lviv, Ukraine*

<sup>2</sup>*Ivan Franko National University of Lviv, Ukraine*

We establish an exact analogue of the equation describing propagation of TE and TM modes in a planar waveguide with arbitrary continuous dependence of electric permittivity and magnetic permeability on coordinates with the stationary Schrödinger equation. The effective potential energies involved in the Schrödinger equation for TE and TM modes are different but in the limit of weak dependence of the permittivity and permeability on coordinates they coincide. In the case when the product of a position-dependent permittivity and permeability is constant, which means that the refractive index is constant, we find that the propagation of TE and TM modes is described by the supersymmetric quantum mechanics. The analogy between quantum mechanics and electromagnetic propagation in waveguides gives a possibility to use the methods developed in one field to another and vice versa. Thus, the methods of quantum mechanics can be effectively applied for the investigations of wave propagation in waveguides and, vice versa, the experiments with wave propagation in waveguides give a possibility to verify many effects in quantum mechanics.

# Relativistic particle dynamics and deformed Poincaré symmetry

Mykola Samar

*Ivan Franko National University of Lviv, Ukraine*

We study the quantized spacetime Lorentz-covariant algebra proposed in [1]. This algebra contains the one of Snyder as a partial case [2]. We present the action of relativistic particle to be invariant under deformed Poincaré symmetry corresponding to chosen algebra. It is shown that the Dirac constraint analysis of the model yields the classical version of the algebra. We also discuss algebraic transformations mapping the deformed symmetries with the undeformed ones. In case of the considered algebra leads to Snyder one, our results yields those obtained in [3].

We also study free motion as well as motion in the electromagnetic field in space with the deformed Poisson brackets being the classical limit of Lorentz-covariant deformed canonical commutation relations leading to minimal length. Calculation of the precession angle of an orbit of the relativistic particle in the Coulomb potential is provided. Comparing our analytical result with the experimental data for precession angle of Mercury's orbit we obtain an estimation of minimal length[4].

1. C. Quesne and V. M. Tkachuk. Lorentz-covariant deformed algebra with minimal length and application to the (1+ 1)-dimensional Dirac oscillator// J. Phys. A. - 2006. - Vol. 39. - P. 10909-10922.
2. H. S. Snyder. Quantized space-time// Phys. Rev. - 1947- Vol. 71. - P. 38-41.
3. R. Banerjee, S. Kulkarni and S. Samanta. Deformed symmetry in Snyder space and relativistic particle dynamics// JHEP. - 2006.- Vol. 05. - Iss. 077. - P. 1- 21.
4. M. Samar and V. M. Tkachuk. Relativistic particle motion in space with the deformed Poisson brackets // Phys. Scripta (in press).

# Supersymmetric approach for quasi-exactly solvable systems with a position-dependent mass

Voznyak O.O., Tkachuk V. M.

*Ivan Franko National University of Lviv, Ukraine*

From the early days of quantum mechanics there has been continuous interest in the potentials, for which the corresponding Schrödinger equation with a constant mass can be solved exactly. Because the number of completely exactly solvable potentials is rather limited much attention has been given to the quasi-exactly solvable (QES) potentials, for which a finite number of the energy levels and the corresponding wave functions are known in an explicit form. As a consequence a large number of different methods for construction of QES potentials was developed. One of them is the supersymmetric (SUSY) method. In [1] the SUSY method was applied for generating quasi-exactly solvable potentials with arbitrary two known eigenstates.

Recently, there has been a growing interest in the study of quantum mechanical systems with a position-dependent effective mass due to their applications in condensed matter physics. Therefore, the search for potentials and corresponding position-dependent mass, for which Schrödinger equation can be solved exactly or quasi-exactly, is topical. Here we generalize the SUSY approach proposed in [1] for generating quasi-exactly solvable potentials with arbitrary two known eigenstates in the case of a position-dependent mass. Explicit examples of potentials and position-dependent mass, for which two energy levels and corresponding wave functions are known in an explicit form, are presented.

1. *V. M. Tkachuk*. Supersymmetric approach for generating quasi-exactly solvable potentials with arbitrary two known eigenstates // *J. Phys. A.* — 2001. — Vol. 34. — P. 6339-6348.

## The impurity states in the liquid Helium – 4

Vakarchuk I. O., Panochko G.

*Department for Theoretical Physics, Ivan Franko National University of Lviv, Ukraine  
College of Natural Sciences, Ivan Franko National University of Lviv, Ukraine*

We consider the effect of impurities the state at behavior many boson system at finite temperatures. The Hamiltonian of such a system contains the Hamiltonian of the Bose-liquid, the Hamiltonian of an impurity and the operator taking into account the interaction of the atoms of liquid with an impurity atom. The background in the study of impurity states in quantum liquids are the Fourier coefficients of the two-particle potential energy of liquid and impurity which is written via the structure factor of liquid  $^4\text{He}$  obtained from X-rays scattering measurements.

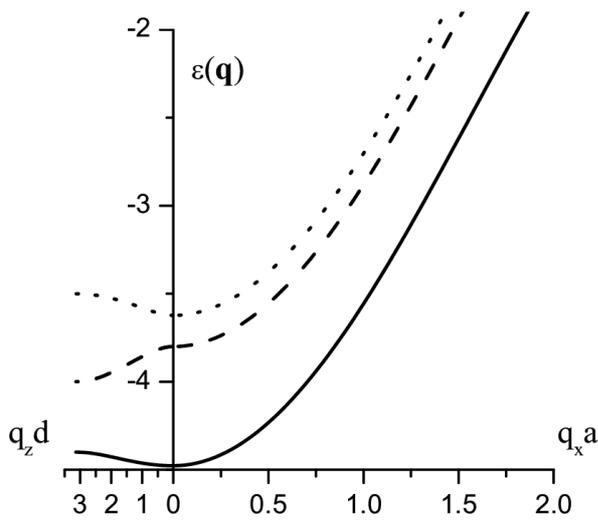
Our task is to find the full density matrix of the system described by the above Hamiltonian for all temperatures by means of the method of collective variables. Its diagonal element integrated over all the variables is the partition function of the system “Bose-liquids + impurity”. Averaging the expression for the full density matrix over the states of the liquid, the one-particle reduced density matrix of the system is found. The Fourier image the one-particle reduced density matrix allows to find the distribution of momenta of the system “liquid helium + impurity”. At low temperature the one-particle density matrix coincides with the one-particle matrix of many body system of bose particles in the approximation of pair correlations. In thermodynamic limit the effective mass of the  $^3\text{He}$  impurity in  $^4\text{He}$  is found.

# The effect of the stage ordering in layered crystals on electron states

I.V. Stasyuk, O.V. Velychko

*Institute for Condensed Matter Physics of NASU, Lviv, Ukraine*

Layered semiconductor selenides GaSe and InSe are well known as the “host” materials due to their pronounced layered structure and the presence of so-called “guest” positions within. Such positions are localized within the van der Waals gaps (oriented perpendicular to the crystallographic axis C) and placed between the layers. Inclusion into the designated intracrystallite intervals of alien ions, atoms or molecules is known as the intercalation phenomenon. Intercalation capability of such systems are greatly improved by subsequent intercalation and deintercalation of sodium nitrate into the “host” matrix. As a result, the  $n$ -stage ordering occurs and the distance between the appropriate packages of layers significantly increases (usually three-layered packages are formed) [1,2].



The anisotropic three-branch electron spectrum ( $t'/t_{\perp} = 0.1$ ,  $t/t_{\perp} = 0.3$ ,  $\delta/t_{\perp} = 0.1$ ,  $\varepsilon(\vec{q})$  is given in  $t_{\perp}$  units).

One could expect a dramatic reconstruction of the electron spectrum for such a modulated multilayered structure. For the case of a three-layered package an equation for the electron spectrum is obtained exhibiting an anisotropic three-branch structure (which reduces to the well-known Fivaz spectrum in the uniform case limit). The dispersion laws for split electron bands are calculated. An analytical expression  $\rho(E) = \int \rho_{\parallel}(y)\rho_{\perp}(E-y)dy$  for the density of electron states (DOS) is derived in the physically explicit form of the convolution of intralayer ( $\rho_{\parallel}$ ) and interpack ( $\rho_{\perp}$ ) densities of states. The peculiarities of DOS arising due to the modulation of the layered structure are studied.

1. Safran S.A. // Solid State Physics: Adv. Res. and Appl. – 1987. – Vol. 40. – P. 246–312.
2. Grigorchak I.I., Netyaga V.V., Kovalyuk Z.D. // J. Phys.: Condens. Mater.– 1997. – Vol. 9. – P. L191–L195.

# Relaxed Optics: problems of development and application

Trokhimchuck P.P

*Lesya Ukrayinka East European National University, Lutsk, Ukraine*

Relaxed Optics (RO) is the part of modern physics of the irreversible interaction light and matter. This part of physics was created for the resolution of the question about the application laser irradiation for the technology: laser annealing of ion-implanted layers of semiconductors, laser implantation and laser evaporation of various materials [1,2]. In more general sense, the RO can be represented as a branch of physics that studies the relaxation of optically-generated primary excitations in the irradiated material. In this case, Nonlinear Optics (NLO) is the part of RO which studies the radiative relaxation of the primary excitation. On the other hand roughly speaking RO may be presented as NLO with non-radiative relaxation of the primary excitation [2]. The temporal-energy classification is the basis of RO [1,2].

RO may be represented as the synthesis of quantum electrodynamics, radiation physics of status solid (RPSS), plasma physics, physics of irreversible phenomena and physical chemistry in one system too [1,2]. So, using methods of RPSS to chemical bonds in the cascade theory of laser-induced excitation in the regime of saturation was allowed to explain the results of laser generation, laser aging, laser implantation and laser annealing of ion implanted layers of InSb, Si, Ge, CdTe and allotropic phases of carbon with unified position [1,2]. Influence of polarization on formation laser-induced surface nanostructures may be explained with help universal polariton-plasmon model [1,2].

Development of RO is caused of the creation new models and theories of mixing (complex) phenomena of irreversible interaction light and matter [1,2]. Among them: problem of creation of homogeneous and heterogeneous surface and volume nanostructures [1,2]; problem of expansion methods of NLO on irreversible processes; creation theory of nonthermal phase transformations in irradiated materials; problem of synthesis methods of plasma physics, quantum electronics and physical chemistry for the creation the theory for the controlling relaxed optical processes.

Basic applications of RO is next: optoelectronic technology, including miniaturization of elements of optoelectronic system and increasing of its life-time [1,2]; laser metallurgy, architecture, arts, biotechnology, medicine and other.

1. P.Trokhimchuck. Foundations of Relaxed Optics. – Lutsk: Vezha, 2011. – 627 p.
2. P.Trokhimchuck. Nonlinear and Relaxed Optical Processes. Problems of Interactions. – Lutsk: Vezha-Print, 2013. – 280p.

# Investigation of the conditions of crystallization suppression by quenching from melt

Kosynska<sup>1</sup> O.L., Dorozhka<sup>2</sup> T.N.

<sup>1</sup> Dneprodzerzhinsk State Technical University, Dneprodzerzhinsk, Ukraine

<sup>2</sup> Dneprodzerzhinsk Energy Technical School, Dneprodzerzhinsk, Ukraine

Recently, more attention is attracted to the study of amorphous materials. This can be explained by the unique combination of corrosion, strength, electromagnetic and other properties in these materials. The preparation of such structures is a scientific and technological interest because it gives an opportunity to establish the degree of influence of various factors on the crystallization kinetics of metals and alloys. So, in this work, using mathematical modeling, developed algorithm of joint solutions of thermal and kinetic problems for a thin melt layer which cooling on a solid substrate.

The mathematical model is based on the Fourier heat equation (1) and the kinetic equation (2) [1], which takes into account the effects of nucleation processes deceleration by decrease of liquid phase volume and a reduction of crystals growth rate by blocking the neighboring crystals:

$$c\rho \frac{\partial T(z,t)}{\partial t} = k \frac{\partial^2 T(z,t)}{\partial z^2} + \Delta H_m \rho \frac{\partial x}{\partial t} \quad (1)$$

$$x(t) = \frac{4}{3} \pi \int_0^{t_e} (1-x(t')) I(t') \left[ R_c(t') + \int_{t'}^{t_e} (1-x(t'')) u(t'') dt'' \right]^3 dt', \quad (2)$$

where  $T_1$ ,  $t$ ,  $z$  – accordingly, temperature, time and coordinate along the heat removing of layer;  $c$ ,  $\rho$ ,  $k$  – specific heat, density and thermal conductivity of explored metal;  $\Delta H_m$  – crystallisation specific heat;  $x$  – fraction crystallized volume;  $t'$  and  $t''$  – current moments of time ( $0 \leq t' \leq t'' \leq t$ );  $I$  – nucleation rate ( $I = I_{hom} + I_{het}$ , where  $I_{hom}$  and  $I_{het}$  – nucleation rate for homogeneous and heterogeneous mechanisms);  $R_c$  – radius of a critical nucleus;  $u$  – linear growth rate of crystals.

Kinetic parameters  $I_{hom}$ ,  $I_{het}$ ,  $u$  and  $R_c$  was calculated according to the formulas of the classical theory of crystallization. As the test material was selected alloy Ag<sub>87</sub>Cu<sub>13</sub>, which is cooled on the copper substrate.

The results of the studies showed that, depending on the thickness of the melt, Ag<sub>87</sub>Cu<sub>13</sub> can be obtained in crystalline, amorphous or partially crystallized state. Thus, in layers thicker than 32  $\mu\text{m}$ , observed complete crystallization of a thin layer ( $x \approx 1$ ). Reducing the thickness of the melted layer from 32 to 30  $\mu\text{m}$  leads to partial crystallization of foils ( $10^{-2} < x < 1$ ) and when the foil thickness is less than 30  $\mu\text{m}$ , there is complete amorphization of the explored volume ( $x \leq 10^{-2}$ ). In this case, the calculated cooling rate is  $1,5 \cdot 10^6$  K/s, which in good agrees with the experimental data.

1. А.Б. Лысенко. Кинетическая модель массовой кристаллизации в приближении эффективных скоростей зарождения и роста кристаллов // Вісник Дніпропетровського університету. Серія «Фізика. Радіотехніка». – 2011. – т.19, №2, вип.18. – С.3–11

# Models of simple crystallographic forms of vapor-phase PbTe nanostructures on Sital

Saliy Y.P., Bylina I.S., Freik I.M.

*Vasyl Stefanyk PreCarpathian National University, Ivano-Frankivsk, Ukraine*

Lead telluride – a narrow-band semiconductor compounds IV-VI, which are used as active elements of optical infrared range and thermoelectricity. New research methodology initial stages of nucleation and growth of nanostructures improves the parameters of thin films and two-dimensional condensates. In this paper, the methods of atomic force microscopy and computer simulation investigated crystallographic properties of condensates PbTe: Sb deposited on sital by methods «hot wall».

On the surface of the films that were grown over 2 min at substrate temperatures of 150 - 250°C, revealed crystalline polyhedra various simple shapes with arbitrary orientation of planes in space, which is likely associated to the properties of the substrate. With increasing deposition time increased the size of polyhedra and their shape changed from shallow to steep.

For films with distinct nano-objects on the surface, some isolated and identified for each face of the object polar and azimuthal angles. Based on these angles showing the angles between the normal to the face sites and are compared with the theoretically derived sets possible.

It is known that ceramics containing a large number of small (<1 μm) crystals, interconnected intercrystalline glassy layer. Therefore, epitaxial objects on the surface of ceramics can follow the orientation of individual crystallites of polycrystalline substrate.

PbTe crystals belong to the substance of the predominant ion-ion bond and have a structure like NaCl. It is known that in these crystals is electrically neutral layers with the highest reticular density is atomic planes of {100} and {110}. It is the plane of these systems under certain conditions, will form nano-objects on the surface of the film. Angles between normals to the faces of these objects on the surface of the film can take the following values 45°, 60°, 90°, 120° and 135°.

Based on the accuracy of the values obtained experimental dihedral angles, one could argue that the hypothesis of a combination of these simple forms is confirmed.

Found that the surface of ceramics are formed variously oriented individual nano-objects in the space of proper crystallographic structure, representing a combination of simple shapes of faces {100} and {110}. From the change in the substrate temperature range 150 - 250°C changes were observed. However, not all possible combinations of the three planes of {100} and {110} met in real nanocrystals.

# Influence of different types of structural disorder on the critical properties of magnets

M. Dudka, Yu. Holovatch

*Institute for Condensed Matter Physics of the National Acad. Sci. of Ukraine, Lviv, Ukraine.*

Influence of a weak structural disorder on the critical behaviour of three-dimensional magnetic alloys is studied. Different forms of quenched disorder are considered: point-like uncorrelated nonmagnetic impurities [1], extended defects [2], disorder in a form of the random anisotropy axis [3] and their combinations [4]. Asymptotic and effective (non-asymptotic) critical characteristics are calculated applying renormalization group methods. Results obtained within the two-loop approximation of field-theoretical renormalization group demonstrate rich critical properties in the non-asymptotic regime.

1. Р. Фольк, Ю. Головач, Т. Яворский, *УФН* **173** (2003) 175.
2. D. Ivaneyko, B. Berche, Yu. Holovatch, J. Ilnytskyi, *Physica A* **387** (2008) 4497.
3. M. Dudka, R. Folk, Yu. Holovatch, *JMMM* **294** (2005) 305.
4. M. Dudka, Yu. Holovatch, *unpublished*.

# **Molecular rotation and volume dependence of the thermal conductivity in liquid nitrogen**

Pursky O.I., Chastokolenko I.P.

*Kyiv National University of Trade and Economics, Kyiv, Ukraine*

The kinetic theory of liquids developed by Ya.I. Frenkel considers a liquid as a dynamic system of particles resembling in part of crystalline state. At temperatures close to the melting point, the thermal motion in liquids is mainly reduced to harmonic vibrations of particles near some average equilibrium position. In general case, the total energy of the molecules in a liquid is due to their random translational motion as well as their vibrational and rotational motions. As indirect, but in no case secondary, experimental data on the thermal conductivity can serve as a source of information on the thermal motion in liquids [1]. A thorough analysis of the thermal conductivity features in liquids allows one to compare them with the results of structural and thermodynamic researches. As compared to atomic liquids the heat transfer in molecular liquids has a number of features. One of these features that can affect the temperature dependence of the thermal conductivity is molecular rotations. Specific features of the dynamics of translational and rotational subsystem of molecular liquids affect their thermodynamic properties and must manifest themselves in one way or another in the relaxation processes. This is related, first of all, to the coupling (known as translation-rotation coupling) between translation displacements and molecular rotations and it is characteristically reflected in the kinetic properties of molecular liquids and, in particular, on the thermal conductivity. In the majority of cases, this coupling is most apparent for liquids at pre-crystallization temperatures in which the formation of orientational subsystem is accompanied by a change of structural ordering. Often this change is preceded by anomalous thermodynamic properties. In the present work, we perform a detailed analysis of heat transfer in liquid nitrogen, paying special attention to influence of molecular rotation on volume dependence of the thermal conductivity. For that purpose, we carried out comparison of the isochoric thermal conductivity of liquid Ar, CH<sub>4</sub> and N<sub>2</sub>. A detailed study of general features of isochoric thermal conductivity coefficients in these liquids let us correlate these features with the results of structural and thermodynamic researches. The distinctions between the volume dependence of liquid Ar, CH<sub>4</sub> and N<sub>2</sub> are explained by influence of rotational motion of molecules. Finally, we give an additional argument by the calculation of the isochoric heat capacity components of liquid nitrogen.

1. O. I. Pursky V. A. Konstantinov, V.V. Bulakh. The thermal conductivity jump at crystal-liquid phase transition in CHCl<sub>3</sub>, C<sub>6</sub>H<sub>6</sub> and CCl<sub>4</sub>: the action of rotational molecular motion// Low Temp. Phys. – 2009. – Vol. 35, №4. – P. 307-310.

# Моделювання структурних перетворень в кристалах класу $A_3^{\text{II}}B_2^{\text{V}}$

Дон Н.Л.

*Херсонський національний технічний університет, Херсон, Україна*

Кристали класу  $A_3^{\text{II}}B_2^{\text{V}}$  ( $Cd_3As_2$ ,  $Zn_3As_2$ ,  $Cd_3P_2$ ,  $Zn_3P_2$ ) є одними з найцікавіших матеріалів для моделювання і симуляції структури та фізичних властивостей, оскільки в них залежно від ступеня упорядкування стехіометричних вакансій металевої підґратки може суттєво змінюватися кристалічна симетрія.

В роботі розвинено комп'ютерні методи візуалізації моделей різних кристалічних форм (політипів) кристалів  $A_3^{\text{II}}B_2^{\text{V}}$ . Сучасними комп'ютерними методами отримано наочні зображення всіх структурних модифікацій сполук класу  $A_3^{\text{II}}B_2^{\text{V}}$  з урахуванням реального розташування атомів, зокрема тетрагональної деформації та локальної дисторсії ґратки. Методами комп'ютерної математики та графіки здійснена візуалізація мотивів розташування стехіометричних вакансій підґраток металів у зазначених сполуках з урахуванням реальних кристалографічних позицій. Проведено глибокий структурний аналіз з метою дослідження мотивів розташування вакансій.

В результаті виявлено, що різні тетрагональні фази матеріалів класу  $A_3^{\text{II}}B_2^{\text{V}}$  є політипами, а всі структурні перетворення, відомі в цих матеріалах фактично є одновимірними структурними перетвореннями – політипією з усіма її характерними наслідками. Політипія, або «одновимірний поліморфізм» – широко відоме явище, однак воно вперше теоретично доведено для кристалічних фаз  $A_3^{\text{II}}B_2^{\text{V}}$ .

Встановлено, що в матеріалах класу  $A_3^{\text{II}}B_2^{\text{V}}$  існує принаймні два різних механізми упорядкування з двома різними скалярними параметрами порядку: позиційне упорядкування (первинне, спостерігається при вищих температурах) та орієнтаційне. Позиційне упорядкування разом з тетрагональною деформацією зумовлює також анізотропію властивостей двопакетних ( $2Q$ ) та чотирипакетних ( $4Q1$ ,  $4Q2$ ) тетрагональних політипів. Орієнтаційне упорядкування додатково зумовлює втрату центру симетрії в політипах  $4Q2$ , стабільних при кімнатних температурах.

# Simulation of the structure of liquid aluminum using fractal theory

V. Kartuzov<sup>1</sup>, Y. Dmytrishyna<sup>2</sup>

<sup>1</sup>*Frantsevich Institute of Materials Science, Kyiv, Ukraine*

<sup>2</sup>*Institute of pulse processes and technologies, Mykolaiv, Ukraine*

Researching the simple methods to describe the liquid alloys, which are dependent on parameters of processing, is urgent. In the considered case a liquid aluminum is treated by electro-hydro-pulse method (EHPT) [1] in the bucket on precasting stage.

The solution, based on synthesis of cluster model of liquid and theory of fractal, is proposed. The modification of the Boltzman formula was used to find the influence of dissipative energy on the lifetime of clusters. The criterion that indicates the destruction of the existing structure is proposed. Probability of the atoms staying in activated condition is based on Bailey criterion and was corrected for structure changes which are occurring during EHPT. The dissipative energies, which provide the structure changes, and energies, which dissipate during one impulse of EHPT, are analysed.

Fractal and multifractal parameterizations are performed according to standard procedures [2] basing on elementary cell (for example 13 with central atom for aluminum). 13-fold number of atoms for each partition in the multifractal parameterization has been varied. Obtained data was compared with data for microstructure of aluminum alloys after EHPT, obtained using the MFR-Drom-1 application of Vstovsky G.V. [3]. Result of simulation are consistent with experimental and other researchers data and shown the need for further development of this model.

1. Цуркин В.Н., Грабовый В.М., Синчук А.В. Функциональные возможности ЭГИ обработки расплава в ковше//. – Электронная обработка материалов. - 2006. – №5. -с. 55-61.
2. С.В. Божокин, Д.А. Паршин. Фракталы и мультифракталы. – Ижевск: НИЦ «Регулярная и хаотическая динамика». – 2001. – 128 с.
3. Vstovsky G.V., Kolmakov A.G., Terentjev V.F. / MEDŽIAGOTIRA (Materials Science). 1999. - №2 (9). – P. 62-65.

# **The study of nanostructures in a single semiflexible macromolecule with inhomogeneous distribution of the chain stiffness by means of Monte Carlo simulation.**

Martemyanova J.A.<sup>1</sup>, Ivanov V.A.<sup>1</sup>, Paul W.<sup>2</sup>

<sup>1</sup> Faculty of Physics, Moscow State University, Moscow, Russia

<sup>2</sup> Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Halle (Saale), Germany

We study the diagram of states of a single multiblock copolymer chain consisting of flexible and semiflexible blocks with regular sequence of these blocks. Monomer units of both kinds (flexible and semiflexible) are equivalent in the sense of the volume interaction potential. We vary the length of the blocks and the value of stiffness parameter. We use Monte Carlo method with Wang-Landau sampling [1] and bond fluctuation lattice model.

We present our data on different non-trivial heterogeneous globular morphologies which we have obtained in our model for different values of the block length and the stiffness parameter. We demonstrate that the collapse can occur in one or in two stages depending on the values of both these parameters and discuss the role of the inhomogeneity of intraglobular distributions of monomer units of both flexible and semiflexible blocks. For short block length the semiflexible monomer units form the core and flexible ones – the shell of a globule, for long block length – vice versa. Transition between these two regimes depends on stiffness – for larger stiffness it occurs at larger block length. For short blocks there are two transitions - between solid globule and liquid globule and between liquid globule and coil. For long blocks with increasing stiffness we observe only a single transition – between the dumb-bell-like globule (semiflexible blocks form a cylinder-like core, and the flexible blocks form two domains at both ends of such a cylinder) or Saturn-like globule (the flexible blocks form a spherical core of a globule while the semiflexible blocks are located on the surface and wrap around this core) globule and coil.

*The financial support from DFG (project PA 473/10-1) and RFBR (grants 12-03-31254-mol and 13-03-91334-NNIO-a) is highly appreciated. We also thank the Supercomputer center of Moscow State University for providing computer time on "Chebyshev" supercomputer.*

1. F. Wang, D.P. Landau, Phys. Rev. Lett. **8**, 2050 (2001); F. Wang, D.P. Landau, Phys. Rev. E **64**, 056101 (2001).

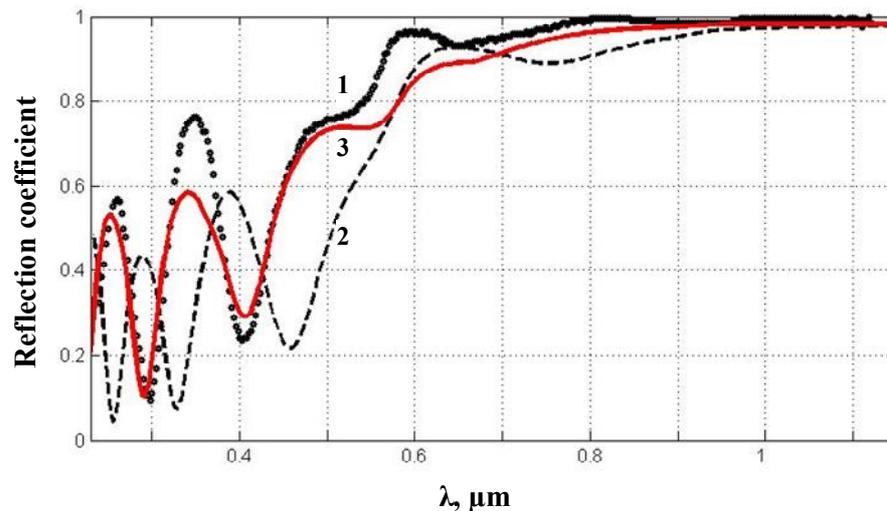
# The aluminium oxide thin film – cooper system's optical properties modeling.

Stashchuk V.S., Stukalenko V.V., Filipov Ya. V., Polianska O.P.

*Taras Shevchenko National University of Kyiv, Ukraine*

The optical properties of aluminium oxide's thin film – bulk aluminium system were modeled. Two-layer model: aluminium oxide – interlayer – bulk metal was used. Measured and calculated reflection coefficient's dispersive dependences  $R(\lambda)$  of bulk cooper mirrors with oxide layer were compared in wide spectral range ( $\lambda = 0,2 - 1.2 \mu\text{m}$ ). The aluminium oxide layer were applied with different thickness (200 -300 nm).

Dispersive dependence  $R(\lambda)$  of discovered system with oxide thickness  $d = 300 \text{ nm}$  was shown of Fig.1: 1- experimental data; 2 – calculated data for one-layer model without system's optical and geometric characteristics; 3 - calculated data for two-layer model with system parameter's variation.



**Fig.1.**

The best harmonization of  $R(\lambda)$  calculated and experimental curves were obtained by the aluminium oxide thin film and interlayer optical constant's variation. Interlayer characteristic's: thickness, refractive index  $n$  and absorption coefficient  $k$  were explored

## The modeling of biocompatible molecular ferroelectrics.

Paramonova E.V.<sup>(1)</sup>, Gevorkyan V.E.<sup>(2)</sup>, Avakyan L.A.<sup>(2)</sup>, Bystrov V.S.<sup>(1)</sup>

<sup>1</sup>*The Institute of Mathematical Problems of Biology RAS (IMPB RAS), Pushchino, Russia,*

<sup>2</sup>*Southern Federal University, Rostov-na-Donu, Russia*

Piezoelectricity in polyvinylidene fluoride (PVDF) is well known, and has been investigated by many authors [1-3]. Nevertheless, the nature of the piezoelectric effect, especially for the “negative piezoelectric effect” in these PVDF materials is still not clear, although several attempts have been made to solve this problem. In this work, computational molecular modeling and exploration was applied to study the nature of the negative piezoelectric effect in the ferroelectric polymer polyvinylidene fluoride (PVDF), and the results confirmed by actual nanoscale measurements. First principle calculations were employed, using various quantum-chemical methods. Both PVDF molecular chains and a unit cell of crystalline  $\beta$ -phase PVDF were modeled. We studied the dependence of the main PVDF electrical properties (dipole momentum, polarization, atomic charges and bond lengths, energies of electron subsystems as well as the total energy of the systems), both without and under an applied electrical field. We explored molecular models of PVDF ferroelectrics with different lengths of the molecular chain, and for a unit cell of the PVDF crystal lattice in the  $\beta$ -phase.

Firstly, we calculate the initial state and all parameters of the PVDF system without an electrical field, taking into detailed consideration the central part of this one PVDF chain. This computational molecular exploration clearly shows that the nature of the so-called negative piezo-electric effect in the ferroelectric PVDF polymer has character, which is connected with the redistribution of electron molecular orbitals, the shifting of charged atomic nuclei, and complex cooperative dipole reorganization in the bonded molecular chain, under the action of applied electrical field. The resulting complicated non-uniform and nonlinear anisotropy deformation of the PVDF molecular chain, arising from both individual interacting and chemically bonded dipoles of  $C_2H_2F_2$ , as well as from the PVDF unit cell, leads to negative deformation in relation to the applied field (OZ axis).

1. Furukawa T// Ferroelectric properties of vinylidene fluoride copolymers. - 1989. -Phase Transit 18:143–211.
2. Bune AV, Fridkin VM, Ducharme S, Blinov LM, Palto SP, Sorokin AV, Yudin SG, Zlatkin A.// Two-dimensional ferroelectric films. -1998. -Nature 391:874–877.
3. Bystrov V, Bystrova N, Paramonova E, Saprionova A.// Computational nanostructures and physical properties of the ultra-thin ferroelectric Langmuir-Blodgett films. -2006. -Ferroelectr Lett 33:153–162.

# Vitrification of B<sub>2</sub>O<sub>3</sub>: Role of hidden polymorphs revealed from molecular dynamics simulations

Ferlat G., Seitsonen A.P., Lazzeri M., Mauri F.

*IMPMC, UMR 7590 CNRS-Université Pierre et Marie Curie, Paris, France;*

*Physikalisch-Chemisches Institut der Universität Zürich, Switzerland*

Understanding the conditions that favour crystallisation or vitrification of liquids has been a long-standing scientific problem. Another connected, and not yet well understood question is the relationship between the glassy and the various possible crystalline forms a system may adopt. In this context, B<sub>2</sub>O<sub>3</sub> represents a puzzling case. It is one of the best glass-forming systems despite an apparent lack of low-pressure polymorphism. Furthermore, the system vitrifies in a glassy form abnormally different from the only known crystalline phase at ambient pressure. Last but not least, it never crystallises from the melt unless pressure is applied, an intriguing behaviour known as the *crystallisation anomaly*.

Here, by means of molecular dynamics simulations employing the density functional theory (DFT), we discover the existence of previously unknown B<sub>2</sub>O<sub>3</sub> crystalline polymorphs with structural properties similar to the glass and formation energies comparable to the known ambient crystal [1,2]. The energy degeneracy of the crystals, which is high at ambient pressure and suppressed under pressure, provides a framework to understand the ability of the system to vitrify and the origin of the crystallisation anomaly. This work reconciles the behaviour of B<sub>2</sub>O<sub>3</sub> with that from other glassy systems and reaffirms the role played by polymorphism in the ability of a system to vitrify.

1. G. Ferlat, A.P. Seitsonen, M. Lazzeri, F. Mauri. Hidden polymorphs drive vitrification in B<sub>2</sub>O<sub>3</sub>// *Nature Materials* **11**, 925-929 (2012); doi: [10.1038/nmat3416](https://doi.org/10.1038/nmat3416)
2. G. Ferlat, T. Charpentier, A.P. Seitsonen, A. Takada, M. Lazzeri, L. Cormier, G. Calas, F. Mauri. Boroxol rings in liquid and vitreous B<sub>2</sub>O<sub>3</sub> from first principles// *Physical Review Letters* **101**, 065504 (2008); doi: [10.1103/PhysRevLett.101.065504](https://doi.org/10.1103/PhysRevLett.101.065504)

# Modelling of thermoelectric modules for low-grade heat recovery

<sup>1</sup>Manyk T.O., <sup>2</sup>Bilynskyj-Slotylo V.R.

<sup>1</sup>*Bukovyna State University of Finance and Economics, Chernivtsi, Ukraine*

<sup>2</sup>*Yuriy Fedkovych Chernivtsi National University, Chernivtsi, Ukraine*

There has been increasing attention to researches aimed at finding ways to improve the efficiency of thermoelectric energy conversion, such as generating modules for the recovery of low-grade heat [1]. A significant proportion of researches are modeling and optimization of these systems. Among the thermoelectric materials which are used to create generator modules on the level of hot temperatures to 773 K materials based on  $\text{Bi}_2\text{Te}_3$  and  $\text{PbTe}$  are conventional. The aim of this paper is design and evaluation of the possibility increasing the efficiency of thermoelectric modules based on  $\text{Bi}_2\text{Te}_3$  and  $\text{PbTe}$  by the use of sectional and cascaded structures.

For researches was conducted selection of materials which produced by SPS-method [2]: for legs of the n-type conduction is chosen:  $\text{Bi}_2(\text{Te}_{1-x}\text{Se}_x)_3$  ( $0 \leq x \leq 1$ ) and  $\text{Sb}_x\text{Pb}_{1-x}\text{Te}_{0.88}\text{S}_{0.12}$  ( $0 \leq x \leq 0.008$ ); for legs of the p-type conduction is chosen:  $(\text{Bi}_2\text{Te}_3)_x(\text{Sb}_2\text{Te}_3)_{1-x}$  ( $0.16 \leq x \leq 0.24$ ) and  $\text{PbTe} + 2\text{mol}\% \text{Na} + x \text{mol}\% \text{SrTe}$  ( $0 \leq x \leq 4$ ). Design and calculation of the generator modules characteristics were carried out by a computer program FemLab, using the experimental temperature dependences of thermoelectric parameters

Two-section module was modeled ( $\text{Bi}_2\text{Te}_3$  was chosen for cold sections and  $\text{PbTe}$  – for hot) with number of thermoelements – 56 couples, height branches of 5.6 mm and cross sectional area of branches  $4.3 \times 1.8 \text{ mm}^2$ . The determination of optimal geometrical parameters two-section  $\text{Bi}_2\text{Te}_3 / \text{PbTe}$  based thermoelement with excluding intersectional losses of electric power made it possible to calculate the main characteristics of the module, operating in the temperature range 303-773 K: maximum efficiency is 13.5% and electrical power – 17 watts. Two-stage module for temperature range 303-773 K was calculated (at cold stage chosen  $\text{Bi}_2\text{Te}_3$  based materials and  $\text{PbTe}$  – at hot stage) with number of thermoelements – 48 couples, cross sectional area of branches  $4.3 \times 1.8 \text{ mm}^2$  at both stages, height branches of 3.3 mm for cold and 2.7 mm for hot stages: efficiency is 15.1% and electrical power – 9.8 watts.

The resulting efficiency value indicates the possibility of increasing the efficiency of thermoelectric modules for low-grade heat recovery.

1. B.I. Ismail, W.H. Ahmed. Thermoelectric power generation using waste-heat energy as an alternative green technology // Recent Patents on Electrical Engineering. -2009. -Vol.2. -P.27-39.
2. T.O. Manyk, V.R. Bilynskyi-Slotylo. Sectional Generating Modules Designing on  $\text{Bi}_2\text{Te}_3$  and  $\text{PbTe}$  Based Materials // Proceedings of XIV International Science-Practical Conference “Modern Information and Electronic Technologies”. Odessa, Ukraine. -2013. P.112-114.

## **Моделювання процесів формування нано-островків конденсату у реакційно-дифузійних системах із пам'яттю**

Д.О.Харченко, В.О.Харченко, С.В. Кохан

*Інститут прикладної фізики НАН України, Суми, Україна*

Розглядається динаміка формування поверхневих структур нано-розмірного масштабу в процесах адсорбції/десорбції в класі реакційно-дифузійних моделях типу Максвела-Катанео, що враховують ефекти кінцевого часу передачі збурень атомовій системі. При дослідженні детерміністичної системи показано, що внаслідок ефектів пам'яті в системі проходять процеси відбору структур та осциляційна динаміка радіусу островків конденсату. Стохастичний випадок із джерелом внутрішніх флуктуацій досліджено у наближенні передемпфованої системи. Виявлено, що внутрішній шум, що задовольняє флуктуаційно-дисипаційне співвідношення за малих інтенсивностей може індукувати проходження нерівноважних фазових переходів між упорядкованими фазами конденсату з островками нано-розмірного масштабу. За великих інтенсивностей такий шум ініціює перехід до неупорядкованої фази з хаотичним розподілом конденсату. Встановлено вплив інтенсивності флуктуацій на період стаціонарних поверхневих структур та відповідний кореляційний радіус.

# **Formation of nano-size structures on the Silicon surface induced by Argon ions sputtering**

Kharchenko V. O.

*Institute of Applied Physics NAS of Ukraine, Sumy, Ukraine*

We study processes of nano-size Si-surface structures formation induced by Ar<sup>+</sup> ion-beam sputtering in the framework of two-level modeling scheme including kinetic Monte-Carlo simulations and continuous theory. To define Silicon target characteristics such as: penetration depth of the ions into the target; widths of the distribution in parallel and perpendicular directions of the incoming beam we use the well known program codes (TRIM and SRIM) for calculating stopping range of ions in matter and transport range of ions in matter. It was shown that both dependencies of penetration depth and longitudinal and transverse widths versus ion energy deviate from the linear law predicted by Bradley and Harper.

Using data from Monte-Carlo simulations and main characteristics for Si target and Ar<sup>+</sup> ions we define the phase diagram (ion energy vs. incidence angle) illustrating possible nano-size structures forming on the silicon target. We have shown that at initial stages of the system evolution the number of surface structures increases (structures formation) and at late stages it remains a constant. We calculated the wavelength dependence on the incident ion energy and the angle of incidence of the formed surface structures. It was found that the wavelength decreases with the ion energy growth according to a power law and varies in the interval from 100 nm to 1 μm. Finally we consider scaling properties of the surface patterns and compute growth and local roughness exponents in the directions normal and parallel to the projection direction of the ion beam at large time interval by analyzing a height-height correlation function.

# Formation of pyramidal islands during epitaxial growth: phase-field modeling

Dvornichenko A.V.

*Sumy State University, Ukraine*

We propose and study properties of pyramidal islands formation in epitaxy within the generalized phase-field approach. By introduction the local temperature field we consider the three-component dynamical system for adsorbate concentration, phase field and temperature. We assume that adsorbed atoms can interact each other.

We show that in the present model at early stages oscillatory regime of pyramidal islands formation can be observed. We define phase diagram illustrating domains of the main system parameters (intensity of the surface re-heat, effective deposition rate and interaction strength) when both temperature of the adsorbate and adatoms concentration grow in the oscillation manner at early stages of the system evolution due to competition of adsorption/desorption processes. Oscillatory regime was studied by means of Lyapunov exponent approach and by computer simulations. By numerical simulations we have shown that the frequency of the temperature field oscillations grows with the deposition flux increasing. Adsorbate interaction strength does not essentially influence on the oscillatory frequency.

We compare obtained results in the proposed generalized three-component phase-field model and results coming from the standard phase-field approach, when temperature of adsorbate is a constant. We have calculated the corresponding probability density functions of the phase field counted off the averaged value at fixed deposition rate and different values for the interaction strength for two kind of models: the standard two-component model at fixed temperature and generalized model at varying temperature field. Finally we discuss the height-height correlation functions and define the corresponding correlation radiuses. It is found that in the proposed generalized three-component model the pyramidal islands are characterized by the small number of terraces and the height between two neighboring terraces is larger than in the standard phase-field model.

The proposed generalization of the standard phase-field approach can be used for the systems (for example, semiconductors), where heating of the condensate plays an essential role in the surface pattern formation.

# ***Ab initio* study of charge correlations in compressed liquid alkali metals**

Klevets I., Bryk T.

*Institute for Condensed Matter Physics, NASU, Lviv, Ukraine*

Modern *ab initio* atomistic simulations of condensed systems allow to study the time evolution of electron density distribution  $\rho_{el}(\mathbf{r},t)$  and total charge density composed of point ions and electron density. For metals at ambient pressures the electron density is very well described by the linear response theory. However one can expect deviation from the linear response for metallic systems at high pressure.

We report *ab initio* molecular dynamics simulations of liquid Li in the pressure range from ambient pressure up to 186 GPa. Static and dynamic total charge correlations were calculated and compared with predictions of the linear response theory. We show that for high pressures the time-dependent total charge correlations reveal different relaxation than the regular density-density correlations, that indeed means a deviation from the linear response. We will discuss the long-wavelength asymptotes for static structure factors of total charge density.

## Thermodegradation kinetics in monolithized spinel ceramics

Klym H.<sup>1,2</sup>, Balitska V.<sup>1,3</sup>, Brunner M.<sup>4</sup>, Shpotyuk O.<sup>1</sup>, Hadzaman I.<sup>1,5</sup>

<sup>1</sup>Scientific Research Company "Carat", Lviv, Ukraine

<sup>2</sup>Lviv Polytechnic National University, Lviv, Ukraine

<sup>3</sup>Institute of Fire Safety, Lviv, Ukraine

<sup>4</sup>Fachhochschule Köln / University of Applied Sciences, Köln, Germany

<sup>5</sup>Drohobych Ivan Franko State Pedagogical University, Drohobych, Ukraine

Functional spinel ceramics are one of the most perspective materials for device application as negative temperature coefficient thermistors. To eliminate the degradation, the method of chemical modification of ceramics at the initial technological stages is used at the example of  $\text{Cu}_{0.1}\text{Ni}_{0.8}\text{Co}_{0.2}\text{Mn}_{1.9}\text{O}_4$  ceramics. Synthesis of optimal thermally-sensitive elements was performed owing to technological conditions for inhibition effects in degradation, the content of NiO phase (1 % - batch 1, 8 % - batch 2, 10 % - batch 3, 12 % - batch 4 and 12 % - batch 5 obtained at different amounts of thermal energy transferred during the sintering) having a decisive role on final ceramics structure.

The results of ageing tests were controlled by relative resistance drift (RRD) caused by ceramics storage at the temperature of 170 °C. The value of RRD for batch 1 (sintered at 1040 °C) with fine grains of 1–3 μm is higher (near 30 %). The extremely small value of RRD near 2.5 % is character for samples of batch 2 (sintered at 1200 °C) having 8 % of additional NiO phase, while ceramics samples of batches 3, 4 and 5 are monolithized having amount of NiO phase near 10 % (for batch 3) and 12 % (for batches 4 and 5). Sintered at higher temperature of batch 5 (1300 °C) demonstrate sharp increase in RRD up to 18%.

This kinetics behaviour in spinel-type ceramics is shown to be adequately described by stretched-exponential relaxation function [1]. The extraction of additional NiO phase from  $\text{Cu}_{0.1}\text{Ni}_{0.8}\text{Co}_{0.2}\text{Mn}_{1.9}\text{O}_4$  ceramics enlarges the dispersivity of the system, while the monolithization of ceramics causes an opposite effect. The non-exponentiality index  $\kappa$  grows from 0.2 (batch 1) to 0.4 for batch 2 ceramics, the similar increase being character for time constant  $\tau$  too. However, the further increase in NiO content from 10 (batch 3) to 12 % (batches 4 and 5) is associated with principally different processes of microstructural evolution corresponding to rash monolithization. The non-exponentiality index  $\kappa$  is most close to 0.4. Such thermodegradation behaviour can be explained in terms topological relaxation model [2].

1. Mazurin O.V. Relaxation phenomena in glass // J. Non-Cryst. Solids. – 1977. – Vol. 25. – P. 130-169.
2. Phillips J.C. Microscopic theory of Kohlrausch relaxation constant  $\beta_k$  // J. Non-Cryst. Sol. – 1994. – Vol. 172-174. – P. 98-103.

# The influence of admixture on the optical properties of the crystals

Stadnyk V.Yo., Kurlyak V.Yu., Romanyuk M.O., Brezvin R.S., Rudysh M.Ya.

*Lviv Ivan Franko National University, Lviv, Ukraine*

Introduction of organic admixtures into the TGS crystal promotes fixing the polarizations  $+P_s$  or  $-P_s$  and appearance of the biasing field  $E_b$ . Due to this, the dielectric parameters of the doped crystals change in the ageing process, the fact that should be properly accounted for when studying and exploring those crystals. Contrary to the TGS, in case of the TGS crystals doped with L-valine (LVTGS) the (110) facets are absent, while the (111) and (100) ones grow only at small dopant concentrations.

In this work we study the influence of L-valine admixture  $(\text{CH}_3)_2\text{-CH-CHNH}_2\text{COOH}$  (L-valine) upon the birefringent and piezooptic properties of the TGS crystals. The temperature and spectral dependences of the  $\Delta n_i$  were measured with the interference technique. The uniaxial mechanical pressure was applied with the aid of a special device, allowing application of stresses as large as  $\sim 500$  bar.

It was determined that the  $\Delta n$  value increases linearly up to the stresses of  $\sigma_i \sim 200$  bar. The general features are as follows: (1) the  $\Delta n_i$  changes are proportional to temperature, (2) the derivative  $\partial\Delta n_i/\partial T$  changes its value while passing through the Curie point, (3) the uniaxial stresses change the absolute value of  $\Delta n_i$ , though remain a qualitative temperature character of  $\Delta n_i$  unchanged, and (4) the PT point is shifted under the influence if the stress.

The PT temperature decreases for the cases of  $\sigma_x$  and  $\sigma_y$  stresses ( $T_c^x = 320.5$  K and  $T_c^y = 320.2$  K), while the  $\sigma_z$  stress increases the PT point ( $T_c^z = 325.2$  K). The relevant temperature shift coefficients are equal to  $\partial T_c/\partial\sigma_x = -0.0064$ ,  $\partial T_c/\partial\sigma_y = -0.0080$  and  $\partial T_c/\partial\sigma_z = 0.0171$  K/bar. The “total” (or hydrostatic) coefficient for the PT temperature shift is 0.0027 K/bar. Those PT shifts have been explained by influence of temperature and stresses on the shifts of structural elements taking place for the PTs. Those slight discrepancies may be caused by both a complex structure of TGS crystals and possible irregularities of introducing the valine admixture into the crystal structure. While the crystal doped with L-valine is growing, the admixture enters into the structure by means of substituting one of the glicines. The glicines I-III are planar in the paraelectric phase, while the glicine I becomes nonplanar in the ferroelectric phase. When the L-valine molecule substitutes the glicine I, the spontaneous polarization  $P_s$  becomes fixed and a biasing field appears, altering all the dielectric parameters of crystals and shifting the PT point. Moreover, a notable shift in the PT point towards higher temperatures should be apparently caused by the influence of uniaxial stresses upon the ferroelectric domains.

## Конфігураційна ентропія змішування розбавлених розчинів $Al_{1-x}Ni_x$ .

Луцишин Т.І., Шевчук О.В., Максимів М.М.

Івано-Франківський національний технічний університет нафти і газу, Україна

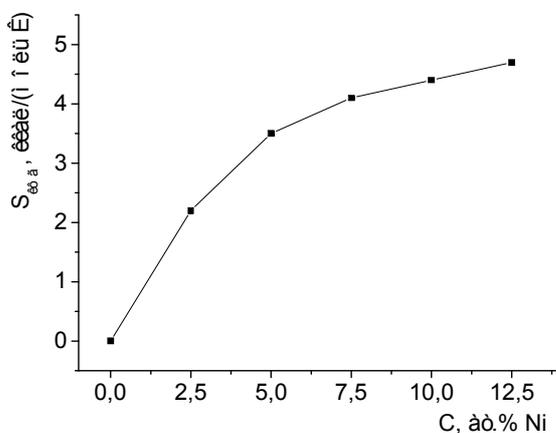
Фазова рівновага системи Al-Ni описується складною діаграмою стану з хімічними сполуками у твердому стані. Така діаграма є наслідком сильної хімічної взаємодії компонентів. Близький порядок чистих Al та Ni характеризуються щільним пакуванням.

Структурні фактори (СФ) розплавів отримані за допомогою рентгенодифракційного дослідження розплавів. Температура перегріву становить 5К вище ліквідус. Для дослідження вибрані сплави  $Al_{1-x}Ni_x$  ( $x=0; 0,025; 0,05; 0,075; 0,1; 0,125$ ), тобто з переважаючим вмістом алюмінію у розплаві. Далі експериментальні СФ використовувались для моделювання RMC-методом [1], як результат розраховані парціальні структурні фактори та парні кореляційні функції.

В наближенні Перкуса-Євіка [2], розраховувалась конфігураційна ентропія змішування за співвідношенням

$$\Delta S = \frac{2\pi k}{\rho} \sum_{i=1}^3 C_i \int g_i(r) \cdot \ln g_i(r) \cdot r^2 dr$$

де  $C_i$  – коефіцієнт який залежить від концентрації та розсіювальної здатності компонента,  $g_i(r)$  – парціальна парна кореляційна функція.



Чисельні значення розрахунків наведені на рис 1. Із отриманих результатів видно, що в області до 5 ат.% спостерігається залежність близька до лінійної, а далі спостерігається значні відхилення від лінійності. Отже термодинамічні властивості даних у концентрації до 5 ат % Ni сплавів можна вважати такими, що підпорядковуються закону Рауля і описуються лінійною залежністю. Такий результат узгоджується із висновками зробленими в роботі [3].

1. McGreevy R.L., Pusztai L. Reverse Monte Carlo simulation: a new technique for the determination of disordered structures // Mol. Simulation. – 1988. – №1. – P. 359-367.
2. Харьков Е.И., Лысов В.И., Федоров В.Е. Физика жидких металлов.- К.: Вища школа.- 1979.- 248с.
3. Mudry S., Lutchyshyn T. Influence of Ni on the structure of liquid aluminum // VIII international conference on crystal chemistry of intermetallc compaunds. Lviv.- 2002.- p106.

# Model pseudopotential calculations for the electronic structure of semiconductors

P.M. Yakibchuk, O.V. Bovgyra, I.V. Kutsa

*Ivan Franko National University of Lviv, Ukraine*

The nonlocal model pseudopotential (MP) [1] has been proposed for electron-ion interactions description in metals in the form

$$w(r) = -\frac{z}{r} + \sum_{l=0}^{l_0} e^{-r/R_l} \left( A_l + \frac{z}{r} \right) P_l,$$

where  $A_l$  and  $R_l$  – parameters of MP,  $P_l$  – projection operator.

In a number of works present MP used to calculate the properties of simple [2], transition [3] and rare metals and in all cases good agreement of calculation results with the corresponding experimental data was obtained.

In this work, the possibility of this MP to describe the electron-ion interaction in semiconductors was considered. We define the parameters of MP for semiconductors with diamond and zinkblende lattice structures, such as Si, Ge, GaAs, AlAs. The calculated MP form factors for all considered semiconductors are in good agreement with the calculated similarly Heine-Abarenkov pseudopotential form factors and experimental data. The Fourier transforms of the model potential was used to obtain the  $q$ -dependent pseudopotential, which is then used to calculate the energy band structures of semiconductors along different crystallographic directions. Note that spin-orbit interaction is not included in these simulations.

We have compared our results of band structure with other pseudopotential calculations and experimental data. It should be noted that good agreement of energy gaps values and dispersion of energy bands in reciprocal space indicates that our model pseudopotential could be applied to investigations of other electronic properties of semiconductors.

1. Ya.I.Dutchak, P.M.Yakibchuk, M.I.Zhovtanetckii. Non-local model potential and atomic properties of non-transition metals // Institute for Theoretical Physics Preprint. – Kiev. – 1975 (in Russian).
2. Ya.I.Dutchak, P.M.Yakibchuk, G.I.Baryljak. Effective potentials of interionic interaction and interionic force constant of simple metals in nonlocal pseudopotential theory // Fiz. Met. Met. – 1977. – Vol. 44. – P.938-944, (in Russian).
3. Ya.I.Dutchak, P.M.Yakibchuk, M.I.Zhovtanetckii, Z.A.Gurskii, V.V.Furman. Model pseudopotential of transition metals. Electronic structure and physico-chemical properties of refractory compounds and alloys. – Kiev, Naukova dumka. –1980, (in Russian).

# Electronic structure and magnetism of 3d transition metal-doped ZnO nanostructures

O.V. Bovgyra<sup>1</sup>, M.V. Kovalenko<sup>1</sup>, R.V. Bovhyra<sup>2</sup>

<sup>1</sup>*Ivan Franko National University of Lviv, Ukraine*

<sup>2</sup>*Pidstryhach Institute for Applied Problems of Mechanics and Mathematics, Lviv, Ukraine*

Diluted magnetic semiconductors (DMS) have attracted scientific interest because of their unique spintronics properties with possible technological applications. Wide band-gap metal oxides such as zinc oxide (ZnO) are among the best candidates for industrial DMS due to their multifunctionality in opticomagnetic applications. In particular, ZnO-based DMS with properties such as transparency in visual region and piezoelectricity have generated huge interest among the scientific community as a strong candidate for the fabrication of spin transistors and spin-polarized light-emitting diodes. In the study of ferromagnetism in DMS we are interested in magnetic exchange coupling between transition metal (TM) impurities; therefore electronic structure calculations at finite impurity concentrations are needed.

The scope of the present work is to study the properties of ZnO clusters ( $\text{Zn}_{12}\text{O}_{12}$ ) and nanotubes (NT) doped with 3d transition metal (TM) elements (TM = V, Mn, Co, Cu) by the density functional theory (DFT). The spin-polarized DFT calculations and the full geometry optimizations on the ZnO nanostructures with and without 3d transition metal atom were performed using the generalized gradient approximation with revised Perdew, Burke and Ernzerhof functional for the exchange-correlation energy. The electronic wave functions were expanded in a plane wave basis set. Charge transfers and magnetic moments are calculated based on the Mulliken population analysis.

The calculated results show that of the pristine ZnO nanostructures are nonmagnetic, TM-doped ZnO nanostructures have large magnetic moment and the ferromagnetic coupling is resulted from the hybridization between the O 2p and 3d states of TM atom. It is found that V-doped ZnO nanostructures are ferromagnetic materials with metallic properties. On the electronic structures, the analyses of total and projected density of states (DOS) indicate that Mn-, Co- and Cu- doped ZnO nanostructures are all half-metals and magnetic with 100% spin polarization and seem to be ideal candidates as DMSs for spintronic applications.

Presented investigations may provide a better understanding on the structural physics and chemistry of magnetic dopants in nanocrystallined DMS materials.

# Structure and dynamic properties of aluminium-copper alloys: a molecular dynamics study

Petro Yakibchuk<sup>a</sup>, Violeta Patsahan<sup>a</sup> and Taras Patsahan<sup>b</sup>

<sup>a</sup>*Department of Metal Physics, Ivan Franko National University of Lviv, Ukraine*

<sup>b</sup>*Institute for Condensed Matter Physics of the NAS of Ukraine, Lviv, Ukraine*

Using the method of molecular dynamics the computer simulations were performed for the different compositions of Al-Cu alloys. The embedded atom model (EAM) [1] was applied to describe the interatomic interactions in the considered systems. There are a few of the EAM potentials developed by the different authors for Al-Cu alloys [2-4]. We tested an ability of these potentials to predict the melting temperature and to give a correct description of the melts structure. To this purpose we built crystalline structures, which were appropriate to the alloy compositions under study. Starting from low temperatures each of the systems was heating until a crystalline structure was destroyed. The internal energy and the alloy density depending on the temperature were obtained. The pair correlation functions of melted Al-Cu alloys were calculated and compared with experimental data. The dynamic properties of the liquid alloys of Al-Cu were studied as well. With this aim the temperature dependencies of self-diffusion coefficient were obtained. It was shown that parameters of the EAM potential proposed in [4] give the best agreement with experiment.

1. S.M. Foiles, M.I. Baskes, M.S. Daw. Phys. Rev. B. -1986. -Vol.33. -P.7983.
2. J. Cai, Y.Y. Ye Phys. Rev. B. -1996. -Vol.54. -P.8398.
3. X.-Y. Liu, C.-L. Liu, L.J. Borucki, Acta Mat. -1999, -Vol.47. -P.3227.
4. X.W. Zhou, R.A. Johnson, H.N.G. Wadley, Phys. Rev. B. -2004. -Vol.69. -P.144113.

# Simulation of advective diffusion in horizontally periodical stratified structures

Chaplya Y.Y.<sup>1,2</sup>, Goncharuk V.Y.<sup>3,1</sup>, Dmytruk V.A.<sup>3,1</sup> and Chernukha O.Y.<sup>1</sup>

<sup>1</sup>Centre of Mathematical Modelling of Pidstryhach Institute for Applied Problems of Mechanics and Mathematics of Ukrainian National Academy of Sciences, Ukraine; <sup>2</sup>Institute of Mechanics and Applied Informatics of Kazimierz Wielki University in Bydgoszcz, Poland; <sup>3</sup>National University "Lviv Polytechnic", Ukraine

Relation between the behavior of mass transfer processes and the structure of a material, where they occur, attracts significant interest. For instance, diffusion influences properties of new composites, when controlling type and distribution of thin channels of fast movement of admixture particles (the domains corresponding to the internal physical surfaces e.g., grain boundary, subgrains) at an initial stage of manufacturing it is possible to obtain a material with properties needed for specific practical applications. Simulation of such processes is based on exact analytical solutions of contact initial boundary-value problems of admixture mass transfer in two-phase periodical structures taking into account both the diffusion in each phase and the advective mechanism in one of them.

For finding these solutions describing the concentration redistribution in the body, we suggest an original method based on integral transforms by the spatial variables separately in the domain of thin channels and in the domain of basic matrix [1]. As partial case of this problem, the Fisher model of advective diffusion along the grain boundary is studied. On this solutions the software is designed and used for investigation of migration processes in two-phase periodical structures. In Fig. 1 for visualization the simulation of saturating steel surfaces with carbon (C) during austenitic steel formation is presented.

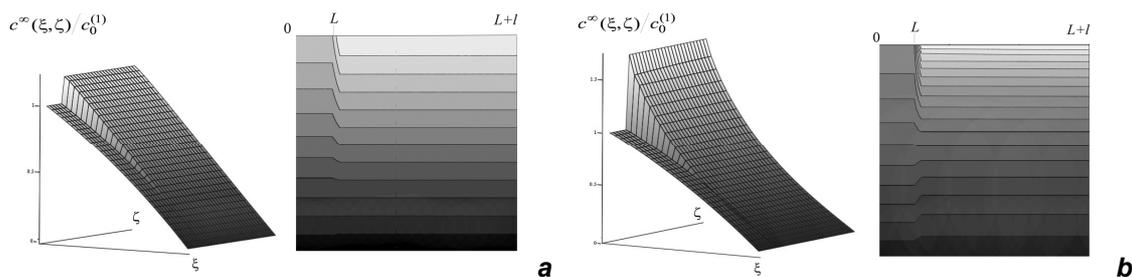


Fig. 1. Redistributions of the carbon concentration in structural elements of a steel layer: a) traditional method of steel cementing; b) thermal cycling

The results of simulation have shown that application of method of thermal cycling leads to the penetration of atomic carbon into the crystal medium in 8 times greater than the quantity of carbon absorbed by a material using a common technology of carburizing steel products.

1. Y. Chaplya, O. Chernukha, V. Dmytruk. Advective-diffusive mass transfer in binary regular structures in the steady-state regime // Applied Mathematical Modelling 37 (2013), pp. 6191-6211.

# Optical activity of disordered gallogermanate crystals

Shopa Y.I., Ftomyn N.Y., Sokolyuk I.V.

*Ivan Franko National University of Lviv, Ukraine*

During the past few years, special attention is paid to correlation between structure and optical properties of crystals e.g., gyrotropic, refractive etc. Phenomena of the rotation of the plane polarization of light traversing a medium is called optical activity (OA) and quantitatively described by the optical rotation (OR)  $\rho = \pi(n_L - n_R)/\lambda$  of the polarization plane (where  $n_L$ ,  $n_R$  denotes refractive indices for left and right circularly polarized light with wavelength  $\lambda$ ). It is well known that the value and the sign of OR is highly sensitive to the structure of the crystals. Furthermore, the possibility to calculate OR using crystal structure data and the information about electronic polarizability volumes of individual atoms gives polarizability theory of OA [1].

The langasite family crystals (Ca-gallogermanate structure type, P321,  $Z = 1$ ) are perspective materials for effective sensors, acoustoelectronic devices, quantum electronics [2]. It necessary to note that most of these crystals are disordered (the occupations of the  $1a$ ,  $3f$ , and  $2d$  Wyckoff positions by Ga/Ge, Ga/Si, etc., atoms are different). These compounds are optically uniaxial, non-centrosymmetric and in addition – optically active with diagonal gyration tensor  $g_{ij}$  (there are two independent components of the  $g_{ij}$  tensor i.e.,  $g_{11} = g_{22}$ ,  $g_{33}$ ).

The aim of our work was to estimate the cite occupancy of  $1a$ ,  $3f$ , and  $2d$  Wyckoff positions of atoms in langasite family crystals applying the results of the OR calculations. The values of polarizability volumes of the  $\text{Ca}^{2+}$ ,  $\text{Ga}^{3+}$ ,  $\text{Ge}^{4+}$ , etc., ions for various crystals with the Ca-gallogermanate structure were calculated in [3], as well as the polarizability volumes of the ions occupying mixed  $1a$ ,  $2d$  and  $3f$  Wyckoff positions (e.g.  $1a - 0.4\text{Ga}+0.6\text{Ge}$ ,  $3f - 0.53\text{Ga}+0.47\text{Ge}$  for  $\text{Ca}_3\text{Ga}_2\text{Ge}_4\text{O}_{14}$  [2]). Using the information about the polarizabilities [3] OR was calculated as a function of cite occupancy of mixed  $1a$ ,  $3f$ , and  $2d$  position for gallogermanate crystals.

Therefore, the comparison of the calculated values of OR with the data of experiment could probably be as the method of refinement of the cite occupancy of mixed positions in the transparent disordered optically active crystals.

1. V. Devarajan, A. Glazer. Theory and computation of optical rotatory power in inorganic crystals// Acta Cryst. – 1986. – Vol. A 42. – P.560-569.
2. B. Mill, A.Klimenkova, B. Maximov, et al. Enantiomorphism of  $\text{Ca}_3\text{Ga}_2\text{Ge}_4\text{O}_{14}$  compound and comparison of the  $\text{Ca}_3\text{Ga}_2\text{Ge}_4\text{O}_{14}$  and  $\text{Sr}_3\text{Ga}_2\text{Ge}_4\text{O}_{14}$  structures// Crystallography Reports – 2005. – Vol. 50, No 5. – P.785-794.
3. Y. Shopa, N. Ftomyn. Calculation of optical rotation and refractive indices in the langasite family crystals// Proceedings of international conference OMEE-2012. – 2012. – P.137-138.

# **Compressed sensing and structure of multicomponent alloys**

Yakibchuk P.M., Volkov O.V., Vakarchuk S.O.

*Ivan Franko National University of Lviv, Ukraine*

Compressed sensing is a signal processing technique for efficiently acquiring and reconstructing a signal, by finding solutions to underdetermined linear systems. This takes advantage of the signal's sparseness or compressibility in some domain, allowing the entire signal to be determined from relatively few measurements. This technique is applied to X-ray studies of metallic alloy structure. Using optimized wavelet transforms which are developed within Polydisperse Hard Sphere approximation we filter experimental noises and increase the precision of the experimental data which allows to detect a lot of subtle effects inaccessible for standard experimental studies

## **Simulation of metallic alloy structure during melting process**

Yakibchuk P.M., Volkov O.V., Vakarchuk S.O.

*Ivan Franko National University of Lviv, Ukraine*

During the recent decade the Polydisperse Hard Sphere approximation was developed and intensively investigated. Here, we are implementing new technique for modeling of structural transformation of atomic distribution in binary alloys in the temperature ranges right above their melting points. Controlling the dispersion factor of each component and the composition of the alloy we calculate partial correlation function (e.g. Structure Factors and Pair Correlation Functions) and receive series of snapshots for each set of control parameters. Comparing the temperature dependencies of real system with the one we calculate within Polydisperse Hard Sphere approximation we may reproduce the dependency of dispersion factors (and other parameters if the model is multivariate) on temperature for the reference system in a whole range of interested states. We have performed these calculations for a set of binary alloys and found the fact there is some classes of the alloys obeys similar rules so the calculation made for some reference metal may be expanded to the whole class of the alloys.

# **Deterministic approach to construction of structure factors for metallic alloys**

Yakibchuk P.M., Volkov O.V.

*Ivan Franko National University of Lviv, Ukraine*

Using Polydisperse Hard Sphere approximation we present the metallic alloy as a set of clustered components. Each of the component is characterized by the sphere diameter dispersion, its effective fraction and the inter-component additivity. These parameters are used as controls to build the multivariate linear programming problem the aim of which is to exactly fit the structure characteristics received from experimental X-ray studies. Using deterministic optimization technics we perform optimization of the theoretical model to experimental data and receive a sparse set of model parameters. These parameters may be used to forecast a set viscoelastic properties of alloys and perform both interpolation and extrapolation of interatomic correlation functions.

# Calculation and experimental study of energy bands of LaPO<sub>4</sub> nanoparticles

Ya. Chornodolskyy<sup>1</sup>, A. Gloskovskii<sup>2</sup>, V. Vistovskyy<sup>1</sup>, O. Shevchuk<sup>3</sup>,  
O. Myagkota<sup>3</sup>, S. Syrotyuk<sup>3</sup>, A. Zaichenko<sup>3</sup>, V. Voloshinovskii<sup>1</sup>

<sup>1</sup>*Ivan Franko National University of Lviv, Ukraine*

<sup>2</sup>*Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany*

<sup>3</sup>*Lviv Polytechnic National University, Ukraine*

Study of band energy structure of luminescent nanoparticles is important for understanding and predicting of their physical properties. Experimental study of the energy band structure is usually performed by means of photoelectron spectroscopy. However, for this method the samples must possess the rather high conductivity to avoid their charge. However, luminescent materials are usually dielectric. In this paper, for the X-ray photoelectron studies the LaPO<sub>4</sub> dielectric nanoparticles were coated with about 1 nm layer of silver.

LaPO<sub>4</sub>-Eu nanoparticles with mean grain size of 16 nm were synthesized via sedimentation nucleation method as it is described in [1]. The synthesis of silver covering onto LaPO<sub>4</sub>-Eu nanoparticle surface was performed as follows. Firstly the dispersion of LaPO<sub>4</sub> nanoparticles (0.2 g) in water (14ml) was prepared and stirred during 2 hours. In another vessel the solution of AgNO<sub>3</sub> (0.21 g) in 1% water-ammonia solution (16ml) was prepared. Then this solution was mixed with the dispersion of LaPO<sub>4</sub>-Eu nanoparticles in a vessel equipped with inlet for argon purging and stirred during 1 hours. After that the solution of NaBH<sub>4</sub> (0.03 g) in water (4ml) was added dropwise into reaction mixture while stirring during 30 min. The synthesis was carried out at 293 K. Nanoparticles with silver covering were separated by centrifugation washed a few times with water and dried until constant weight.

The calculations of band structure of LaPO<sub>4</sub> crystal was performed using the PAW formalism and taking into account the strong local correlations in the PBE0 GGA approximation. The calculation of the partial electron state density of LaPO<sub>4</sub> crystal is performed and the nature of the various states in the overall density formation is explained. The obtained results are in good agreement with the experimental ones obtained from the X-ray photoelectronic spectra in the range of LaPO<sub>4</sub> valence and nearest core bands.

1. V. Vistovskyy, N. Mitina, A. Shapoval et al., Opt. Mater. 34, 2066-2070 (2012).

## Секція 2

*Структура неупорядкованих систем*

*Фізичні властивості розплавів і аморфних сплавів.*

*Наноматеріали і наноккомпозити.*

# Scaling functions and critical amplitude ratios for the Potts model on scale-free networks

M.Krasnytska<sup>1,2</sup>, B. Berche<sup>2</sup>, Yu. Holovatch<sup>1</sup>

<sup>1</sup>*Institute for Condensed Matter Physics NAS Ukraine, Lviv, Ukraine*

<sup>2</sup>*Institute Jean Lamour, University of Lorraine, Nancy, France*

Recently, much attention is being paid to analysis of phase transition models on complex networks [1]. Possible applications of spin models on complex networks can be found in various segments of physics, starting from problems of sociophysics to physics of nanosystems, where the structure is often much better described by a network than by geometry of a lattice. In this case, the disorder of an underlying structure is modeled in terms of a random graph, rather than a random lattice.

In this report we present analysis of phase transition behaviour of a Potts model which is the standard model of statistical physics and has numerous physical realizations [2]. We consider the  $q$ -state Potts model on an uncorrelated scale-free network for which the node-degree distribution manifests a power-law decay governed by the exponent  $\lambda$ . In our previous paper [3] we have shown that, depending on particular values of  $q$  and  $\lambda$ , one observes either a first-order or a second-order phase transition or the system is ordered at any finite temperature. In the present study we further analyze the model in the second-order phase transition regime. In particular, we analyze the equation of state and get scaling functions which are of fundamental interest in the theory of critical phenomena and have previously been theoretically and experimentally explored in the context of various magnetic and fluid systems [4]. Here, we obtain general scaling functions for the order parameter, entropy, the constant-field heat capacity, magnetic susceptibility and the isothermal magnetocaloric coefficient near the critical point. Moreover we present critical amplitudes ratios, that appear to depend on the node-degree distribution exponent  $\lambda$ .

1. S. N. Dorogovtsev, A. V. Goltsev, J. F. F. Mendes. *Rev. Mod. Phys.* **80** (2008) 1275.
2. F. Y. Wu, *Rev. Mod. Phys.* **54** (1982) 235.
3. M. Krasnytska, B. Berche, Yu. Holovatch. *Condens. Matter. Phys.*,16, No. **2**, (2013) 23602.
4. C. von Ferber, R. Folk, Yu. Holovatch, R. Kenna, V. Palchykov. *Phys. Rev. E* **83**, (2011) 061114.

## Defect Subsystem of Solid Solutions

### PbTe-Sb<sub>2</sub>Te<sub>3</sub> and PbTe-Bi<sub>2</sub>Te<sub>3</sub>

<sup>1</sup>Freik D.M., <sup>2</sup>Mudry S.I., <sup>3</sup>Kryskov C.A., <sup>1</sup>Gorichok I.V., <sup>1</sup>Lyuba T.S.,  
<sup>1</sup>Turovska L.V., <sup>1</sup>Krynycky O.S., <sup>1</sup>Matkivskyi O.M.

<sup>1</sup>*Vasyl Stefanyk PreCarpathian National University, Ivano-Frankivsk, Ukraina*

<sup>2</sup>*National University "Lviv Polytechnics", Ukraina*

<sup>3</sup>*Kamyanets-Podilsky State University, Ukraina*

Lead telluride is a promising semiconductor material for conversion of thermoelectric energy devices that operate in high temperature range (500-850) K. Doping with antimony and bismuth can significantly improve the thermoelectric properties of the material. In particular, substituting ions of lead, atoms of fifth group of the periodic table that are in the valence shell with one electron more than the matrix atom, giving it into the conduction band, which leads to increase the concentration of free carriers  $n$  and conductivity  $\sigma$ . The solid solutions of PbTe-Sb<sub>2</sub>Te<sub>3</sub> and PbTe-Bi<sub>2</sub>Te<sub>3</sub> are less researched, although thermoelectric properties of such systems can be much better, particularly by significantly reducing the effectiveness of solutions' thermal conductivity due to phonon scattering on defects in the crystal lattice. However, reliable data about the mechanism of occurrence of antimony and bismuth atoms into the lattice is absent. Therefore, the goal of this research is to discover the structural and thermoelectric properties PbTe-Sb<sub>2</sub>Te<sub>3</sub> and PbTe-Bi<sub>2</sub>Te<sub>3</sub> solid solutions' crystal chemistry and establishing mechanisms for their formation.

Synthesis of solid solutions was performed by fusion in quartz ampules evacuated to a pressure of  $2 \cdot 10^{-4}$  Pa. The initial used components were purified Pb, Te, Sb and Bi. These bars were crushed in an agate mortar and after selecting fractions sized (0,05 - 0,5) mm were compressed under the pressure of 0,5 GPa. These cylindrical samples with  $d = 5$  mm and  $h \approx 8$  mm were subjected for annealing in air at a temperature of  $T = 230$  ° C for 5 h.

A conclusion of the research is that increasing Sb<sub>2</sub>Te<sub>3</sub> content in solid solution leads to a monotonic decrease of the lattice constant and reducing of Zeebek's index with saturations on back end with concentrations  $> 1$  mol.% and non-monotonic change in conductivity with a minimum at 1 ml.% Sb<sub>2</sub>Te<sub>3</sub>.

The functional dependence between PbTe-Bi<sub>2</sub>Te<sub>3</sub> solid solutions' lattice constant and content of Bi<sub>2</sub>Te<sub>3</sub> is characterized by nonmonotonic dependence of the minimum in the vicinity of 2 ml.% Bi<sub>2</sub>Te<sub>3</sub>. Concentrational dependence of conductivity is also nonmonotonic with a maximum at 1 mol.% Bi<sub>2</sub>Te<sub>3</sub>; Zeebek's index decreases in all the studied concentration range while increasing content of Bi<sub>2</sub>Te<sub>3</sub>. Crystal quasychemical analysis the defect subsystem indicates that dominant mechanism for formation PbTe-Sb<sub>2</sub>Te<sub>3</sub> solid solution is substituting lead antimony to form interstitial tellurium. The same conclusion is in case of PbTe-Bi<sub>2</sub>Te<sub>3</sub> solid solutions: the position of lead bismuth substitution with the formation of interstitial tellurium was realized only at concentrations of Bi<sub>2</sub>Te<sub>3</sub>  $\geq 2$  mol.%.

# The EXAFS and DFT Study of Doped Nickel Phthalocyanine as a Potential Room-Temperature Molecular Magnet

L. A. Avakyan<sup>1</sup>, A. S. Manukyan<sup>2</sup>, A. A. Mizarkhanyan<sup>2</sup>, E. G. Sharoyan<sup>2</sup>, Y. V. Zubavichus<sup>3</sup>, A. L. Trigub<sup>3</sup>, N.A. Kolpacheva<sup>1</sup>, L. A. Bugaev<sup>1</sup>

<sup>1</sup>*Southern Federal University, Rostov-na-Donu, Russia*

<sup>2</sup>*Institute for Physical Research National Academy of Sciences of Armenia, Yerevan, Republic of Armenia*

<sup>3</sup>*National Research Centre Kurchatov Institute, Moscow, Russia*

Magnetic properties of compounds are usually originated of localized d- and f-electronic states of metal ions. Recently a new class of magnetic materials was revealed, where noncompensated spin magnetic moment is formed by p-electrons of nonmetal atom [1, 2]. Application of these materials is drastically limited by weak spin coupling so that magnetic order vanishes at temperature of several dozens Kelvin, and, in most cases, compounds are antiferromagnetic and unstable at ambient conditions.

In this work Nickel Phthalocyanine (NiPc,  $\text{Pc}=\text{N}_8\text{C}_{16}\text{H}_{32}$ ) doped by Kalium was studied as a potential Room-temperature ferromagnet with molecular origin of its magnetism [3] via the EXAFS spectroscopy tool which provides detailed information about local structure of selected type of absorbing atom. The EXAFS study revealed unchanged NiPc molecules together with Nickel clusters, which should not influence magnetic properties due to small concentration of metallic Nickel. Consequently the simulation within density functional theory framework of NiPc electronic structure was performed. The obtained distribution of electronic and magnetic density confirmed the molecular origin of magnetism, XANES, UV/vis spectra were simulated using Abinit [4] software.

1. P.-M. Allemand, K. C. Khemani, A. Koch, F. Wudl, K. Holczer, S. Donovan, G. Grüner, J. D. Thompson Organic molecular soft ferromagnetism in a fullerene C60// *Science*, 1991, 253 (5017), 301-302.
2. J. M. Clemente-Juan, E. Coronado, A. Gaita-Ariño Magnetic polyoxometalates: from molecular magnetism to molecular spintronics and quantum computing // *Chem. Soc. Rev.*, 2012, 41, 7464-7478.
3. S. Manukyan, A. A. Mirzakhanyan, T. I. Butaeva, A. A. Guda, A. V. Soldatov, L. A. Bugaev, H. R. Asatryan, P. G. Baranov, E. G. Sharoyan Room-temperature molecular ferromagnetism based on nickel phthalocyanine. Magnetic resonance, optical and xanes spectra// *Armen. J. Phys.* -2010. -Vol.3 -P.272-275.
4. Abinit Software Project <http://www.abinit.org>

# Spatial periodic structures in the system of charged Fermi particles above the surface of liquid dielectrics

Lytvynenko D.M., Slyusarenko Yu.V.

*Akhiezer Institute for Theoretical Physics NSC KIPT, Kharkiv, Ukraine*

We propose a consistent theory of equilibrium states of same sign charges above the surface of liquid dielectric film located on solid substrate in the presence of external attracting constant electric field. The theory is based on the variation principle [1] that allows obtaining the self-consistency equations for the parameters describing the system: the distribution function of charges above the liquid dielectric surface, the electrostatic field potentials in all regions of the system and the surface profile of the liquid dielectric. The self-consistency equations are used to describe the phase transition associated with the formation of spatially periodic structures in the system of charges on liquid dielectric surface. Assuming the non-degeneracy of the gas of charges above the surface of liquid dielectric film the solutions of the self-consistency equations near the critical point are obtained. In the case of the symmetric phase we obtain the expressions for the potentials and electric fields in all regions of the studied system [1, 2]. The distribution of the charges above the surface of liquid dielectric film for the symmetric phase is derived. The system parameters of the phase transition to nonsymmetric phase – the states with a spatially periodic ordering are obtained. We derive the expression determining the period of two-dimensional lattice as a function of physical parameters of the problem – the temperature, the external attractive electric field, the number of electrons per unit of the flat surface area of the liquid dielectric, the density of the dielectric, its surface tension and permittivity, and the permittivity of the solid substrate. We take the temperature of the system, external pressing electric field and the number of charges above dielectric surface unit as the control parameters for the researched phase transitions. The numeric estimations of the critical values of the control parameters are made. The obtained values are similar to the experimental data [3].

1. D.M. Lytvnenko, Yu.V. Slyusarenko and A.I. Kirdin. The Thomas-Fermi model in the theory of systems of charged particles above the surface of liquid dielectrics// J. Math. Phys. -2012. –Vol.53, 103302
2. D.M. Lytvynenko, Yu.V. Slyusarenko. On equilibrium charge distribution above dielectric surface// Condensed Matter Physics. –2009. -Vol.1. –P.19-34.
3. P. Leiderer, M. Wanner. Structure of the dimple lattice on liquid  $^4\text{He}$ // Physics Letters A.-1979, -Vol.73, -№3, -P.189-192.

# Amorphization of the ice near melting point

V.M.Silonov, V.V.Chubarov

*Moscow State University named after M.V.Lomonosov, Moscow, Russia*

The enormous quantity of scientific works were dedicated to the problems of water structure and different forms of ice. The authors of the work [1] approved that amorphous ice can be created only at the temperature lower the temperature of vitrification 130K. In all cases the attempts of formation of the amorphous ice by quickly direct cooling of liquid water led up to appearance of ice Ih [2].

The exploration of X-ray scattering and the revelation of nature of X-ray diffusion scattering from water ice was the main aim in present work. For X-ray diffractometer, specially, the precision semi-automatic low temperature attachment was elaborated for the investigations of the X-ray diffusion scattering from water ice near the melting point 00C [3].

The reflections of hexagonal phase Ih were discovered by authors on X-ray diffraction pattern simultaneously with the intensive diffusion scattering, caused by amorphization of the ice. In the present work this was obtained both on the samples of water ice, recorded at the temperature range from 00C to –250C, prepared at temperature of liquid nitrogen, and on the samples, recorded at temperature –100C. The existence of both the X-ray reflections of crystal phase and intensive X-ray diffusion scattering points to coexisting in water ice the crystalline and amorphous conformations. The splitting of the first maximum on the radial distribution function was detected by using the X-ray diffraction pattern of the ice sample at the temperature –30C. At present work this splitting was explained by increasing of interatomic distances between nearest-neighbor atoms located on different levels. The same splitting was obtained on the radial distribution function by using the X-ray diffraction pattern of the ice sample at the temperature –100C.

1. Mishima O., Stanley H.E. // Nature. 1998. V. 396. P. 329.
2. Fletcher N.H. // Rep. Prog. Phys. 1971. V. 34. P. 913.
3. Silonov V.M., Chubarov V.V. Preprint № 2/2013. Moscow: Moscow State University by M.V. Lomonosov, Physic's Department.

## Calculation of the mass fraction of spinel $\text{MgAl}_2\text{O}_4$ that formed at the operation with ceramic welding fluxes

O. O. Davydenko, V. E. Sokolskii, I.O. Goncharov

*Tharas Shevchenko National University, Kyiv, Ukraine*

*The E.O. Paton Electric Welding Institute, Kyiv, Ukraine*

New approaches should be elaborated to meet quality demands for a weld, which is produced at automatic arc welding under a flux. These requirements are due to the fact that modern industry has need in a significant increase of the welded joints strength and of the rate of the welding process. To produce defect-free joints the molten flux, the latter should be characterized by gradual increase of viscosity with the temperature decrease. This increase of viscosity should realize in a wide temperature interval, that reduces temperature-dependent fluctuations in the metallic part of the weld pool. So, it seems to be reasonable to use for this purpose the crystalline spinel ( $\text{MgAl}_2\text{O}_4$ ), which is formed at heating of the ceramic fluxes of  $\text{MgO}-\text{Al}_2\text{O}_3-\text{SiO}_2-\text{CaF}_2$  system. The spinel remains crystalline up to  $2100^\circ\text{C}$ , and, thus, increases the viscosity of the molten ceramic flux by the spinel crystallites inclusion into fluxed matrix. In such a way the increase of amount of spinel in the ceramic flux causes the increase of viscosity. The qualitative determination of spinel in the molten ceramic flux matrix is the main aim of the present study. For this reason two automatic X-ray diffractometers, which are recorded solid state and melts diffraction spectra, were used. Quantitative X-ray diffraction (QXRD) analysis with the internal standard and chemical analysis were used to examine the fluxes. Tungsten trioxide was used as the internal standard at the QXRD experiments. Monoclinic  $\text{WO}_3$  was chosen as the standard due to the fact that its reflection does not overlap with the main reflections of the spinel and that of other crystalline phases could be registered in the samples. The QXRD and the chemical analysis show that the content of spinel in the samples is in the range of 20-29.4 wt. %. It was found that all  $\text{Al}_2\text{O}_3$  of the initial flux composition was spent on the spinel formation, thus  $\text{MgO}$  left in an excess. The ratio of composed oxides in the spinel phase is 70 wt.%  $\text{Al}_2\text{O}_3$  and 30 wt.%  $\text{MgO}$ . The spinel phase is formed completely at  $1500^\circ\text{C}$ . It was found from the X-ray diffraction determined quantitative ratios of the spinel found in the welding slag after the welding and in the molten model samples, which were obtained at different temperatures. The quantitative relations determined by XRD correspond within  $\pm 2$  wt.% confidence interval to the chemical analysis results. An experimental correlation between the viscosity and the content of the spinel phase in the samples was determined. The method elaborated by us can be recommended for the practical use.

## X-Ray Diffraction Study of the NaF–LiF–NdF<sub>3</sub> and NaF–LiF–LaF<sub>3</sub> Eutectic in the Liquid and Solid States

V. E. Sokol'skii, A. S. Roik, O. O. Davidenko, S. A. Fesenko, N. V. Faidyuk, and R. N. Savchuk

*Tharas Shevchenko National University, Kyiv, Ukraine  
Vernadsky Institute of General and Inorganic Chemistry, Kyiv, Ukraine*

The ternary eutectic alloy with the composition 33 mol % NaF + 53 mol % LiF + 14 mol % NdF<sub>3</sub> and 44 mol % NaF + 42 mol % LiF + 14 mol % LaF<sub>3</sub> has been studied in the liquid and crystalline states using X-ray diffraction at room and high temperatures. Room-temperature XRD measurements were made on a DRON-3 diffractometer (CuK $\alpha$  radiation). Analogous studies at higher temperatures were carried out in a helium atmosphere on a diffractometer adapted for studies of melts (DRON-2), using a high-temperature vacuum chamber and  $\theta$ – $\theta$  goniometer. We used MoK $\alpha$  radiation monochromatized by balanced differential Zr + Y filter pair. High-temperature XRD examination at 350, 450, and 550°C showed that the phases present in the material were in the crystalline state. At 600, 700, and 800°C, the sample was in the liquid state. Structural models of melts at different temperatures were derived from SF curves using reverse Monte-Carlo simulations.

The results demonstrate that the alloy undergoes no phase transformations below its melting point: the only phases identified with certainty are NaF, LiF, and NaLnF<sub>4</sub> (Ln=La, Nd). However, in these systems, there are minor differences, which affects the results of the experiment in the liquid state [1-2]. The unit cell parameters, with temperature increasing of NaF, LiF and NaNdF<sub>4</sub> are linear functions of temperature.

In contrast to the lanthanum trifluoride containing melt, the fluorine anions in the neodymium trifluoride containing melt do not form close\_packed microgroups. The lanthanum melt is not structurally uniform but consists of a mixture of microgroups that differ quantitatively in cation composition. The neodymium cations do not form any locally ordered centers with attached fluoride polyhedra having sodium or lithium atoms in their center.

1. Sokol'skii, V.E., Roik, A.S., Kazimirov, V.P., et al., X-ray diffraction study of the NaF–LiF–LaF<sub>3</sub> eutectic in the liquid and solid states, *Inorg. Mater.*, 2012, vol. 48, no. 4, pp. 416–422.
2. V. E. Sokol'skii, A. S. Roik, A. O. Davidenko., et al., X-Ray Diffraction Study of the NaF–LiF–NdF<sub>3</sub> Eutectic in the Liquid and Solid States, *Inorg. Mater.*, 2013, vol. 49, no. 8, pp. 904–912.

## Atomic structure of the binary and ternary Al-based liquid alloys

Roik O.S., Kazimirov V.P., Sokolskii V.E.

*Taras Shevchenko National University of Kyiv, Ukraine*

Using the results of the X-ray diffraction and the RMC simulations, the comparative analysis of the short-range order (SRO) in the liquid binary Al–TM (TM = Mn, Co, Ni and Cu) alloys and liquid ternary Al–Ni–TM (TM = Fe, Co), Al–Cu–TM (TM = Mn, Fe, Co, Ni), Al–Mn–TM (Co, Ni) alloys was carried out. It was established that the atomic structure of the liquid binary and ternary Al-based alloys depends on the type of the transition metal atoms.

The presence of the chemical short-range order (CSRO) in the liquid alloys has been found. The CSRO is characterized by strong interaction between Al and TM atoms and higher coordination of Al atoms around TM in comparison with stoichiometrical one that leads to the repulsion of TM–TM first neighbours. The shortest interatomic distances are between aluminum and transition metal atoms. It is shown that partial the partial substitution of the Cu or Mn atoms in the liquid binary Al–Cu or Al–Mn alloys by another TM (Fe, Co Ni) leads to reduce the  $R_1(\text{Al-TM})$  distances and to a strengthening of the role of the CSRO in formation atomic structure of the metallic melts. It is also shown that the degree of chemical ordering in the liquid binary Al–TM alloys increases with filling of the 3d-electron shell of the transition metal (Mn  $\rightarrow$  Co  $\rightarrow$  Ni). In case of the completion of 3d-electron shell (Cu) the CSRO not only becomes weaker, but its nature is changed that the coordinations between Cu atoms in binary liquid Al–Cu alloys is dominant.

The origin of the prepeak appearance on experimental total structure factor of the liquid Al-based alloys has been found. The prepeak is a sign of the MRO in the liquid alloys that caused by correlation between TM atoms at distances ranging from 0.4 to 0.5 nm. These correlations between TM atoms are realised primarily due to the existence of the CSRO in the liquid alloys.

It was found that the atomic packing density plays a significant role in the formation of the SRO of the liquid Al-based alloys. The high atomic packing density is achieved by the formation of dense non-crystalline polytetrahedral clusters whose size can reach up to 1-2 nm. The atoms located in the centre of these clusters are characterised by polytetrahedral order (PTO). The asymmetric shape of the second peak of total structure factor is associated with the existence of the PTO in the melts.

# Origin of the shoulder on the high Q side of the main peak on the structure factors of liquid Si and Ge

Roik O.S., Muratov O.S., Kazimirov V.P.

*Taras Shevchenko National University of Kyiv, Ukraine*

The short-range order in the liquid semiconductors like Si and Ge is more complicated compared with one in the most liquid metals. The structure factors  $S(Q)$  of liquid Si, Ge are characterized by the shoulder on the high Q side of the main peak. There are two explanations of this feature on the  $S(Q)$  curve. The first one is existence of the covalent bonds in the liquid semiconductors [1]. Another is related with the difference between the effective core radius and the wavelength of the Friedel oscillation in the interatomic potentials [2]. To investigate the origin of this shoulder on the  $S(Q)$ , the X-ray measurements of liquid silicon at 1743 K have been performed. The models of the liquid semiconductors have been generated by reverse Monte Carlo (RMC) method using obtained  $S(Q)$  of the liquid Si and previously reported X-ray diffraction data for the liquid Ge at 1233 K [3].

The atomic configurations obtained by the RMC method were analyzed for the presence of the short distances between the atoms that are less than the length of covalent bond in crystal Ge (0.245 nm) and Si (0.235 nm). The RMC models were divided into two parts: the atoms that have neighbors at the distance less than the length of covalent bond (further mentioned as atoms of type A) and the other atoms (atoms of type B). Thus the single-liquids Si and Ge were considered as the binary systems. The numbers of atoms of type A in the RMC models of the liquid Si and Ge were 64 and 34 %, respectively.

It was found that the first peak of the partial  $S_{AA}(Q)$  coincides with the shoulder on the first peak of the  $S(Q)$  of the liquid Si and Ge. The first peaks of  $S_{AB}(Q)$  and  $S_{BB}(Q)$  coincide with the first peak on the  $S(Q)$ . The SRO was analyzed by a tessellation of the models space into Voronoi polyhedra and the analysis of their metric and topological properties. The stronger distinction of local atomic environments between atoms of type A and atoms of type B in the liquid semiconductors has been established. The results of the study suggest that the shoulder originates from the presence of short distances between the atoms that are less than the length of covalent bond in the crystal Ge and Si.

1. M.P. Tosi. Structure of covalent liquids // J. Phys.: Condens. Matter. A. - 1994. - Vol.6. - P.13–28.
2. Ya. Chushak, J. Hafner, G. Kahl. Dynamical properties of the liquid polyvalent elements: soft modes in liquids // Phys.Chem.Liquids - 1995. - Vol.29. - P.159-168.
3. V.P. Kazimirov, V.E. Sokol'skii, V.A. Shovskii at al. Structure of liquids germanium // Metally - 1996. - N.6. - P. 97-103 [in Russian].

# Compositional disordering in amorphous $\text{Ti}_{1-x}\text{Zr}_x\text{O}_2$ thin films

Nahusko O.T., Studenyak I.P.

*Uzhhorod National University, Ukraine*

Titanium dioxide ( $\text{TiO}_2$ ) and zirconium dioxide ( $\text{ZrO}_2$ ) are materials which have been extensively studied because of their hardness, high chemical stability, excellent dielectric properties, large transparency range from UV to IR and relatively high refractive indices [1, 2]. The present study is aimed at the optical investigation of  $\text{Ti}_{1-x}\text{Zr}_x\text{O}_2$  thin films, because they are promising materials for various optoelectronic devices, in particular for creation of multilayer dielectric coatings for optical elements of laser engineering.

The films were deposited onto a silica glass substrate by electron-beam evaporation, their thickness being 0.4–0.6  $\mu\text{m}$ . The structure of the deposited films was analyzed by X-ray diffraction; the diffraction patterns have shown the films to be amorphous. The substrate temperature was 200–300  $^\circ\text{C}$  and standard evaporation rates ( $\sim 1\text{--}2$  nm/s) were applied. High-purity initial materials were used, the film composition was controlled by chemical analysis. Ellipsometric parameters were measured at room temperature by a LOMO LEF-3M-1 laser ellipsometer ( $\lambda=632.8$  nm). Transmission spectra of the films at room temperature were studied by a LOMO MDR-3 grating monochromator.

The performed studies have enabled the character of the dependence of the optical pseudogap  $E_g^*$  and refractive index  $n$  on the film composition to be elucidated. With substitution of Ti atoms by Zr atoms the optical pseudogap  $E_g^*$  is shown to increase nonlinearly (with downward bowing) from 3.25 eV for  $\text{TiO}_2$  to 4.55 eV for  $\text{ZrO}_2$ . Contrary, the refractive index  $n$  (at  $\lambda=632.8$  nm) of the films decreases nonlinearly (with upward bowing) with the increase of Zr content from  $n=2.281$  for  $\text{TiO}_2$  to  $n=2.016$  for  $\text{ZrO}_2$ .

The influence of different types of disordering on the Urbach energy  $E_U$  of optical absorption edge in  $\text{Ti}_{1-x}\text{Zr}_x\text{O}_2$  thin films is studied. It is well known that the Urbach energy  $E_U$  is the measure of disordering degree in solids. In  $\text{Ti}_{1-x}\text{Zr}_x\text{O}_2$  thin films, besides the temperature and structural disordering, the compositional disordering should also be revealed. The temperature disordering is mainly caused by the thermal vibrations of atoms and structural units while the structural disordering is caused by defects of structure (e.g. oxygen vacancies), inhomogeneities, pores, etc. The character of compositional behaviour of  $E_U$  is determined by the nonlinear compositional dependence of the contribution of compositional disordering caused by the substitution of Ti atoms by Zr atoms.

1. J. Robertson, *J. Vac. Sci. Technol. B*, 18, 1785 (2000).
2. D. Luca, L.S. Hsu, *J. Optoelect. Adv. Mat.*, 5, 835 (2003).

## Electron structure and magnetic properties of the new ternary intermetallic compounds

I.D.Shcherba<sup>1,2</sup>, M.V.Sacharevycz<sup>2</sup>, A.O. Stosyk<sup>2</sup>,  
L.O.Dobryanska<sup>2</sup>, B.M.Jatsyk<sup>3</sup>

<sup>1</sup>*Institute of Techniques, University of Pedagogy, Krakow, Poland*

<sup>2</sup>*Lviv National University by Ivan Franko, Lviv, Ukraine*

<sup>3</sup>*University of Forestry and Wood Technology, Lviv, Ukraine*

High-energy spectroscopy has been used to study the electron structure and valence state of new ternary intermetallic compounds, which crystallize in the  $\text{ThM}_{12}$ ,  $\text{CeGa}_2\text{Al}_2$  and  $\text{YbNi}_4\text{In}$  types. The calculations of electron energy bands  $E(k)$  and partial DOS for compounds were performed by the semi relativistic linear muffin-tin orbital method (LMTO) without considerations of spin-orbit interactions. Effective filling numbers of electrons in different bands of components in  $\text{R.E.M}_2\text{X}_2$  ( $\text{R.E} = \text{Y, Sc, Er}$ ;  $\text{M} = \text{Mn, Fe, Co, Ni, Cu, Pd, Rh}$ ;  $\text{X} = \text{P, Si, Ge}$ ) compounds have been calculated. On the basis of the obtained, photoelectron, X-ray emission spectra and calculation of density of total and partial electron states in  $\text{R.E.M}_2\text{X}_2$  compounds, the localization of electron of s- and p-states of Si (P) has been established within the energy ranges 14-7 eV and 7-2 eV, respectively. These states of Si (P) are hybridized with 4p-states of M atoms. The electron occupation of the d-states of the M atoms has a dominant influence on the degree of their hybridization. Between the experimental and calculated X-ray emission spectra  $\text{R.E.M}_2\text{X}_2$  good agreement has been obtained.  $L_{\text{III}}$  - absorption spectra Ce and Yb in ternary  $\text{YbNi}_4\text{In}$ ,  $\text{YbNiIn}_4$ ,  $\text{Ce(Yb)M}_2\text{X}_2$  and  $\text{Ce(Yb)M}_4\text{X}_8$  compounds were obtained at 78K and 300K using a tube spectrometer equipped with an RKD-01 co-ordinate detector. The mixed valence state of Ce and Yb was obtained in the  $\text{YbNiIn}_4$ ,  $\text{Ce(Yb)M}_2\text{X}_2$  and  $\text{Ce(Yb)M}_4\text{Al}_8$  compounds.

# Hybrid quantum-classical approach for dynamical simulations of metallic systems

J. Dziejczak<sup>1,2,3</sup>, J. Rybicki<sup>1,2</sup>

<sup>1</sup>*Faculty of Technical Physics and Applied Mathematics, Gdansk University of Technology, Gdansk, Poland*

<sup>2</sup>*TASK Computer Centre, Gdansk University of Technology, Narutowicza 11/12, 80-952 Gdansk, Poland*

<sup>3</sup>*[also at] School of Chemistry, University of Southampton, Highfield, United Kingdom*

The increasing technological significance of nanoscale systems is the driving force for their study. High costs and difficulties of experimental analysis lead to the use of computer simulation at the atomistic level for the investigation of the properties and behaviour of such systems. Simulations of this kind traditionally fall into one of two categories – classical (e.g. molecular dynamics, MD) or quantum-mechanical (QM, ab initio). The conceptual simplicity of the MD approach allows treating larger systems, but simple empirical interatomic potentials usually cannot capture all the relevant effects. Ab initio methods are of use only in the smallest systems, up to a thousand of atoms, because of their high computational effort. Multiscale approaches, which combine the two methodologies are a new addition to the toolbox of the computational material scientist [1].

We present a multiscale method targeted at atomistic simulations (including non-equilibrium) of metals in which selected regions are modelled using a quantum-mechanical approach (tight-binding, TB [2] or density functional theory, DFT), while the rest of the system is treated with molecular-dynamics employing (in this case) the Sutton-Chen [3] many-body interaction potential. The parameters of the underlying MD potential are re-parametrized locally on-the-fly by the employment of an extension to the Learn-on-the-Fly [4] technique, in order to reproduce the forces obtained by local QM calculations. The technique is parallel-ready, with both the quantum-based calculation and the force-fitting procedure scalable to several tens of processors [5]. Apart from the presentation of the method and implementation in computer code, the results of a series of validation and production simulations will be presented, demonstrating the accuracy and practicality of the approach.

1. Bernstein N, Kermode J R and Csányi G // Rep. Prog. Phys. -2009. -72 026501.
2. Cohen R, Mehl M and Papaconstantopoulos D // Phys. Rev. B – 1994. -50. 14694.
3. Sutton A P and Chen J // Phil. Mag. Lett -1990. -61 139.
4. Csányi G, Albrecht T, Payne M C and De Vita A // Phys. Rev. Lett – 2004. – 93. 175503.
5. Dziejczak J, Bobrowski M, Rybicki J // Phys. Rev. B - 2011 83.

# Structure and conditions for forming amorphous films of the GaSb – Ge system

Lutsyk N.Yu.<sup>1</sup>, Balitska V.O.<sup>2</sup>, Mykolaychuk O.G.<sup>1</sup>

<sup>1</sup> *Ivan Franko National University of Lviv, Ukraine*

<sup>2</sup> *Lviv State University of Life Safety, Ukraine*

Films of the GaSb-Ge system with the thickness near 500Å were prepared using method of a flash vacuum evaporation. Ceramic, glass and spallings NaCl monocrystals were served as substrates. Structure, substructure, concentration areas of existence of metastable solid solutions and an amorphous state and kinetics of structural transformations depending on technological conditions of evaporation of thin films of system GaSb-Ge were studied by methods of electronography and transmission electron microscopy. Equilibrium of system GaSb-Ge in a massive state is featured by the diagram of the eutectic type, and mutual solubility of components on the molar composition does not exceed 1 %. The composition of films is more convenient to represent using the formula  $(\text{GaSb})_{1-x}(\text{Ge}_2)_x$  because in the investigated system solid thin-film solutions are formed by substitution.

The temperature of a substrate supported in a precipitation process of films has dominant effect on structure formation of explored films. Films of all explored compositions, precipitated on substrates at room temperature, were amorphous. In amorphous films GaSb threefold coordination in distribution of the proximate atoms is observed. At concentrations  $\text{Ge}_2$  about 20 % transferring from threefold coordination to tetrahedral is observed. Amorphous films at heat crystallized, but phases of a solid solution it is not observed. Initial crystallization phases are crystal grains GaSb. The growth of crystallite sizes of GaSb takes place with the temperature increase. A speed of continuous heating has essential influence on the density and sizes of crystallites of GaSb formed in the amorphous semiconductor matrix based on Ge.

With an increase of temperature of a substrate there is a forming the nonuniform amorphous films. Areas of initial ordering on a basis GaSb are observed. With the further increase of temperature of substrates on the isotropic substrates polycrystalline films of a metastable solid solution of substitution are formed, and on spallings NaCl monocrystals are formed textured and epitaxial films. In case of epitaxial films the feeble modulation of a composition detected by transmission electron microscopy is observed. Disorder of solid solutions on phases GaSb and Ge at temperatures is higher 700K is observed.

## Temperature investigations of the structure of $\beta'$ - and $\gamma$ -phases of $\text{Ag}_8\text{SnSe}_6$ argyrodite

Chekaylo M.V.,<sup>1</sup> Akselrud L.G.,<sup>2</sup> Gladyshevskii R.E.,<sup>2</sup>  
Ilchuk H.A.,<sup>1</sup> Ukrainets V.O.,<sup>1</sup> Ukrainets N.A.<sup>1</sup>

<sup>1</sup>*Lviv Polytechnic National University, Ukraine.*

<sup>2</sup>*Ivan Franko National University of Lviv, Ukraine.*

The argyrodites, in particular  $\text{Ag}_8\text{SnSe}_6$ , are characterized by probabilistic fill of positions of crystalline structure by Ag atoms, and they can be considered to be non-ordered semiconductors with electron-ionic conduction.

With a use of X-ray powder diffraction, we have investigated the structure of  $\text{Ag}_8\text{SnSe}_6$  argyrodite at fixed values of temperature from the interval  $\Delta T = (250 - 420)$  K, as well as its electronic properties. Unlike in the work [1], where the determination of the structure was carried out with the use of a “rigid” model of crystalline lattice [2], our experimental diffractogram enabled us to achieve agreement only with the use of the concept of probabilistic fill of some positions by Ag atoms.

In the low-temperature  $\beta'$ - $\text{Ag}_8\text{SnSe}_6$  phase, atoms of Ag occupy seven positions, three of which of (Ag5 ( $P = 0,922$ ), Ag6 ( $P = 0,048$ ), Ag7 ( $P = 0,103$ )) at  $T = 295$  K have probabilistic fill. In spatial aspect, these positions forms chains oriented along the [100] crystallographic direction, along which on tetrahedral voids, drift of Ag ions is possible. In the high temperature ( $T > 356$  K)  $\gamma$ - $\text{Ag}_8\text{SnSe}_6$  phase, for all positions of Ag atoms the probability of the fill is essentially less than unity.

Modelling of  $\beta'$ - $\text{Ag}_8\text{SnSe}_6$  structure and that of  $\gamma$ - $\text{Ag}_8\text{SnSe}_6$  phase (with the use of Frank-Kasper polyhedron) have carried out. The coordinates of atoms in elementary cells of  $\beta'$ - $\text{Ag}_8\text{SnSe}_6$  and  $\gamma$ - $\text{Ag}_8\text{SnSe}_6$ , the values of the parameters of the elementary cells, as well as their temperature dependences are determined. Electrochemical cells of solids which are fabricated on the basis of monocrystals of  $\text{Ag}_8\text{SnSe}_6$  argyrodite in potentiostatic mode show relaxation of electric current caused by ionic component of the conductance.

1. L.D. Gulay, I.D. Olekseyuk, O.V. Parasyuk, Crystal structure of  $\beta$ - $\text{Ag}_8\text{SnSe}_6$ . J. Alloys Compd. -2002. Vol.339. -P.113-117.
2. D. Carré, R. Ollitrault-Fichet, J. Flahaut, Structure de  $\beta'$ - $\text{Ag}_8\text{GeSe}_6$ . Acta Crystallogr. -1980. Vol.B36. -P. 245-249.

# **The X-ray study of relaxation processes in amorphous Fe<sub>75</sub>Mo<sub>5</sub>Si<sub>6</sub>B<sub>14</sub> alloys**

S.Mudry, Yu.Kulyk, S.Zhovniruk.

*Ivan Franko National University of Lviv, Ukraine*

It is well known that heating of amorphous alloys is accompanied by two main processes-structure relaxation and crystallization. Before the structure relaxation the state of amorphous alloy deviates from metastable equilibrium one and only upon heating it can reach this state. The transition from non-equilibrium to equilibrium state reveals the change of structure that results in formation of more regular structure which is more close to amorphous than crystalline one. On that reason the structure relaxation is not pre-crystallization process and has as features, which are far from complete understanding.

We have studied the structure changes in Fe<sub>75</sub>Mo<sub>5</sub>Si<sub>6</sub>B<sub>14</sub> amorphous alloy at heating within temperature range 383-683 K by means of X-ray diffraction method. Structure factors show change their parameters especially in the region of second maximum. As is seen the second sub-peak of second maximum is most sensitive to annealing temperature and becomes most pronounced at annealing within temperature range 598-673 K. But for more accurate conclusion the more accurate analysis of such sub-maximum parameters should be done. We have analyzed the half height width at different annealing temperatures.

Similar dependence was observed in plot of half height peak width of pair correlation functions, calculated from structure factors, but in this case maximum has symmetric profile contrary to one in structure factor. Thus, the structure relaxation is accompanied by formation of less size clusters due to which an atomic distribution becomes more close to ideal amorphous structure.

In order to confirm the such mechanism of structure relaxation we have estimated a temperature dependence of distance to nearest neighbors. Such dependence allowed us to conclude that due to rearrangement of clusters the change in short order structure occurs too that results in decrease of free volume in alloy.

# Structure changes in laser irradiated iron and cobalt-based amorphous alloys.

Nykyruy Yu.

*Ivan Franko Lviv National University, Lviv, Ukraine.*

Under the influence of various external influences in amorphous metallic alloy (AMA) transition from the metastable to the equilibrium state occurs, which is accompanied by the formation of nanocrystalline phase, and causes changes in material properties. Therefore, the investigation of conditions of nanocrystalline structures formation and methods of control of their physical and technical characteristics in order to optimization of existing and/or developing more efficient than existing methods for structuring the AMA is very interesting. In these studies laser radiation was used for structuring AMA. Thus the task of the research is study the laser-induced structural changes in amorphous metallic alloys based on iron and cobalt depending on radiation parameters and to establish the relationship between the laser-induced structural changes and changes in their properties.

Amorphous ribbons, based on iron and cobalt, obtained by rapid cooling from the melt, were irradiated by laser pulses of wavelength 1.06 microns with different values of energy  $E$  and pulse duration  $\tau$  -  $10^{-7}$ ,  $10^{-6}$ ,  $10^{-5}$ ,  $10^{-4}$  s. Laser-induced structural changes was investigated by X-ray diffraction. The structure of the irradiated samples surface was studied by scanning electron microscopy.

Values of  $E$  for the corresponding values of  $\tau$ , which can be used for laser annealing of AMA without their destruction, were defined. It was also found that at laser irradiation at all values of  $\tau$  and the corresponding ones of  $E$  alloy surface is heated to a temperature that is much higher than the temperature of the starting of crystallization, but the crystalline phase was detected only at  $\tau > 10^{-5}$  s. This suggests the existence of a threshold value of pulse duration that is accompanied with influence of laser irradiation on structure. Under the influence of the pulse, which duration is below the threshold value, at temperate values of  $E$  the processes of structural relaxation and the pre-crystallisation structural changes occur, while at larger values of  $E$  nonequilibrium phase transitions and, intense melting and evaporation take place, so it is extremely difficult to achieve the crystallization process due to damping of diffusion processes. When the pulse duration is close to the threshold value ( $\sim 10^{-5}$  s) in alloys based on Fe (Co) the iron (cobalt) phases and borides are formed at crystallization, but the silicides as a result of such exposure haven't been identified. However, for alloy  $\text{Fe}_{73.5}\text{Nb}_3\text{Cu}_1\text{Si}_{15.5}\text{B}_7$  it was found that at some higher pulse duration the  $\text{Fe}_{1.72}\text{Si}_{0.28}$  phase, containing silicon 14%, is formed, while at much higher pulse durations ( $10^{-3}$  s) phase  $\text{Fe}_3\text{Si}$  (15% Si) is observed.

## Atomic structure of SiO<sub>2</sub> after alpha irradiation.

Koman B. P, Yuzevich V.M.

*Lviv National Ivan Franko University, Ukraine  
Physical Mechanical Institute G. Karpenko NASU, Lviv, Ukraine*

Modern microelectronics technology uses radiation processing structures Si-SiO<sub>2</sub> as an essential stage production cycle in order signifies our strong radiation modification of semiconductor materials, microelectronic devices and chips in their manufacture. In particular, one of the areas of radiation is radiation modification of semiconductor doping, which is controlled by the introduction of semiconductor own electrically active structural defects.

The aim was to study the structural changes in the atomic structure of SiO<sub>2</sub> under alpha irradiation.

Conductance changes in short-range order. We used the technique of X-ray using the installation DRON -3,0 (Cu<sub>α</sub>). Calculation of short-range order was carried out using the technique of even functions.

The paper used in Si-SiO<sub>2</sub> structures produced by industrial technology through the combined oxidation in dry and wet oxygen at a temperature of 1100°C in a КДБ –type silicon wafers (100) with  $\rho = 20$  Ohm \* cm. The source of alpha radiation isotope <sup>238</sup>Pu was the energy of particles 4 ... 5 MeV and flux density equal to  $5 * 10^7 \text{s}^{-1} * \text{cm}^{-2}$ .

Found that irradiation thermal oxide SiO<sub>2</sub> leads to a small increase in bond length Si-O from 1,615 up to 1,625 Å. The value of the first coordination number increases from 4.04 to 4.10 Å. The most significant changes recorded in the bond length variation. Irradiation is also accompanied by increased dispersion of interatomic distances Si-O (0,15 and 0,24 Å), O-O (0,29-0,43 Å), Si-Oii (0,29 and 0.36 Å) in the source and irradiated samples, respectively. Irradiation reduces the average angle of communication Si-O-Si from 109 to 107°. The mean angle blackout Si-O-Si irradiated sample is equal to 139.5° shifted towards larger values of the angle relative to unirradiated (137.6°).

Thus, alpha radiation is accompanied by a slight increase in the first coordination number, but a significant increase in bond length Si-O values from 1,615 to 1,625 Å. Significant variance values at the corners O-Si-O, compared with the original samples. Found that thermal annealing leads to a decrease in variation in the corners connection O-Si-O compared to the irradiated samples.

## **Structure of $(\text{PbTe})_x(\text{Bi}_2\text{Te}_3)_{1-x}$ molten alloys**

A.Korolyshyn, V.Vus, M.Lytvyn, S.Mudry

*Lviv National Ivan Franko University, Ukraine*

Pseudo-binary PbTe-Bi<sub>2</sub>Te<sub>3</sub> system reveals the existence of ternary compositions in solid state. Interest to alloys of this system is due to potential application as thermoelectrical materials.

In this work the structure of short order of liquid alloys has been investigated at temperatures in vicinity of liquid – solid phase transition. Particular interest was focused to alloys with concentration corresponding to existence of ternary compositions in solid state. The question arises how this type of interatomic distribution correlates with short range order structure before solidification.

On that reason the X-ray diffraction studying was carried out in liquid state. The structure factors have been obtained and used for calculation of pair correlation functions. The concentration step was equal to 10 percent in order to determine the concentration dependences of structure parameters in liquid state. Analysis of the structure factors and radial distribution function show that atomic arrangement of liquid alloys has the similar topological and chemical short range order within some composition range.

## Heat flow researching in the fluid at the process of electrical activation arising

S. Mudry, S. Prokhorenko\*, I. Bordun\*, V. Ptashnyk\*

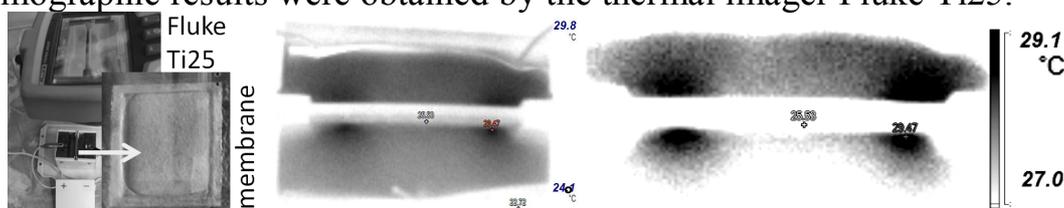
*Ivan Franko National University of Lviv, Ukraine*

*\*Lviv Polytechnic National University, Ukraine*

Melting electroactivation processes (MEA) solutions at last time received essential value. Process of transferring water solution to a metastable state caused by structure-energy and electrochemical changes in the electric field as MEA of water solution is understood. MEA is carried out in dilute solutions (generally at a concentration less than 0.01 M) at a high value of the external polarizing electromotive force. In such solutions, along with the products of electrolysis of dissolved solids, grow up the role of a solvent electrolysis, occur an intermediate states of the reacting particles - ions of different oxidation states, radicals and molecules. Resulted of water solution MEA in this solutions anomalous properties in the physical and chemical transformations show for a period of relaxation.

Researches of colleagues of the State research institute of especially pure biological products [pat. RU 2378058], improvements of generating of anolyte procedure (numerous work of prof. Bakhir's group) given the opportunity to consciously decide on the importance of in-depth study of energy-activated liquids. The main constraining factors for the development of technologies based on MEA of water solutions are the metastability of its characteristics and the absence of a complete theoretical description of the process. As a result, there are still many unanswered questions, especially the concept of structural ordering of the activated water solution.

The preliminary results of the determination of heat flow distribution of the MEA process are following. MEA of the water was carried out in a stationary cell with two graphite electrodes and separating diaphragm made of nonwoven polypropylene of mark FS 2226-14E (pore volume 55%, the predominant pore radius of 10  $\mu\text{m}$ ). Diaphragm was glued hermetically to the plastic frame. Electrode voltage was 220 V during treatment with tap water. Thermographic results were obtained by the thermal imager Fluke Ti25.



# Influence of the temperature-temporal prehistory of the melts on crystallization kinetics of the Fe-Si-B amorphous alloys

Mazur Yu.P., Nosenko A.V.\* , Semen'ko M.P., Zakharenko M.I.

*Taras Shevchenko National university of Kyiv, Ukraine*

*\*Institute for Metal Physics, NASU, Kyiv, Ukraine*

Here we present the results concerning the crystallization kinetics of the METGLAS-type Fe<sub>80</sub>Si<sub>6</sub>B<sub>14</sub> amorphous metallic alloys (AMAs) prepared by single-roll quenching technique after different heat treatment of the melts. The performed investigations allow to conclude that the crystallization of the studied AMAs is the two-stage process. The values of the apparent activation energy of crystallization  $E_a$  have been determined by the Kissinger method. However, the routine approach provides no distinct evidence for the complexity of the processes occurring upon crystallization. So, the further analysis has been performed using Kolmogorov-Johnson-Mahl-Avrami equation, that in a case of constant heating rate could be expressed as [1]:

$$x(T) = 1 - \exp\left(-\frac{K_0(RT^2)/(vE_a)}{\exp(E_a/RT)}\right)^n \quad (1)$$

Here,  $x$  is a fraction of the formed crystalline phase,  $n$  is the Avrami index and  $K_0$  is the reaction rate constant. Using Eq. (1), the expression for  $E_a$  as a function of  $x$  has been deduced. Reasoning from kinetic curves obtained by the resistivity measurements the dependencies of the Avrami index on temperature have been calculated.

$E_a$  was found to be substantially dependent on  $x$  for AMAs quenched after the exposure of the melt at the temperatures  $T_L$  higher than 1450°C, which is known to be close to so-called critical temperature for this composition [1]. Moreover, just for these AMAs  $n$  occurs to be strongly dependent on temperature. Since the value of  $n$  reflects the mechanisms of nucleation and growth, the obtained  $n(T)$  dependencies could be interpreted from the viewpoint of reducing of the nucleation rate and transition of the growth rate from the linear to the parabolic diffusion controlled one. If  $T_L$  is less than the critical value,  $n$  and  $E_a$  were revealed to be independent on temperature and  $x$ , respectively. The obtained results are consistent with the common conceptions on the structure of melts at different thermal conditions and its influence on the AMAs atomic structure.

1. V. V. Maslov, V. I. Lad'yanov, A. G. Ilinsky, V. K. Nosenko. The influence of melt atomic structure on structure and properties of amorphous Fe-based alloys // J. Phys.: Conf. Ser. – 2008. – Vol. 98. – 072007, 6 p.

# **Correlation between electro-transport properties of the disordered systems and their electronic and atomic structures**

Semen'ko M.P.

*Taras Shevchenko National university of Kyiv, Ukraine*

This presentation deals with finding the regularities of electrical resistivity, magnetoresistivity and tensor resistivity of the binary and multicomponent amorphous metallic alloys on the base 3d-transition metals, ascertaining of the physical mechanisms of charge carrier scattering and creation the physical models describing transport parameters of the disordered metallic systems of different nature.

Therewith the influence of composition, production conditions and external actions (temperature, magnetic field, mechanical stresses, etc.) on the kinetics of conductive electrons has been studied. The role of the electronic and atomic structures peculiarity on electronic transport has been clarified.

It was shown that the main contribution to conduction electron scattering arises from their diffraction on the disordered, heterogeneous atomic structure, while peculiarities arising on a series of transport characteristics are the consequence of the presence of atomic clusters that are characterized by special scattering mechanisms.

# **Physical properties, phases' stability and electronic structure parameters of the random metallic systems**

Zakharenko M.I.

*Taras Shevchenko National university of Kyiv, Ukraine*

This presentation deals with the finding the regularities of the influence of electronic structure parameters and peculiarities of electronic correlations on the temperature and compositional ranges of phases' stability in metallic systems with chemical and topological disordering (in particular, in amorphous alloys and composite materials containing nanocrystalline constituent). The physical principles of the formation of magnetic characteristics have been considered for these systems. Here, the influence of composition, structural state and preparation conditions on magnetic state of the constituent atoms has been investigated for antiferromagnetic chromium-based alloys, amorphous, nanocrystalline systems and composite materials containing 3d-element. Besides, the role of the exchange correlations and electronic structure parameters (namely, density-of-electronic-state spectra) in the specification of the temperature and compositional ranges of phases' stability in the listed systems has been evaluated. Magnetic state of transition metal atoms has been determined and two types of atomic clusters (with parallel and antiparallel spin alignments) have been proved to exist in the alloys under study. The principal characteristics of these clusters have been ascertained.

# The synergetic theory of plastic deformation

Yushchenko O.V., Yurko D.S.

*Sumy State University, Ukraine*

Despite the fact that processes occurring during the deformation of solids at the moment are well studied [1], the questions associated with plastic deformation are attracted the great attention of scientists today [2,3]. Besides according to [2] it turns that some properties (elasticity and viscosity) are not unique to solids, but they are inherent in continuous media (e.g. granular materials, supercooled liquid polymers, etc.).

Moreover the plastic deformation, on the one hand, is typical for many natural and technological processes and, on the other hand, is difficult in terms of the theoretical description. Our task is to construct a synergetic scheme, which allows to describe the transition of solids to the plastic flow state. Since the plastic flow always arises at the microscopic level, the influence of point defects on the behaviour of solids under the action of the given stress will be an actual task.

It is known that a simple three-parameter synergetic scheme, describing the self-organizing system is the Lorenz system. Furthermore the understanding of the basic laws of plastic flow can be achieved in the framework of the hydrodynamic theory, where the concentration of vacancies (characterizing the state of the material) was introduced

$$m = \delta\rho / \rho + u_{ii},$$

where  $\rho$  is an average density of the material,  $\delta\rho$  is a density deviation, and  $u_{ii}$  is a strain tensor. As a result, we built a three-parameter scheme based on the Lorenz system, where the order parameter was the concentration of vacancies, the conjugate field was the velocity profile of the shear displacement, and the internal stress was a control parameter.

On the basis of this system the dependencies of the internal stresses and curvature of the velocity profile of the shear displacement on the order parameter were found. Obtained from the Ginzburg-Landau-Khalatnikov the vacancy formation energy was built.

1. L.D. Landau, E.M. Lifshitz. Theory of Elasticity (Theoretical Physics, Volume 7. – Elsevier, Oxford 1986.
2. Liu, S.R. Nagel. Jamming and Rheology: Constrained Dynamics on Microscopic and Macroscopic Scales. – Taylor and Francis, London 2001.
3. Ikeda, L. Berthier, P. Sollich. Unified study of glass and jamming rheology in soft particle systems // Phys. Rev. Lett. – 2006. – Vol.109.– P.018301.

# Structural and dielectric studies of disordered solid electrolytes of Ag-As-S system

Neimet Yu. Yu., Studenyak I.P.  
*Uzhhorod National University, Ukraine*

Chalcogenide glasses, doped with metals, have attracted wide interest due to increased ionic conductivity therefore they are the promising materials for creation of solid electrolytes, electrochemical sensors, electrochromic displays etc. It should be noted that in comparison with crystalline solid electrolytes they are more technological, simple and lower-cost in production. The remarkable place among them is taken by glasses of Ag-As-S system due to the high value of electrical conductivity [1]. Structurally Ag-As-S glasses become phase separated after adding of 7 at.% of silver [2].

Synthesis of Ag-As-S glasses was carried out at a temperature of 700°C during 24 h with following melt homogenization during 72 h. Measurements of complex electrical conductivity were carried out in the frequency range from 1 Hz to 1 GHz and in the temperature range 300-400 K using a coaxial impedance spectrometer setup.

X-ray studies have shown that glasses of Ag-As-S system get separated after adding the proustite  $\text{Ag}_3\text{AsS}_3$  crystal to the base  $\text{As}_2\text{S}_3$  glass. Glass  $(\text{Ag}_3\text{AsS}_3)_x(\text{As}_2\text{S}_3)_{1-x}$  with  $x=0.3$  was found to be fully amorphous, whereas the spectrum of glasses with  $x=0.6$  and 0.8 have bands, similar to those of  $\text{AgAsS}_2$  and  $\text{Ag}_3\text{AsS}_3$  crystals, accordingly.

This fact is confirmed by the behavior of electrical conductivity as well as of dielectric permittivity in the given glasses. Electrical conductivity has one dispersion in  $(\text{Ag}_3\text{AsS}_3)_x(\text{As}_2\text{S}_3)_{1-x}$  ( $x=0.3, 0.4$ ) glasses and two dispersion regions in  $(\text{Ag}_3\text{AsS}_3)_x(\text{As}_2\text{S}_3)_{1-x}$  ( $x=0.8, 0.9$ ) glasses, which is as a matter of fact a sign of disordered phase separated structure.

Compositional behavior of real and imaginary part of dielectric permittivity and electrical modulus in  $(\text{Ag}_3\text{AsS}_3)_x(\text{As}_2\text{S}_3)_{1-x}$  glasses showed that the most significant changes are seen after the transition from  $x=0.4$  to  $x=0.5$ . Revealed features, as well as in the case of electrical conductivity, are related to the transition from glassy structure at  $x \leq 0.4$  to composite structure at  $x \geq 0.5$ .

1. E. Bychkov, D.L. Price, C.J. Benmore, A.C. Hannon. Ion transport regimes in chalcogenide and chalcogen halide glasses: from the host to the cation-related network connectivity // *Solid State Ionics*. - 2002. - Vol.154-155. - P.349.
2. Bychkov E., Bychkov A., Pradel A., Ribes M. Percolation transition in Ag-doped chalcogenide glasses: comparison of classical percolation and dynamic structure models // *Solid State Ionics*. - 1998. - Vol.113-115. - P.691.

# Hydrogen adsorption on non-polar surfaces of ZnO: *Ab initio* calculations

A.Usseinov<sup>1</sup>, E.A. Kotomin<sup>2</sup>, Yu.F. Zhukovskii<sup>2</sup>, J. Purans<sup>2</sup>, A. Akilbekov<sup>1</sup>,  
A.K. Dauletbekova<sup>1</sup>

<sup>1</sup>*L.N. Gumilyov Eurasian National University, Astana, Kazakhstan*

<sup>2</sup>*Institute of Solid State Physics, University of Latvia, Riga, Latvia*

Understanding of the atomic and electronic structure of defective/doped ZnO is of great importance for improving performance of electrodes in optoelectronic devices based on transparent conducting oxides, *e.g.*, light-emitting diode (LED). Particular interest in this case is connected with clarification of a role of hydrogen impurities penetrating into ZnO thin films from plasma.

We report results of *ab initio* modeling of atomic hydrogen adsorption onto the two nonpolar  $(10\bar{1}0)$  and  $(11\bar{2}0)$  surfaces of ZnO positioned into two sites: *i*) atop surface O atom; *ii*) atop surface Zn atom. Our calculations of the corresponding 2D supercells have been performed using the hybrid DFT method (using PBE0 exchange-correlation functional) within the formalism of linear combination of atomic orbitals (LCAO) as incorporated into the CRYSTAL-2009 computer code [1]. This approach allows us to obtain very accurate calculations of the optical gap and defect level positions therein. The defect-induced electronic charge redistribution, lattice distortion, adsorption energy as well as the density of electronic states (DOS) and band structure have been calculated for both  $(10\bar{1}0)$  and  $(11\bar{2}0)$  surfaces of ZnO.

As a result, we have shown that energetically favorable position of hydrogen atom on both surfaces is atop the surface oxygen with similarly adsorption energies, whereas hydrogen locations atop the surface Zn is unstable. It should be noted also that hydrogen incorporation induces the defect states, which contribute below and within the surface conduction band. Thus, it is characterized as a shallow donor. Analysis of the charge redistribution has shown that hydrogen atom forms strong chemical bond with surface oxygen atom, unlike that in bulk. Based on our calculations, we have shown that hydrogen adsorption leads to decrease of both  $(10\bar{1}0)$  and  $(11\bar{2}0)$  surface relaxations and reduces the surface energy, in consistence with results of other DFT calculations [2].

1. Dovesi R, Saunders V R, Roetti R, Orlando R, Zicovich-Wilson C M, Pascale F, Civalleri B, Doll K, Harrison N M, Bush I J, D'Arco P and Llunell M 2009 *CRYSTAL09 User's Manual* University of Torino, Torino.
2. Siao Y I, Liu P L and Wu Y T 2011 *Appl. Phys. Express* **4** 125601

## The influence of thermocycling and cryotreatment on stability of amorphous alloys

Lysov V.I., Tsaregradska T.L., Turkov O.V., Saenko G.V.

*Kyiv Taras Shevchenko national university, Ukraine*

The researches of influence unisothermal heat treatment on the thermal stability of multicomponental amorphous alloys on the basis of transitional metals has been carried out. The monitoring of thermodynamic stability of amorphous alloys in initial state and after unisothermal heat treatment was carried out with help of highly sensitive dilatometrical techniques. The temperature dependences of relative change of volume for amorphous alloys for initial state and after heat treatment at  $T' = T_k^0 - 50K$  ( $T_k^0$  – is the temperature of beginning of intensive crystallization): 3 cycles of heating to  $T'$  (thermocycling) and heating to  $T'$  with subsequent immersion in liquid nitrogen (cryotreatment) were obtained. The changes of temperatures beginning of intensive crystallization after heat treatment were certain; the obtained results are presented in table.

Composition of amorphous alloy	$T_k^0, K$ for initial sample	$T_k^1, K$ after 3 cycles of heating	$T_k^2, K$ after cryotreatment
Fe <sub>80</sub> B <sub>14</sub> Si <sub>6</sub>	773	788	803
Fe <sub>70</sub> Cr <sub>15</sub> B <sub>15</sub>	753	763	773
Fe <sub>77,5</sub> B <sub>16</sub> Si <sub>2</sub> Ni <sub>3,5</sub> Mo <sub>1</sub>	753	773	773
Fe <sub>76,2</sub> B <sub>14</sub> Si <sub>6</sub> Ni <sub>3,8</sub>	773	793	793

The heat treatment brings to the increase of stability of amorphous alloys, to what testifies the increase of temperature of beginning of intensive crystallization. It is set that thermocycling is extended by the interval of thermal stability on (10-20) K; cryotreatment results in expansion of interval of thermal stability on (20-30) K. It is rotined that the unisothermal heat treatment allow to influence on the size of „freezes” centers of crystallization: thermocycling allows to regulate the size of nanocrystals and cryotreatment fixes the existent size of nanocrystals, which is confirmed the results of X-rays diffraction researches.

Thus, the results of the carried out researches confirm the conclusions of the theory of thermodynamic stability amorphous alloys, which predict the possibility of shift of phase equilibrium in the system „amorphous matrix”– „freezes” centres of crystallisation due to directed modification of exterior actions and is defined by modes of the extension of temperature interval of existence of amorphous state.

## Thermal conductivity of molecular glass

Krivchikov A. I., Vdovichenko G. A., Korolyuk O. A. Romantsova O. O.

*B.Verkin Institute for Low Temperature Physics and Engineering of NASU, Kharkov, Ukraine*

The work is devoted to an experimental research of thermal conductivity of row of molecular disordered solids at low temperatures [1]: structural and orientation glasses, glass-like crystals and crystals with the different degree of orientation disorder.

The unique experimental setup was created for research of samples of and molecular glasses at temperatures from 2 to 200 K [2].

New effects explored in the thermal conductivity of glass alcohol - isomer, the mass, the isotope. For the first time shown that the thermal conductivity of solid ethyl alcohol in the orientational glass has a temperature dependence is close in magnitude and behavior to the temperature dependence of the structural glass. We will show that orientation glasses behave similarly to canonical glass formers as far as Boson peak and Ioffe-Regel crossover are concerned on the basis of the soft potential model [3]. It is found of new universal dependence of thermal conductivity of molecular orientation of glass - a universal behavior, according to the soft-potential model for glass and diffuse maximum thermal conductivity characteristic of the crystal structures.

1. O.A. Korolyuk, I.V. Sharapova, O.O. Romantsova, F.J. Bermejo, C. Cabrillo, R. Fernandez-Perea, I. Bustinduy. Thermal conductivity of glassy primary mono-hydroxyl alcohols // *J. Non-Cryst. Solids.* — 2011. — V. 357, № 2. — P. 483—486.
2. A.I. Krivchikov, B.Y. Gorodilov, O.A. Korolyuk. A Setup for studying the low-temperature thermal conductivity of powder samples// *Instruments and Experimental Techniques.* -2005. – Vol.48. –P.417-421.
3. M. Hassaine, M. A. Ramos, A. I. Krivchikov, I. V. Sharapova, O. A. Korolyuk, R. J. Jimenez-Rioboo. Low-temperature thermal and elasto-acoustic properties of butanol glasses: Study of position isomerism effects around the boson peak // *Phys. Rev. B.* — 2012. — V. 85, № 10. — P. 104206-1—104206-11.

# Vapour-liquid phase diagram and surface tension for a fluid of two-level atoms with taking into account short-range order

<sup>1</sup>Myhal V.M., <sup>1,2</sup>Derzhko O.V.

<sup>1</sup>*Ivan Franko National University of Lviv, Ukraine*

<sup>2</sup>*Institute for Condensed Matter Physics of NASU, Lviv, Ukraine*

We consider a fluid of two-level atoms, discussed previously for a microscopic analysis of the effect of an external electrical field or excited atoms on the macroscopic properties of the nonuniform system [1]. In contrast to these previous studies, where for the long-range interaction contribution to the density functional of the grand thermodynamical potential

$$\frac{1}{2} \int d\mathbf{r}_1 d\mathbf{r}_2 \rho^{(2)}(\mathbf{r}_1, \mathbf{r}_2) U(\mathbf{r}_1, \mathbf{r}_2), \quad \rho^{(2)}(\mathbf{r}_1, \mathbf{r}_2) = \rho(\mathbf{r}_1) \rho(\mathbf{r}_2) g(|\mathbf{r}_1 - \mathbf{r}_2|, \bar{\rho})$$

it was assumed that

$$g(|\mathbf{r}_1 - \mathbf{r}_2|, \bar{\rho}) = \Theta(|\mathbf{r}_1 - \mathbf{r}_2| - \sigma)$$

(here we used the Heaviside step function  $\Theta(x)$  and denoted by  $\sigma$  the diameter of the atom), in the present study we assume a more precise expression for  $g(|\mathbf{r}_1 - \mathbf{r}_2|, \bar{\rho})$ , which was obtained recently for the hard-sphere system in Ref. 2. The adopted form for  $g(|\mathbf{r}_1 - \mathbf{r}_2|, \bar{\rho})$  reflects a short-range order emerging due to the repulsion. After obtaining the vapour-liquid phase diagram, we consider the case of the planar vapour-liquid interface and calculate the density profiles and the surface tension. We demonstrate that the present choice of  $g(|\mathbf{r}_1 - \mathbf{r}_2|, \bar{\rho})$  leads to a certain improvement of previous findings reported in Ref. 1.

Further details can be found in Ref. 3.

1. О.В.Держко, В.М.Мигаль, Журн. фіз. досл. **1**, 402 (1997); **2**, 339 (1998); **4**, 424 (2000); O.V.Derzhko, V.M.Myhal, J. Mol. Liquids **92**, 15 (2001);
2. О.В.Держко, В.М.Мигаль, Журн. фіз. досл. **9**, 156 (2005); **10**, 203 (2006); O.Derzhko, V.Myhal, Condens. Matter Phys. **9**, 703 (2006).
3. А.Трохымчук, І.Незбеда, J.Jirsák, D.Henderson, J. Chem. Phys. **123**, 024501 (2005); **124**, 149902 (2006).
4. В.М.Мигаль, О.В.Держко, надіслано до Журн. фіз. досл. (2013).

## Dynamics of chemical bond formation in iron based materials

<sup>1</sup>Ashcheulov A.A., <sup>1</sup>Manyk O.M., <sup>2</sup>Manyk T.O., <sup>1</sup>Bilynskyj-Slotylo V.R.

<sup>1</sup>*Yuriy Fedkovych Chernivtsi National University, Ukraine*

<sup>2</sup>*Bukovyna State University of Finance and Economics, Chernovtsi, Ukraine*

There is great relevance to the issues with regard to study of the structural peculiarities of iron based solid solutions depending on the composition and conditions of receipt at this time. FeSe and FeTe are characterized by the highest values of the superconducting transition temperature among binary compounds. In this regard, is reasonable to research chemical bond peculiarities of iron-based materials, the dynamics of its formation by force and energy characteristics calculation.

It is necessary, first of all, to establish the relationship between the theories of elasticity and crystal lattice by comparing their movement equations for the calculation of force parameters of the chemical bond [1]. The mathematical models that enable to describe nature of microparticles movement, their thermodynamic properties of the resulting harmonic and anharmonic vibrations considered at this paper. Consistency between the obtained values of the quantities which found by solving the inverse problem of chemical bond theory, theory of elasticity and calorimetric measurements confirms the correctness of the molecular models. This leads to further improvement and their successful application to the refinement of process conditions to obtain materials with desired properties [2].

Evaluation of characteristic temperatures of the respective chemical bonds was conducted with the influence of anharmonic effects. It is allowed using this model to find the “effective” temperature characteristics of non-equivalent chemical bonds. Analysis of anharmonic corrections showed that the values of the anharmonic parameters for the various non-equivalent interatomic distances which described by the non-equivalent hybrid orbitals are significantly different. This is due to the change of the form of movement and deformation effects.

The obtained results give a possibility to trace the dynamics of iron based materials polymorphism, the relationship with the structure, the elastic properties and also physical and chemical parameters of substance which defining its properties, forming the structure, and hence the valence and fine structure of the chemical bond.

1. A.A. Ashcheulov, O.M. Manyk, T.O. Manyk, A.I. Savchuk, V.R. Bilynskyj-Slotylo. Peculiarities of the chemical bond of FeSe and FeTe // Physics and Chemistry of Solid State. -2012. -Vol. 13, №1. -P.136-141.
2. Patent 67792, Ukraine. Process for producing of monocrystalline ingots of FeSe, FeTe and solid solutions of  $\text{FeSe}_x\text{Te}_{1-x}$  / A.A. Ashcheulov, O.M. Manyk, T.O. Manyk, V.R. Bilynskyj-Slotylo, A.I. Savchuk. -2012. Bul.№5.

# Mathematical morphology and electronic structure of the amorphous metal alloy $\text{Fe}_{77}\text{Si}_8\text{B}_{15}$ surface at thermal effect

V.L. Karbivskyy, O.I. Slukhovskyy, N.A. Kurgan

*G.V. Kurdyumov Institute for Metal Physics NAS of Ukraine, Kiev, Ukraine*

Scanning tunneling microscopy and spectroscopy methods were used to study the relaxation processes on the surface of amorphous tapes of  $\text{Fe}_{77}\text{Si}_8\text{B}_{15}$  depending on the annealing and cooling temperatures. The effects of temperature and rate of heating on the surface morphology and nanocrystals size were shown. Investigated samples of amorphous tape were produced by rapid cooling of the melt composition  $\text{Fe}_{77}\text{Si}_8\text{B}_{15}$ , annealed for one hour at temperatures from 300 °C to 600 °C (Fig. 1) by direct current heating in a vacuum chamber of the microscope. The residual pressure during annealing process was not higher  $10^{-7}$  Pa.

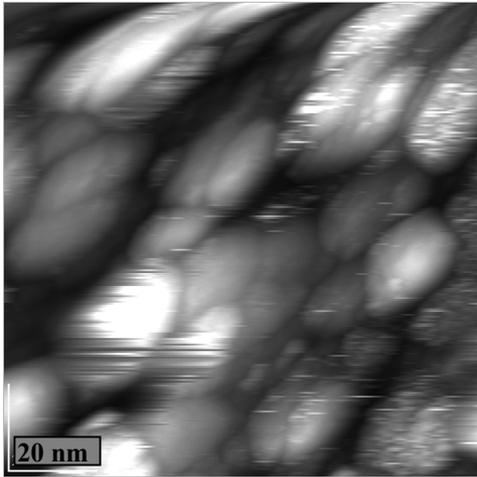


Fig. 1. The surface of the amorphous tape annealed at 600 °C.

It was found that the annealing process at the tape surface leads to formation of nanocrystalline phase of  $\alpha$ -Fe or  $\alpha$ -Fe (Si) located in an amorphous matrix, what is caused by a local stabilization of the amorphous structure.

During fast annealing at low temperatures was found formation of nanoclusters with close to spherical surface morphology. Such morphology of clusters is most optimal in terms of achieving the desired soft magnetic properties of amorphous tapes.

Observed nanocrystals at moderate annealing temperatures have size of about 15 nm what is comparable with the length of magnetic exchange correlation. The distribution of the average cluster size like that leads to a spatial averaging of the magnetic anisotropy and, consequently, to a significant decrease in the coercive force.

Depending on the local atomic ordering, what has an impact on the process of nucleation of nanocrystals, the small areas separated by an amorphous phase forms in the early stages of crystallization and then consolidates with subsequent increase of temperature and time of annealing.

# Long-wave high-frequency plasma oscillations in alkali-halid liquid salts

Stupka A.A.

*Oles Honchar Dnipropetrovsk National University, Ukraina*

High-frequency long-wave electromagnetic oscillations in an ionic liquid with two species of ions are considered. Lets ignore the thermal motion and suppose an environment is homogeneous and isotropic and do not take into account for the high-frequency oscillations the resiliency force, proportional to the gradients, that leads to the acoustic oscillations. Lets study small oscillations in the non-magnetic environments, whereas it is possible to drop a nonlinear magnetic part of the Lorentz force. An electronic polarization of ions that arises up self-consistently because of the presence of the field, equivalent to the origin of an additional electric field. It would result in a self-action in the equations of motion for oscillating ions, i.e. to the force that counteractive to the mean field, that must be dropped. Then the related system of linearized equations for a self-consistent electric field and polarized ions is obtained  $\partial \varepsilon \mathbf{E} / \partial t = -4\pi e n_0 (\mathbf{v}_+ - \mathbf{v}_-)$ ,  $\partial \mathbf{v}_+ / \partial t = e \mathbf{E} / M_+^*$ ,  $\partial \mathbf{v}_- / \partial t = -e \mathbf{E} / M_-^*$ . Here  $\varepsilon$  is relative permittivity of the ionic liquid,  $n_0$  is an equilibrium density of the ions of a certain sign. Effective masses for alkali metal and halogen ions are entered  $M_{\pm}^* = M_{\pm} / (1 + 4\pi \alpha_{\pm} / \nu_{\pm})$ , where  $\alpha_{\pm}$  - is an electronic polarizability of an ion of the corresponding sign,  $\nu_{\pm}$  is its volume [1]. An expression for eigenfrequency of plasma oscillations in such a system through physical characteristics of the salt is found  $\omega = \sqrt{4\pi e^2 n_0 (1/M_+^* + 1/M_-^*) / \varepsilon}$ . The obtained frequency is the plasma frequency of the polarized ions in a dielectric environment. As known, optical characteristics for the ionic crystals and for the same ionic melts are similar [2]. Then the transversal optical phonon  $\omega_T$  and the phonon-polariton  $\omega_L$  frequencies of alkali-halid crystals correspond to obtained  $\omega$  with a static relative permittivity  $\varepsilon_0$  and a high-frequency (electronic) relative permittivity  $\varepsilon_{\infty}$  accordingly. The Lyddan-Sachs-Teller formula [1]  $\omega_L / \omega_T = \varepsilon_0 / \varepsilon_{\infty}$  is obtained. Good accordance of the calculated values of the indicated frequencies to experimental data is found.

1. N.W.Ashcroft, N.D.Mermin, Solid state physics (Cengage Learning, Inc , New York, 1976).
2. E.A.Ukshe, Structure and properties of molten salts// RUSS. CHEM. REV. -1965. -Vol.34. P. 141–159.

# Optical conductivity peculiarities and electronic parameters of Fe-rich amorphous metallic alloys

Poperenko L.V.<sup>1</sup>, Manko D.Yu.<sup>2</sup>, Yurgelevich I.V.<sup>1</sup>.

<sup>1</sup>*Kyiv Taras Shevchenko University, Ukraine*

<sup>2</sup>*Institute for information recording NASU, Kyiv, Ukraine*

Amorphous metallic alloys are characterized by improved characteristics compared to their crystalline analogs. The aim of this work is to establish the significance of substituting of small concentration of one transition metal to another in the  $\text{Fe}_{80}\text{TM}_5\text{B}_{15}$  (TM=Ti, Cr, V) metallic amorphous alloys and its influence on its optical properties. Parameters of electronic subsystem, namely plasma and relaxation frequencies give us important information about concentration of charge carriers and even estimation the topological structure of an amorphous alloy surface. On the other hand, calculations of parameters of electronic subsystem, performed by different numeric methods could end up with totally different results. Its being caused due to considering of single an optical function (real part of dielectric function or imaginary part of dielectric function or optical conductivity) in calculations. The aim of this work is to make a proposition how optimize such calculations using a few optical functions simultaneously and thus, get more reliable results.

The obtained parameters indicate much higher concentration of charge carriers near Fermi level in the case of TM=Ti, Cr than TM=V and simultaneously smaller free length path of them. The results of analysis of spectroellipsometric data established that in amorphous metallic alloys Fe atoms at condition of substitution of Fe atoms into atoms of such 3d metals as Ti, V, Cr Fermi level became closed to mobility edge of density of electronic states (at certain concentration of Fe atoms such level may occur into pseudo-slit). The improved method of calculation of electronic subsystem parameters is proposed and discussed.

It was found, that the most effective way of calculation of parameters of electronic subsystem is to make simultaneous fitting of both: real and imaginary part of dielectric function. The analysis of optical functions of investigated samples with TM=Cr, Ti makes us sure that in observed optical phenomena there are only a particular type of charge carrier takes place, despite of quite complicated shape of the Fermi surface. In contrast to TM=V there are two groups of charge carriers having different concentration and mobility.

# Influence of Co and Cu additions on the enthalpy of mixing of liquid Li-Sn alloys

Yakymovych A., Flandorfer H., Fürtauer S., and Ipser H.

*Department of Inorganic Chemistry / Materials Chemistry, University of Vienna, Austria*

The heat balance is an important factor for any process development. Therefore, the enthalpy of mixing is one of the most requested thermodynamic properties of the liquid state. The knowledge of this quality is also necessary to model the phase diagrams of multi-component systems with the CALPHAD method as well as for the prediction of different thermo-physical properties including viscosity, surface tension, diffusion, etc.

Development of new materials for Lithium-Ion Batteries is a key issue in current electronic industry. Various systems which are able to reversibly uptake lithium are in discussion as alternatives to the commonly used carbon anodes. Promising candidates are the systems Cu-Li-Sn and Co-Li-Sn, where  $\text{Li}_{17}\text{Sn}_4$  should be the active phase and pure copper or Cu-Sn-phases (cobalt or Co-Sn-phases) form the stabilizing matrix. This work provides thermodynamic data of the liquid range which are needed to predict phase relations to fully understand the phase diagrams of the investigated ternary systems.

The calorimetric measurements were carried out using a Calvet-type twin microcalorimeter system based on a commercial wire wound resistance furnace (HTMC-1000, SETARAM, Lyon, France). This device and all measuring facilities are controlled by a user-assembled software in LabVIEW, and the obtained data were evaluated by using the HiQ program. The enthalpy of mixing for the Co-Li-Sn system was determined at 1173 K by the addition of lithium to mixtures  $x_{\text{Co}}/x_{\text{Sn}} \approx 3:97$ ,  $x_{\text{Co}}/x_{\text{Sn}} \approx 1:9$ , and  $x_{\text{Co}}/x_{\text{Sn}} \approx 3:17$ , as well as by the addition of cobalt to mixtures of  $x_{\text{Li}}/x_{\text{Sn}} \approx 3:1$ ,  $x_{\text{Li}}/x_{\text{Sn}} \approx 1:1$ ,  $x_{\text{Li}}/x_{\text{Sn}} \approx 1:2$  and  $x_{\text{Li}}/x_{\text{Sn}} \approx 3:17$ . In the Cu-Li-Sn system, lithium was dropped at 1073 K to liquid mixtures with ratios of  $x_{\text{Cu}}/x_{\text{Sn}} \approx 1:1$ ,  $x_{\text{Cu}}/x_{\text{Sn}} \approx 2:3$  and  $x_{\text{Cu}}/x_{\text{Sn}} \approx 1:4$ , and copper was dropped to mixtures of  $x_{\text{Li}}/x_{\text{Sn}} \approx 1:1$  and  $x_{\text{Li}}/x_{\text{Sn}} \approx 1:4$ . The integral molar enthalpies of mixing in the ternary systems were described with a least square fit, according to a Redlich-Kister-Muggianu-polynomial.

*This work was supported by the Austrian Science Foundation (FWF) under the Projects No. 21507-N19, No. M 1324-N19. and by the Austrian Agency for International Cooperation in Education and Research (OeAD-GmbH) under Project No. UA 03/2013.*

## Radiation-induced defect formation in glassy As-S/Se

M. Shpotyuk<sup>1,2</sup>, O. Shpotyuk<sup>1</sup>, M. Vakiv<sup>1,2</sup>, S. Kozyukhin<sup>3</sup>

<sup>1</sup> SRC "Carat", Lviv, Ukraine

<sup>2</sup> Lviv Polytechnic National University, Ukraine

<sup>3</sup> M.S. Kurnakov Institute of General and Inorganic Chemistry of RAS, Moscow, Russia

The role of charged coordination topological defects (CTD) in different types of induced structural transformations in chalcogenide glasses (ChG) has been still an matter of discussions since the time of first experiments on photostructural transformations in these materials performed yet in the early 1970-s [1,2]. Primarily, such situation is caused by often misunderstanding on principal difference in the origin of native (technological) and induced CTD.

In our research, we proposed the formulism to calculate the content of induced CTD in ChG of different chemical compositions. It was assumed that CTD's concentration depends on the energy of broken covalent bond, bond-switching energy balance, correlation electron energy, optical band-gap and energy of excitation light. It was shown that theoretically calculated maximally possible content of radiation-induced defects in glassy As<sub>2</sub>S<sub>3</sub> was about 1.6 % while concentration of native defects is negligible in this specimen.

Based on the concept of destruction-polymerization transformations [2,3], we have developed the estimation methodology for structural modification of network ChG. Our approach is grounded on the assumption that induced optical effects are associated mainly with transformations revealing in local misbalances in distribution of covalent bonds, atomic coordination and intrinsic electric fields. The contribution of each misbalance into a total value of induced structural modification was estimated at the examples of As-S/Se ChG. It was shown that compositional dependence of structural modification criteria could be associated with charged CTD for arsenic sulphides in a vicinity of stoichiometric As<sub>2</sub>S<sub>3</sub> composition. In case of As-Se system, the external influence causes only slight bond alteration.

This investigation was partially supported by State Fund for Fundamental Research of Ukraine within research project # F53.2/022.

1. V.M.Lyubin, *Photographical processes on the base of vitreous chalcogenide glasses* // In: *Nonsilver photographical processes*, A.L.Kartuzhanskii, ed., Leningrad: Khimia, 1984.
2. S.B.Gurevich, N.N.Ilyashenko, B.T.Kolomiets, V.M.Lyubin, V.P.Shilo // *Phys. Stat. Sol.* **A26** 2 (1974) K127.
3. O.I.Shpotyuk, *Radiation-induced effects in chalcogenide vitreous semiconductors* // In: *Semiconductors and Semimetals*, R.Fairman and B.Ushkov, eds., Elsevier Academic Press, 2004.

# On the problem of self-organization effect in Ge-Se system

V. Boyko<sup>1</sup>, V. Gurin<sup>2</sup>, O. Shpotyuk<sup>1</sup>, M. Vakiv<sup>1</sup>

<sup>1</sup> SRC "Carat", Lviv, Ukraine

<sup>2</sup> Physico-Chemical Research Institute, Belarusian State University, Minsk, Belarus

Chalcogenide glasses possessing fully-saturated covalent bonding in respect to known 8-N rule have been in a sphere of tight interests because they exhibit a large variety of useful practical applications in IR optoelectronics and photonics. They exist in many glass-forming compositions in dependence on their connectivity defined in mean coordination number  $Z$  taken as average number of covalent bonds per one atom of structural unit. The stressed-free intermediate phase having just 3 Lagrangian constrains per atom appears so as to avoid stress, forming a so-called reversibility window. In device application, the self-organized intermediate-phase glasses having optimal space filling are most attractive since they reveal unique non-aging ability.

Quantum mechanical calculations were performed using HyperChem/GAMES programs, ab initio RHF and DFT (B3LYP functional) calculations with 3-21G/6-311G\* and LANL2DZ basis sets being used to determine the total energies of  $\text{Ge}_m\text{Se}_n$  clusters. All boundary Se atoms belonging to two clusters were terminated by H atoms to be two-fold coordinated. Only half-part contributions from these atoms were considered after subtraction both energies of H atoms and  $-\text{Se-H}$  bonds from total cluster energy. This value was taken as a measure for cluster formation probability. The hydrogen H atom having an extremely low bonding energy in covalent structures is the most suitable ones to be used in this way [1].

The performed calculations showed that directly linked edge- and corner-shared  $\text{GeSe}_{4/2}$  tetrahedrons are basic glass-forming blocks in the studied glasses, the former being more energetically preferential. These overconstrained tetrahedrons are specifically interconnected in a space within more extended structural blocks forming a so-called outrigger raft structural motive [2]. Despite overconstrained nature of constituting blocks, they are specifically distributed in a glassy network via optimally-constrained intercation linking elements. In such a way, the pseudo-reversibility window appears in glass compositions between  $Z$  ranging from 2.4 to 2.5.

This investigation was partially supported by State Fund for Fundamental Research of Ukraine within research project # F54.1/021.

1. Phillips J.C. Phys. Rev. B 73, 024210-1-8 (2006).
2. Phillips J.C. J. Non-Cryst. Sol., 34, 153-181 (1979).

## Електропровідність склоподібних сплавів системи $\text{Ag}_2\text{S}-\text{GeS}_2-\text{AgBr}$

Мороз М.В.\*, Миколайчук О.Г.\*\*, Прохоренко М.В.\*\*\*

\*Національний університет водного господарства та природокористування, Рівне, Україна

\*\* Львівський національний університет ім. Івана Франка, Україна

\*\*\* Національний університет “Львівська політехніка”, Україна

В системі  $\text{Ag}_2\text{S}-\text{GeS}_2$  гомогенні стекла отримано в інтервалі концентрації 45–100 мол. %  $\text{GeS}_2$ . Сплави на їх основі є чисто іонними ( $\text{Ag}^+$ ) провідниками в інтервалі 45–70 мол. %  $\text{GeS}_2$ . Перехід в чотириелементний концентраційний простір вздовж розрізу  $\text{Ag}_3\text{GeS}_3\text{Br}-\text{GeS}_2$  дозволив покращити значення питомої іонної електропровідності стекел [1]. Параметри та механізми електро- та масопереносу значної частини чотириелементних склоподібних сплавів системи  $\text{Ag}_2\text{S}-\text{GeS}_2-\text{AgBr}$  залишаються недостатньо вивченими.

Для синтезу стекел використовували хімічні елементи напівпровідникової чистоти. Склоподібні сплави масою  $\sim 1$  г отримували гартуванням розплавів у воду з льодом від температур  $\sim 1250$  К. Електропровідність досліджено в інтервалі температур 250–495 К на постійному струмі зондовим методом, під тиском аргону  $p \sim 10^5$  Па. В дослідженнях використовували електрохімічні комірки (ЕХК) типів:  $\text{Ag}|\text{скло}|\text{Ag}$ ,  $\text{Ag}|\text{скло}|\text{Ag}_3\text{SBr}|\text{Ag}$  та  $\text{Ag}|\text{скло}|\text{Ag}_3\text{SI}|\text{Ag}$  з зондами  $\text{Ag}|\text{Ag}^+\text{Ag}_3\text{SBr}|\text{скло}$ . Шари сполук  $\text{Ag}_3\text{SBr}$  та  $\text{Ag}_3\text{SI}$  в ЕХК слугували для інжекції аніонів галогенів в сплави та блокування електронної складової електропровідності. Порошкоподібні складові комірок пресували до значень густини  $\rho = (0.93 \pm 0.02)\rho_0$ , де  $\rho_0$  – густина литого склоподібного сплаву.

Встановлено, що скло складу  $\text{Ag}_3\text{Ge}_2\text{S}_5\text{Br}$  є чисто іонним провідником. Електро- та масоперенос в електричному полі забезпечують катіони срібла та інжектвані в структуру сплавів аніони галогенів. Запропоновано механізми дрейфового переміщення іонів  $\text{Ag}^+$ : вакансійний по вільним катіонним позиціям “формульного” срібла в сплавах; естафетний за участі зарядових центрів захоплення в каналах; естафетний за участі інжектованих аніонів галогенів. За параметрами електропровідності ( $\sigma = 1.71 \cdot 10^{-2}$  1/(Ом·м) при  $T = 300$  К) скло належить до класу суперіонних матеріалів.

1. Moroz M.V., Demchenko P.Yu., Mykolaychuk O.G., Akselrud L.G., Gladyshevskii R.E. Synthesis and electrical conductivity of crystalline and glassy alloys in the  $\text{Ag}_3\text{GeS}_3\text{Br}-\text{GeS}_2$  system // Inorganic materials. – 2013. – V. 49. N. 9. – P. 867–871.

# Sigmoid tendencies in the kinetics of natural physical ageing in As<sub>10</sub>Se<sub>90</sub> glass

Balitska V.O.<sup>1,2</sup>, Golovchak R.Ya.<sup>1,3</sup>, Shpotyuk O.I.<sup>1</sup>

<sup>1</sup>*Institute of Materials, Scientific Research Company “Carat”, Lviv, Ukraine*

<sup>2</sup>*Lviv State University of Vital Activity Safety, Kleparivska str., Lviv, Ukraine*

<sup>3</sup>*Dep. of Physics and Astronomy, Austin Peay State University, Clarksville, USA*

It is shown that kinetics of enthalpy losses caused by prolonged storage of glassy g-As<sub>10</sub>Se<sub>90</sub> in a dark at room temperature during more than two decades (natural physical ageing) exhibits a well-expressed sigmoid behavior – the plateaus and steep regions. The microstructure mechanism of ageing explains well the observed stretch-exponential behavior in relaxation kinetics in terms of hierarchically-constrained mixed serial-parallel relaxation events having different atomic precursors. This kinetics can be decomposed into elementary components, each of them being single exponential.

The model of natural physical ageing in g-As<sub>10</sub>Se<sub>90</sub> is developed at the basis of detailed kinetics study. Structural data for Se-rich As-Se glasses suggest that physical ageing initiated by the elementary twisting of inner Se atoms within specific double-well potentials associated with high flexibility of Se bonds [1]. In the first approximation, these twisted Se atoms can be accepted as elementary Johari-Goldstein (JG)  $\beta$ -relaxation precursors. They should result in the appearance of aligned Se-based regions in a glassy network and, consequently, local free volumes released by twisted Se atoms. Appearance of such free volumes around collapsed Se-based regions is assumed to be accompanied by elastic strains in their immediate atomic surrounding. This initial stage is responsible for the lowering of glass transition temperature during first period of ageing. If the accumulated elastic energy is high enough, the further cooperative rearrangements occur, eliminating redundant free volumes from the considered local atomic regions, which lead to the lowering internal energy of the system at this particular scale. Happening at a larger scale, these relaxation processes should lead to general shrinkage of glassy network. Therefore, in subsequent stages of ageing, a general shrinkage of network takes place, which can be attributed to JG  $\beta$ -relaxation facilitated further  $\alpha$ -relaxation. This process is a reason for increase in the glass transition temperature and enthalpy losses in conventional differential scanning calorimetry measurements [2].

1. R.Golovchak, O.Shpotyuk, A.Kozdras, M.Vlcek, B.Bureau, A.Kovalskiy, H.Jain, J. Phys.: Condens. Matter **20**, 245101-1-7 (2008).
2. R.Golovchak, O.Shpotyuk, A.Kozdras, Phys. Lett. **A370**, 504-508 (2007).

# **Notes on functional metastabilities in chalcogenide semiconductor glasses: the role of free-volume deviations as probed by positron annihilation**

Shpotyuk O.I.

*Scientific Research Company “Carat”, Lviv, Ukraine*

Positron annihilation (PA) is known to be high informative tool to study atomistic imperfections in solids (free-volume defects – vacancies, vacancy-like clusters, voids and void agglomerates) despite their structural organization (crystals or glasses, fine-grained or coarse powders, ceramics or bulk alloys, etc.) [1]. Recently this method has been also applied to characterize induced metastabilities in chalcogenide semiconductor glasses (ChSG), an important class of disordered materials possessing excellent IR functionality [2]. Nevertheless, possibilities of PA technique are often treated too ambiguously and speculatively, without any connection with realistic physical models of tested objects. The most often are speculations with compositional trends in the treatment of PA data performed in a so-called lifetime measuring mode, when physically real annihilation channels are mistakenly substituted by mathematical fitting parameters and annihilation from delocalized defect-free states is ignored at all. These misleading “explanations” significantly distort correct understanding of realistic models of induced effects in ChSG like as in case of numerous speculations incorrectly treating data of positron annihilation lifetimes [3] and Doppler broadening [4] measurements.

In this report, we shall discuss the methodological possibilities of PA technique to characterize compositional dependences of free-volume evolution in typical ChSG under a condition of changes possible in both defect-free bulk and defect-related annihilation channels. Application of PA techniques is analysed for different types of void-evolution processes proper to intrinsic and external metastabilities exemplified by ChSG of binary As-S system.

1. R.Krause-Rehberg, H.S.Leipner, Positron Annihilation in Semiconductors. Defect Studies, Springer-Verlag, Berlin-Heidelberg-New York, 1999.
2. B.Bureau, X.Zhang, F.Smektala, J.-L.Adam, J.Troles, H.Ma, C.Boussard-Pledel, J.Lucas, D.LeCoq, M.R.Riley, J.H.Simmons// J. of Non-Crystalline Solids. -2004. -Vol.345-346. -P.276-283.
3. T.Kavetsky, J.Borc, P.Petkov, K.Kolev, T.Petkova// Solid State Ionics.- 2011.-Vol.183.-P.16-18.
4. T.Kavetsky, V.Tsmots, A.Sausa, A.L.Stepanov// Phys. Stat. Sol.-2012.- Vol.C9.-P.2420-2423.

# The charge carriers transfer in amorphous (GeS)<sub>1-x</sub>Bi<sub>x</sub> films

Romanyuk R.R.<sup>a</sup> Mykolaychuk O.G.<sup>b</sup>

<sup>a</sup>Western Scientific Centre of the NAS of Ukraine and the MES of Ukraine, Lviv, Ukraine

<sup>b</sup>Ivan Franko National University of Lviv, Ukraine

The influence of Bi additions on the electrical and photoelectrical properties of amorphous (GeS)<sub>1-x</sub>Bi<sub>x</sub> films ( $0 \leq x \leq 0.15$ ) has been investigated.

Bulk samples (GeS)<sub>1-x</sub>Bi<sub>x</sub> ( $x = 0; 0.03; 0.07; 0.11; 0.15$ ) were obtained in ampoules by melting stoichiometric GeS with the addition of Bi of certain concentrations. The ampoules were subjected to vibration and hardening in cold water. The thin films under investigation (thickness of nearly 0.3-1.2  $\mu\text{m}$ ) were obtained by using a method of discrete evaporation of a fine-dispersive mixture on the surface in a vacuum ( $10^{-4}$  Pa) from substrates of quartz and ceramics at 293 K followed by annealing in a vacuum at  $T = 350$  K. A pre-sputtering method was applied to the substrate contact with copper. The photovoltaic properties of the samples were studied by using methods of unmodulated and modulated lighting depending on the temperature and the spectral composition of the exciting light. Temperature dependences of static conductivity and photoconductivity of amorphous films were investigated in the temperature range 150-350 K.

Supplementing Bi to amorphous condensates leads to changes in the mechanism of conductivity and the conductivity type inversion. Bi-additives reduce the activation energy of photoconductivity and photosensitivity of GeS films. It is found that amorphous GeS films have an activation mechanism of conductivity in the temperature range  $T=150-350$  K. Bi-additives in the GeS condensates cause an increase of conductivity and the appearance of hopping conductivity through localized states near the Fermi level with the variable length of hopping. Increasing the concentration of Bi reduces the photoconductivity and the spectral region of photosensitivity of GeS films. In the concentration range  $0.11 < x < 0.15$  the conductivity type inversion from  $p$ - to  $n$ -type takes place. Changes of the physical properties of the films are explained in the framework of the heterogeneous structure of the condensates and defect states in the mobility gap [1].

1. R. R. Romanyuk, Y. V. Boyko, O. G. Mikolaychuk. Structure and optical absorption edge in (GeS)<sub>1-x</sub>Bi<sub>x</sub> amorphous films ( $0 \leq x \leq 0.15$ ) // Physics and Chemistry of Solids State. – 2010. - Vol. 11, N 4. - P. 971-975.

# Electrophysical and structure-sensitive properties of liquid Ag-Sb-Sn and Bi-Cu-Sn alloys

Yu. Plevachuk<sup>a</sup>, V. Sklyarchuk<sup>a</sup>, A. Yakymovych<sup>b</sup>, I. Kaban<sup>c</sup>

<sup>a</sup>*Ivan Franko National University of Lviv, Ukraine*

<sup>b</sup>*University of Vienna, Department of Inorganic Chemistry / Materials Chemistry, Austria*

<sup>c</sup>*Leibniz Institute for Solid State and Materials Research, Dresden, Germany*

On implementation of the EU RoHS and WEEE directives extensive investigations have been carried out to find lead-free alloys instead of traditional Pb–Sn solders. Progress has been made in the area of low-temperature lead-free solders, while the research is seriously lacking into replacements of Pb–Sn solder alloys, where the Pb-content is above 85 wt.%. High-temperature solders with melting temperatures above 550 K are widely used in the electronics industry for advanced packing technologies. Sb–Sn alloys are considered among the high-temperature solder candidates. Indeed, Sn-rich Sn–Sb alloys exhibit good electrical properties and a wide range of melting temperatures that make them appropriate in the step-soldering technology. The solders used at the early stages should be characterized by higher melting temperatures in order not to be molten during the subsequent soldering.

As silver is one of the main materials for the conduction lines and pads in multilayer low-temperature ceramic substrates, Sb–Sn solder joints form Ag–Sb–Sn contacts because of the dissolution and interfacial reactions. Thus, binary Sb–Sn solders with intake of Ag are transformed into the ternary Ag–Sb–Sn phases. The ternary Ag–Sb–Sn alloys are characterized by enhanced mechanical properties, fatigue resistance, and thermal resistance with respect to the eutectic Ag–Sn solder, thus rendering it suitable for use in high temperature service environments. The Bi–Cu–Sn ternary system is a promising candidate for lead-free solders because of the suitable melting temperature, good thermal resistance, and low cost.

In this work, the electrical conductivity and thermal conductivity, thermoelectric power and viscosity studies, surface tension and density of liquid Ag-Sb-Sn and Bi-Cu-Sn alloys were carried out in a wide temperature range above the liquidus. The surface tension experimental data were analysed by the Butler thermodynamic model in the regular solution approximation. The Sn-rich liquid alloys show better wetting behaviour on the Cu substrates as compared to the Ni substrates. The new experimental results were compared with the calculated values as well as with data available in the literature. Corresponding temperature scaling relations have been derived and recommended as input data for thermodynamic simulations.

# Thermophysical properties of the liquid Au<sub>15.9</sub>Pb<sub>84.1</sub> eutectic alloy

Yu. Plevachuk<sup>a</sup>, V. Sklyarchuk<sup>a</sup>, A. Yakymovych<sup>b</sup>

<sup>a</sup>*Ivan Franko National University of Lviv, Ukraine*

<sup>b</sup>*University of Vienna, Department of Inorganic Chemistry / Materials Chemistry, Austria*

Lead-gold eutectic alloy (LGE) is under consideration as target material of spallation sources. The thermohydraulic design of such a target or related coolant systems requires a reliable data basis regarding the temperature dependent physical properties of such alloys. However, the recently reported corrosion behaviour of the liquid LGE in contact with 316L stainless steel was found to be worse than that of the lead-bismuth eutectic (LBE). This fact requires detailed investigations on steels with higher corrosion resistance towards LGE, as for instance the more resistant T91. The modeling and thermohydraulic design of such a target requires a reliable database regarding the temperature dependent physical properties of such alloys over a broad range of temperatures above the melting point, where the structure-sensitive characteristics play a prominent role.

In this work some electrophysical (electrical conductivity, thermal conductivity, thermoelectric power) and structure-sensitive (viscosity, surface tension) properties for liquid Au<sub>15.9</sub>Pb<sub>84.1</sub> alloy were investigated for the first time over a wide temperature range between the liquidus  $T_m = 485$  K and 1000 K. The electrical conductivity and thermoelectric power measurements were carried out by the 4-point contact method. An experimental arrangement based on the steady-state concentric cylinder method was used for thermal conductivity measurements. The dynamical viscosity was measured by the oscillating cup method. The surface tension has been studied by the sessile drop method. Corresponding temperature scaling relations have been derived and recommended as input for thermodynamic simulations.

## **Structure and thermophysical properties of Au-Ag-based alloys**

V. Sklyarchuk, Yu. Plevachuk, S. Mudry, Yu. Kulyk, I. Shtablavyi,  
A. Korolyshyn

*Ivan Franko National University of Lviv, Ukraine*

Thermophysical properties of gold- and silver-based alloys as the basic input data for their thermodynamic description, were investigated. A currently missing reliable and accurate thermodynamic modeling of these alloys is necessary for effective reduction of the cost and for improvement of the casting technology in the jewelry industry.

The gold- and silver-based alloys, covering the color variation range from white gold to yellow and red ones, and are widely used in jewelry industry were studied. Such alloys are easily processed and resistant to darkening.

Comprehensive study of temperature dependence of the thermophysical properties, structure and microstructure of the Au and Ag based alloys were carried out in the liquid and solid states from the room temperature to 1400 °C during heating and cooling cycles in order to detect structural changes in these alloys. An influence of impurity elements such as Ag, Cu, Pd, Zn, Sn, Ga on structure transformations were analyzed.

The influence mechanism of a heating - cooling process on alloy properties in the solid state, and the influence of impurity elements on the alloy solidification have been studied. The structural models for a variety of the alloy condensed phases, as well as mechanisms for interpretation of the correlations between structure, microstructure and properties, were developed.

# Effect of structural disordering on the optical properties of $\text{Li}_2\text{B}_4\text{O}_7:\text{Cu}$

Popovich K.P., Holovey V.M., Prymak M.V., Birov M.M.

*Institute of Electron Physics, Ukr. Nat. Acad. Sci., Uzhhorod, Ukraine*

Copper-doped crystalline lithium tetraborate ( $\text{Li}_2\text{B}_4\text{O}_7:\text{Cu}$ , LTB:Cu) has found application in dosimetry of ionizing radiation. Due to the specific features of its structure LTB can be rather easily obtained in both crystalline and glassy forms. The transition from crystalline to glassy LTB is characterized by a decrease of structural ordering, a variation of the ratio between boron-oxygen tetrahedra and triangles in the anion sublattice in favour of the latter as well as an increase of the degree of oxidation of part of impurity ions. We have performed a study of the effect of structural disordering on the photoluminescence (PL) and optical absorption of LTB and LTB:Cu. The measurements were performed for single-crystalline and glassy samples with identical stoichiometric composition and impurity content.

The PL of glassy LTB:Cu at room temperature is much weaker in intensity in comparison with the single-crystalline samples. The only emission peak of glassy LTB:Cu has a broad smeared spectral maximum in the range of 2.52–2.66 eV and remains unchanged with temperature. It is strongly redshifted in comparison with the single-crystalline LTB:Cu. Such specific features of the spectral distribution of the PL intensity can be explained by an increase of the oxidation degree of part of copper impurity ions  $\text{Cu}^+ \rightarrow \text{Cu}^{2+}$  as well as by a variation of the local environment of  $\text{Cu}^+$  copper ions. The PL intensity of the glassy LTB:Cu rapidly decreases with temperature and at 623 K comprises near 15% of that for the room temperature.

In glassy LTB:Cu, contrary to the single-crystalline material, no impurity-related absorption bands are observed in the range 1.50–6.00 eV. Irradiation of the glassy LTB:Cu leads to an essential increase of the absorption intensity in the whole energy range under consideration and a shift of the absorption band edge from 3.75 до 3.25 eV. The most intense absorption for glassy LTB and LTB:Cu is observed in the range of lower energies; however, no pronounced bands of the induced absorption are formed.

# Inelastic-elastic properties and defect nanostructure changing of amorphous MgBa alloys and automated system of ultrasonic anisotropy visualization

Onanko A.P., Lyashenko O.V., Kulish M.P., Prodayvoda G.T., Onanko Y.A., Lyashenko I.O.

*Kyiv National University, Ukraine*

Mechanical properties of amorphous  $Mg_{0.95}Ba_{0.05}$  alloy were explored. For the determination of temperature position and relaxation depths of elastic module  $\eta = \frac{E_0 - E_{min}}{E_0}$  at the same time with IF the temperature dependence elastic module  $E(T) \sim f^2$  of amorphous  $Mg_{0.95}Ba_{0.05}$  alloy were measured on fig.1.

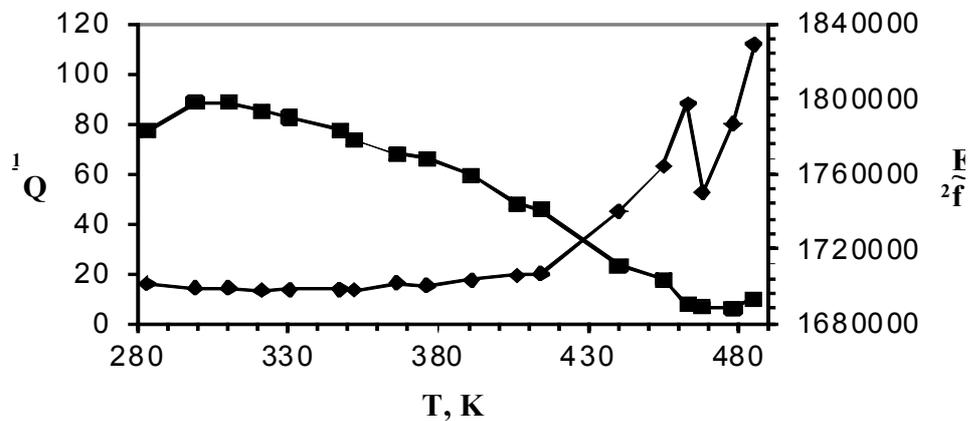


Fig. 1. Temperature dependence internal friction  $Q^{-1}(T)$  and elastic module  $E(T) \sim f^2$  of amorphous  $Mg_{0.95}Ba_{0.05}$  alloy.

The relaxation depths of elastic module was  $\eta \approx 1\%$  at  $T \approx 450$  K. Impurity atoms may decelerate vacancies moving to dislocations from the interaction impurity atoms with vacancies V. This phenomenon play visible role at concentrations  $C_0 \square 1$  at.%, that's more higher, then that's, which are necessary for Kottrell atmospheres creation. The pair number "I-V" – "impurity-vacancy" were determined from the relation:

$$\frac{N_{I-V}}{N_{0V}} = \frac{C_0 Z e^{\frac{E_d}{k_B T_M}}}{1 + C_0 Z e^{\frac{E_d}{k_B T_M}}}, \quad (1)$$

where  $N_{0v}$  – number free vacancies,  $C_0$  – impurity concentration,  $E_d$  – pair dissociation energy,  $Z$  – coordination number.  $E_d \approx 0,1$  эВ, then for  $C_0 \approx 5 \times 10^{-2}$  and temperature  $T_M \approx 460$  K there are  $\frac{N_{I-V}}{N_{0V}} \approx 4 \times 10^{-1}$ , that is  $\sim 40\%$  equilibrium vacancies  $Mg_{0.95}Ba_{0.05}$  alloy are connected with impurity atoms and few movable, then free vacancies.

## X-Ray Er<sup>3+</sup> Luminescence in the Glassy Lithium Tetraborate Matrix

Puga P.P.<sup>1</sup>, Danyliuk P.S.<sup>2</sup>, Popovych K.P.<sup>1</sup>, Turok I.I.<sup>1</sup>, Krasylynec V.M.<sup>1</sup>,  
Birov M.M.<sup>1</sup>, Vuchkan V.I.<sup>1</sup>, Puga G.D.<sup>2</sup>, Chychura I.I.<sup>1</sup>

<sup>1</sup> *Institute of Electron Physics, Ukrainian Academy of Sciences, Uzhgorod, Ukraine*

<sup>2</sup> *Uzhgorod National University, Ukraine*

During last years, a special attention has been drawn to the wide-band borates based on the lithium tetraborate (LTB) being activated by the rare-earth elements (REE). In the above matrix, the REE ion replaces the cation sublattice node, while formation of one or another polyhedron around Er<sup>2+</sup> or Er<sup>3+</sup> depends on the character of chemical bonds between the vicinity ions and the REE ions, as well as on the participation of the valence shell in those bonds formation. Therefore the REE ion and its vicinity produce a thermodynamically stable optical center that is, first of all, revealed in the optical spectra of the 4f<sup>N</sup>-configuration. As of today, the problem of the nature of the X-ray luminescence (XRL) in LTB activated by lanthanoids remains open. This is specially related to the LTB:Er<sub>2</sub>O<sub>3</sub>, the spectra of which are almost not studied.

As the analysis of the experimental results shows, introduction of Er<sub>2</sub>O<sub>3</sub> into the glassy LTB matrix results in the appearance of a series of narrow luminescence bands that by their energy position coincide with the luminescence spectra of free triply ionized Er<sup>3+</sup> ions and are due to the optical transitions between the f-shell transitions/ Since the 4f-shell is screened by the filled 5s<sup>2</sup>5p<sup>6</sup>- shell, the XRL spectra reveal the narrow bands, the energy positions of which completely agree with the energy-level diagram that corresponds to the 4f<sup>1</sup> configuration of the free Er<sup>3+</sup> ion with principal multiplet term being <sup>4</sup>I<sub>15/2</sub>.

The analysis of the XRL LTB spectra indicates that in the weak crystalline field approximation it is convenient to deal with the free Er<sup>3+</sup> ion terms taking into account the multiplet structure in a form of a series of closely located energy levels that correspond to different values of the total moment **J**. In this case the XRL spectra of the Er<sup>3+</sup> ion in the glassy LTB matrix are due to the optical transitions between the electronic states realized within the limits of the 4f<sup>N</sup>- configuration (the f→f transitions) and are characterized by the energy transfer from the 4F<sub>j</sub> (**j** = 3/2, 5/2, 7/2, 9/2); <sup>4</sup>G<sub>j</sub> (**j** = 9/2, 11/2); <sup>2</sup>G<sub>7/2</sub>; <sup>4</sup>D<sub>5/2</sub> i <sup>2</sup>I<sub>13/2</sub> spin-orbital levels to the ground <sup>4</sup>I<sub>15/2</sub> multiplet.

# DFT calculation of clusters within vitreous germanium selenide

Gurin V.S.<sup>1</sup>, Kislyakov E.F.<sup>2</sup>, Ratkevich S.V.<sup>2</sup>, Shpotyuk O.I.<sup>3</sup>, Boyko V.<sup>3</sup>

<sup>1</sup>Research Institute for Physical Chemical Problems, Belarusian State University, Minsk, Belarus;

<sup>2</sup>Belarusian State University, Minsk, Belarus;

<sup>3</sup>Institute of Materials of SRC "Carat", Lviv, Ukraine

Vitreous chalcogenides are of great interest as perspective materials for application in telecommunication, optoelectronics, nanophotonics, etc. Their structure features have been simulated using different approaches, however, there remain many open questions about details of atomic-scale structure of these materials. In the present communication for vitreous germanium selenide we develop the approach based on featured clusters which structure partially correspond to the bulk crystalline GeSe<sub>2</sub>. The clusters were built on the basis of GeSe<sub>4</sub> tetrahedral units interlinked by different ways leading to Ge<sub>2</sub>Se<sub>6</sub> and Ge<sub>2</sub>Se<sub>7</sub> clusters (edge-sharing, corner-sharing and corner-sharing tetrahedra with Se-Se bridge). A series of model clusters were built from these basic units: Ge<sub>6</sub>Se<sub>16</sub>, Ge<sub>6</sub>Se<sub>18</sub>, Ge<sub>6</sub>Se<sub>20</sub>, etc. They retain GeSe<sub>4</sub> tetrahedral units, but include various number of Se atoms between the constituents, intra- and inter-cluster selenium bridges.

The quantum chemical treatment was done at the level of density functional theory (DFT) including also the time-dependent version (TDDFT) to calculate optical properties. We obtain the electronic structure of model clusters, their relative stability, optical features, and vibrational spectra. Fig. 1 displays an example of calculation for a couple of clusters with different location of Se atoms. The more favorable structures include lateral selenium forming 6-atoms-rings.

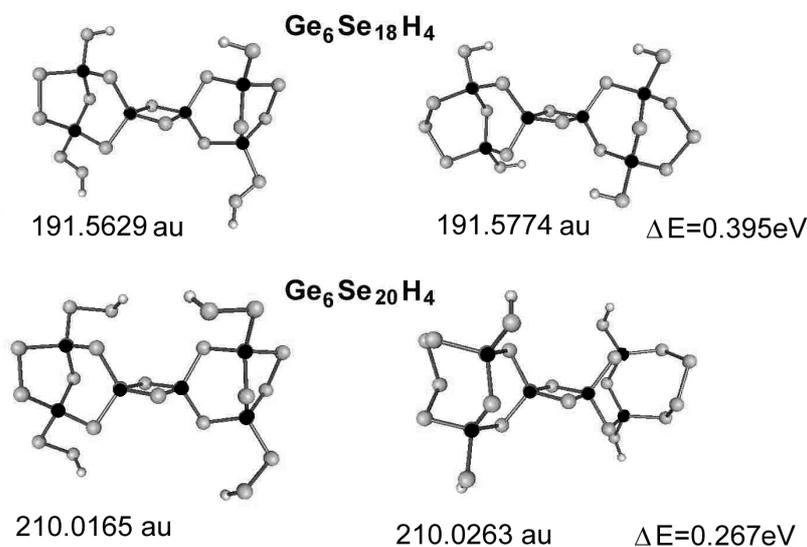


Fig. 1. Geometry of H-terminated Ge<sub>6</sub>Se<sub>18</sub> and Ge<sub>6</sub>Se<sub>20</sub> clusters with different location of Se-Se chains. Ge – black, Se – grey and H – small circles. A comparison of total electronic energies results in relative stability (ΔE) of the models.

## Electrophysical properties of Pb-Mg based eutectic melts

Peleshchyshyn R<sup>1</sup>., Sokolovskyi B<sup>2</sup>., Vus V.<sup>2</sup>

<sup>1</sup> *Secondary school №54, Lviv, Ukraine*

<sup>2</sup> *Ivan Franko National University of Lviv, Ukraine*

Physical properties of Pb-Mg based alloys in recent is the subject of intense research because of their use as liquid metal coolant in nuclear power industry. Particularly noteworthy are Pb<sub>83</sub>Mg<sub>17</sub> based eutectic alloys due to increased demands on the safety of nuclear reactors [1]. Due to the fact that continuously circulating coolant is in direct contact with the heat exchanger and other materials of the reactor, the effect of possible chemical interactions and corresponding changes in physical properties become particularly important [2]

In this work, the electrical conductivity and thermo-e.m.f. of Pb<sub>83</sub>Mg<sub>17</sub> eutectic melt with Al, Ga, Ni, Bi, Cu admixtures have been investigated.

1. P.N.Alexeev, V.P.Didoukh, Yu.O.Plevachuk, V.M.Sklyarchuk, B.I.Sokolovskii, S.A.Subbotin. Jahrestagung Kerntechnik '92, INFORUM GmbH, Bonn -1992. - P.31-34.
2. Yu.Plevachuk, V.Sklyarchuk. Experimental Study on the Electrical Conductivity and Thermo-Electromotive Force of Liquid Pb-Mg-Based Alloys // Z.Metallkd. -2001. Vol.92(6). -P.600-603.

# Prospects for the use of low melting metal alloys

Pazdry I. P.

*National university «Lviv polytechnic», Ukraine*

Team of scientists, headed by Prof. Ya J. Dutchak and Prof. V. Ya. Prokhorenko, investigated the structure, thermal properties and the possibility of applying of metal alloys based on low-melting metals (Gallium, Bismuth, Lithium) at objects of new technology, especially in nuclear power and thermometry. Obtained significant results in the direction of using eutectic alloys as liquid metal carriers of nuclear reactors as well as heat sensitive elements of liquid metal thermocouples and resistance thermometers [1].

The use of metal-based alloys Ga, Bi, Li as advanced functional materials of nuclear power is caused by the fact that they are maintaining a high thermal and electrical conductivity and heat capacity, acquire useful new skills through strength. The combination of convective heat transfer properties and radiation stability of the structure provides indispensability of metal alloys as heat carriers of nuclear reactors, the working fluid of magnetohydrodynamic devices, electrocontact elements, hermetic sealing nodes, inertial elements of power mechanical engineering and thermometry.

Experimentally researched that in a high level of penetrating radiation the radioactive damages of the alloy structure are instantly self-regenerating due to the high mobility of atoms and therefore thermophysical properties remain stable. This feature of the alloys is the basis for creating of physical principles of liquid metal heat sensitive elements of the primary thermal converters that can be used to measure high temperatures under high radiation levels. Is shown that we can purposefully control the structural state of the alloy using the methods of thermal temporal processing as well as overlapping sound and magnetic fields that contribute to the homogenization of the alloys and their degassing, removal of suspended impurities. Passivation of structural materials surfaces which contact with the alloys can be controlled using the method of thermodiffusion applying of protective coatings from the liquid metal environment and the method of laser modification and alloying of the surface.

1. V. Ya. Prokhorenko, I. P. Pazdry, S. V. Prokhorenko. Experience of using of liquid metals as heat carriers and heat-sensitive elements // X Russian conference “Structure and properties of the metal and slag alloys” — Ekaterinburg, 2001. — pp. 101–104.

# Magnetoresistance of RE-M(Cu, Ni)-X(Si,Sn) ternary compounds

Kuzhel B.S.<sup>[1]</sup>, Salamakha L.P.<sup>[1,2]</sup>, Romaka L.<sup>[1]</sup>, Belan B.D.<sup>[1]</sup>

<sup>1</sup>Ivan Franko National University of Lviv, Ukraine

<sup>2</sup>Technical University of Vienna, Austria

The electrical resistivity of the number of ternary compounds with rare-earth metals, copper or nickel and silicon or tin had been studied under magnetic fields up to 12 T in the temperature region down to 0.3 K. For those compounds displaying magnetic transitions, the transition temperatures were analyzed (see table and figures).

Compound	Crystal structure	Space group	<i>a</i>	<i>b</i>	<i>c</i>	$\rho$ , $\mu\Omega\text{cm}$ <i>T</i> =280-285 K	<i>T</i> <sub>mag</sub> , K
Ce <sub>3</sub> Cu <sub>4</sub> Sn <sub>4</sub>	Gd <sub>3</sub> Cu <sub>4</sub> Ge <sub>4</sub>	<i>Immm</i>	0.459	0.702	1.509	138	~7.7 ~3.5
Nd <sub>3</sub> Cu <sub>4</sub> Sn <sub>4</sub>	Gd <sub>3</sub> Cu <sub>4</sub> Ge <sub>4</sub>	<i>Immm</i>	0.454	0.698	1.495	39	~1.9
Sm <sub>3</sub> Cu <sub>4</sub> Sn <sub>4</sub>	Gd <sub>3</sub> Cu <sub>4</sub> Ge <sub>4</sub>	<i>Immm</i>	0.450	0.695	1.482	53	4,8; 6,5; 8,5
GdNiSn <sub>2</sub>	LuNiSn <sub>2</sub>	<i>Pnma</i>				80	~10.5, ~3.7
DyNiSn <sub>2</sub>	LuNiSn <sub>2</sub>	<i>Pnma</i>	1.599	0.441	1.453	60	~9.0
HoNiSn <sub>2</sub>	LuNiSn <sub>2</sub>	<i>Pnma</i>				68	~3.6, ~2.1
DyNiSi	TiNiSi	<i>Pnma</i>	0.682	0.415	0.716	173	~8.5
DyNiSi <sub>3</sub>	ScNiSi <sub>3</sub>	<i>Cmmm</i>	0.392	2.095	0.394	71	~9.6

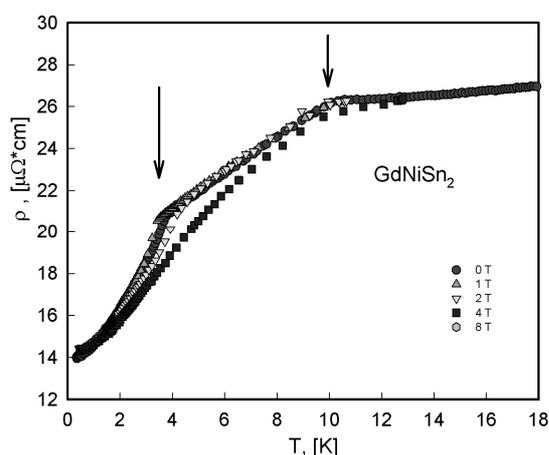


Fig. 1 The temperature dependence of the electrical resistivity GdNiSn<sub>2</sub> in various values of a magnetic field. Arrow points to the transition.

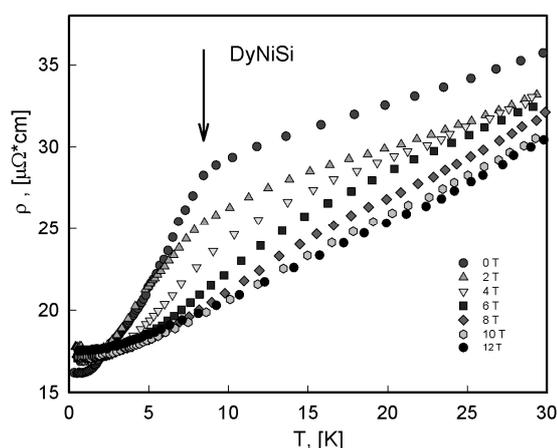


Fig. 2 The temperature dependence of the electrical resistivity DyNiSi in various values of a magnetic field. Arrow points to the transition.

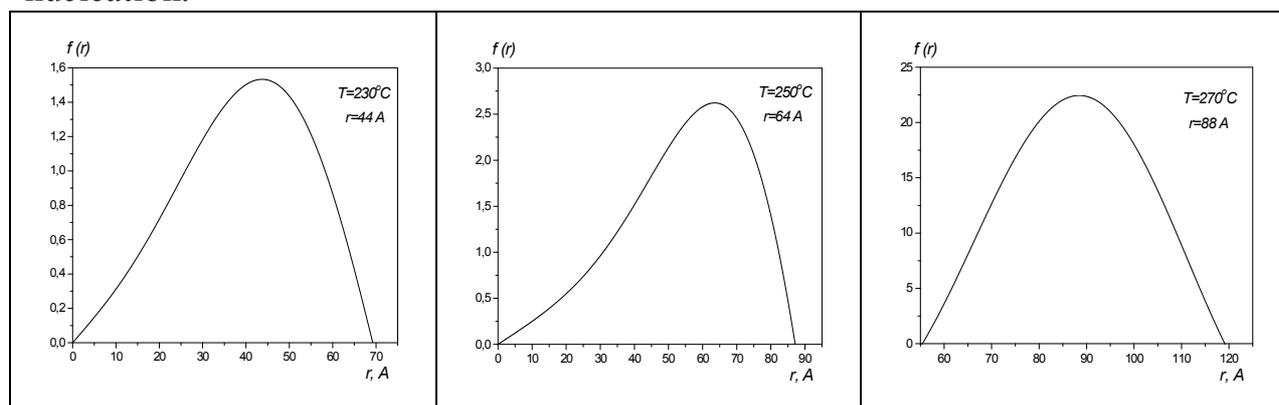
Effect of magnetic field on the nature of the temperature dependence of the electrical resistivity of the investigated compounds is considered as the result of the influence on the strengths of hybridization between the (*sd*)-conduction electrons and localized f-electrons including the change of mobility of the charge carriers due to possible compensation of spin interaction.

## Evolution of nanocrystalline structure in amorphous $\text{Al}_{86}\text{Ni}_8\text{Ho}_6$ alloy.

Kulyk Yu. Zhovneruk S., Mudry S.  
*Ivan Franko National University of Lviv, Ukraine*

Producing of materials with improved properties is one of the most important aims of industry and is related with fundamental problems of physics, chemistry and material science. In particular, such materials as Al-based nanocrystalline alloys, obtained by means of controlled crystallization of initial amorphous alloy reveal significantly better mechanical properties in comparison with traditional aluminium-based alloys obtained by casting method. At annealing of amorphous alloy the formation of Al nanocrystals of 5-20 nm size and density of  $10^{23}$ -  $10^{25}$   $\text{nm}^{-3}$  occurs. Up date understanding of nucleation and growth mechanism of nanocrystals in amorphous matrix is far to be clear. На сьогодні, залишається актуальним питання стосовно механізму зародження та росту нанокристалів в аморфній матриці. On that reason studying of nanocrystallization features at annealing of  $\text{Al}_{87}\text{Ni}_8\text{Ho}_5$  amorphous alloy, obtained by rapid cooling from liquid state was the aim of this work. Main methods, which have been used to measure the structure parameters were high temperature X-ray diffraction and small angle X-ray scattering (SAXS) methods.

It was shown that annealing results in formation of nanocrystals, randomly distributed in amorphous matrix that evidently follows from SAXS measurements. Analysis of intensity curves by Guinier interpretation allowed us to conclude that Al nanocrystals of 5-20 nm size are mixed with larger nanocrystalline particles of 50-80 size that indicates the formation of inhomogeneities in residual amorphous matrix. Fig.1 illustrates size of nanocrystals distribution function, calculated from measured data of SAXS – measurements. As is seen the increasing of annealing temperature to  $250^\circ\text{C}$  leads to shift of this function to larger interatomic distances that is suggested to be caused the increasing of fraction of comparatively larger clusters. Besides, the sample, annealed at  $270^\circ\text{C}$  in fact has no the nanocrystals of small size. Such distribution occurs in alloys with heterogeneous mechanism of cluster nucleation.



# The viscosity and electrical conductivity of liquid Bi-In alloys

Vus V.<sup>1</sup>, Yakymovych A.<sup>2</sup>, Mudry S.<sup>1</sup>, Plevachuk Yu.<sup>1</sup>

<sup>1</sup>*Department of Metal Physics, Ivan Franko National University, Lviv, Ukraine*

<sup>2</sup>*Department of Inorganic Chemistry / Materials Chemistry, University of Vienna, Austria*

The structure of binary liquid alloys is in correlation with the equilibrium phase diagram. It has been shown early that the existence of chemical compounds or of eutectic points in the phase diagram is often linked to a deviation of the structure of the liquid from a random atomic distribution and that there is interrelation between the phase diagram and physical-chemical properties.

X-ray diffraction data of Bi-In melts revealed an anomalous behavior, which was attributed to a competition between BiIn<sub>2</sub>- and BiIn-like atomic distributions in the liquid state [1]. It seemed of interest to investigate if such an assumption agrees with transport properties, and this was the reason for the measurements of the viscosity and electrical conductivity of liquid Bi-In alloys.

The viscosity measurements were carried out using an oscillating-cup viscometer [2]. In this method, a graphite crucible containing the sample is placed in a stainless steel container which is attached to the torsion wire inside the high temperature furnace. The temperature was determined by WRe-5/20 thermocouples. Using the modified Roscoe equation, the dynamic viscosity was calculated from the logarithmic decrement and the period of oscillations [3].

A home-made experimental facility based on the 4-point method, was used for electrical conductivity measurements. The experiments were performed in an argon atmosphere. Graphite electrodes for current and potential measurements were placed in the wall of the vertical cylindrical boron nitride ceramic measuring cell along its vertical axis. For further details of this method and its experimental realization we refer to [4].

Taking into account the obtained transport properties values in comparison with literature data, one can suppose that stoichiometry of chemically ordered clusters. Such atomic rearrangement also influences on the interaction between each kind of clusters and is revealed on anomalous behavior of temperature dependence of the viscosity and electrical conductivity.

1. R. Bek, E. Nold, S. Steeb. *Z. Naturforsch. A*, 36, 150 (1980).
2. S. Mudry, V. Sklyarchuk, A. Yakymovych, *J. Phys. Studies* 12, 1601 (2008).
3. R. Roscoe, *Proc. Phys. Soc.* 72, 576 (1958).
4. Yu. Plevachuk, V. Sklyarchuk, *Meas. Sci. Technol.* 12, 23 (2001).

## Structure of $\text{Ni}_{1-x}\text{In}_x$ molten alloys within near-eutectic ( $\zeta + \delta$ ) concentration region

Vus V., Shevernoga I., Mudry S., Korolyshyn A.  
*Ivan Franko National University of Lviv, Ukraina*

Eutectic alloys attract an attention of researchers because they have a low melting point in comparison to alloys of other concentration. Numerous structure studies of these alloys in liquid state by means of diffraction methods [1-3] as well as structure sensitive properties measurements [4,5] shown the deviation of atomic distribution from one for liquid atomic solution. Most of such melts reveal the tend to preferred interaction of like kind atoms that results in formation of self-associated atomic groups (clusters), which upon increasing of their size at cooling become the nuclei of solid phase at crystallization. Therefore, existence of clusters on the base of like kind atoms is a suitable condition for formation of eutectic structure at crystallization. In case, when structure before solidification is close to one of atomic solution, the significant atomic rearrangement at crystallization should be realized. Such rearrangement is impossible if diffusive processes are damped as it occurs at rapid cooling resulting in formation of amorphous structure.

More complicated structure is observed in eutectic melts, whose components are chemical compounds [6,7]. Unfortunately, experimental data on structure of such systems are scarce. For that reason we have investigated the structure of  $\text{Ni}_{1-x}\text{In}_x$  molten alloys at few temperatures ( $T = 5, 50$  and  $100$  K above the melting point for each concentration) within the concentration region 28-61 at%, including high temperature  $\zeta$  and  $\delta$  – phases and eutectic alloy.

The structure studies have been carried out by means of X-ray diffraction method. Structure parameters have been obtained from experimental dependences of scattered intensities versus scattering angle.

Structure of  $\text{Ni}_{1-x}\text{In}_x$  molten alloys shows the tendency to chemical ordering within concentration range, from  $\zeta$  to  $\delta$  - phase, including eutectic point. Topology of atomic distribution is close to structure of solid intermetallics, which remains even when melts were overheated by 100 K above the melting point.

1. S. Mudry, T. Lutsyshyn, I. Shtablavyi, A. Yakymovych, Yu. Plevachuk, J. Non-Cryst. Solids 353 (2007) 2982-2986.
2. Shtablavyi, S. Mudry, V. Mykhaylyuk, J. Rybicki, J. Non-Cryst. Solids 354 (2008) 4469-4474.
3. Yanwen Bai, XiufangBian, Xubo Qin, Jingyu Qin, Xiaoqian Lv, Junzhe Sun, J. Non-Cryst. Solids 356 (2010) 1823-1828.
4. R.K. Gupta, R.A. Singh, J. Crystal Growth 267 (2004) 340-347.
5. R.K. Gupta, S.K. Singh, R.A. Singh, J. Cryst. Growth 300 (2007) 415-420.
6. I. Kaban, Th. Halm, W. Hoyer, J. of Non-Crystalline Solids 288 (2001) 96-102.
7. A. Il'inskii, S. Slyusarenko, O. Slukhovskii, I. Kaban, W. Hoyer, J. of Non-Crystalline Solids 306 (2002) 90-98.

## **Magnetic properties of Gd-Fe system (Films and Bulk)**

Prysyazhnyuk V.I., Mykolaychuk O.G.

*Ivan Franko National University of Lviv, Ukraine*

We conduct investigation of magnetic properties of films of  $\text{GdFe}_2$ ,  $\text{GdFe}_5$  and  $\text{Gd}_2\text{Fe}_{17}$  compounds. Films have been gained by a method of thermal evaporation on teflon substrates at room temperatures.

Values of Curie temperature, curves of specific magnetisation, and hysteresis curves for massive and thin-film samples are determined. It is spotted that the Curie temperature of massive samples corresponds to references. At examination of thin-film samples Curie temperature reduction was observed. Such depression of Curie temperature speaks expansion of a crystalline lattice owing to formation of microdefect (films were is amorphous-crystal).

Temperature dependences of magnetic saturation for compounds and films of Gd-Fe system are determined. The given dependences characteristic for materials of such class. Magnetic saturation of films  $\text{Gd}_2\text{Fe}_{17}$  at room temperature makes  $4.8 \mu\text{b}$ . The given value gets to an interval  $6.21\text{-}1.84 \mu\text{b}$  for rhombic and hexagonal modification properly. It means that our films are an intermixture of these modifications.

It is made attempt to unite methods of the phase magnetic analysis with structural analysis.

## **Concentration dependence of physical properties of liquid NaF–LiF–NdF<sub>3</sub> alloys**

L. Bulavin<sup>1</sup>, Yu. Plevachuk<sup>2</sup>, V. Sklyarchuk<sup>2</sup>, A. Omelchuk<sup>3</sup>, N. Faidiuk<sup>3</sup>,  
R. Savchuk<sup>3</sup>, I. Shtablavyi<sup>2</sup>, V. Vus<sup>2</sup>

<sup>1</sup> *Kyiv National Taras Shevchenko University, , Ukraine*

<sup>2</sup> *Ivan Franko National University, Lviv, Ukraine*

<sup>3</sup> *V.I.Vernadsky, Institute of General and Inorganic Chemistry, Kyiv, Ukraine*

The molten salt fuel mixtures are considered as a good environment for controlled accelerator transmutation of the long lived radionuclides in transmutation reactors, created for deep burning weapons-grade isotopes and disposal of radioactive waste. Because of good heat transfer capacity, radiation insensitivity, high boiling point and wide range solubility for actinides, the molten fluorides are particularly interesting for a possibility to be used either for the whole heat transfer between two places or as both heat and fuel carriers in reactors. A mixture of metal fluorides with small thermal neutron capture cross sections was recommended as a nuclear fuel carrier.

In this work, experimental studies of viscosity, thermoelectric power and electrical conductivity of the ionic liquid alloys NaF–LiF–NdF<sub>3</sub> were carried out in the wide temperature intervals above the melting points. Similar temperature dependences of these properties for different melt compositions have been revealed. The alloy composition has a significant influence on the interval of melt homogeneity and behaviour of the thermoelectric power temperature coefficient. It was found that a small shift from the peritectic to eutectic composition increases considerable the viscosity. A correlation between the structure and thermophysical properties has been analyzed. The results can be used in modelling a blanket for the liquid salt reactor.

# Temperature dependence of structure in eutectic melts

V. Klanichka<sup>1</sup>, I. Shtablavyi<sup>2</sup>, S. Mudry<sup>2</sup>

<sup>1</sup> *Vasyl Stefanyk Precarpathian National University, Ivano-Frankivsk, Ukraine*

<sup>2</sup> *Ivan Franko National University of Lviv, Ukraine*

Most of eutectic alloys reveal the inhomogeneous atomic distribution at temperatures not far from melting point. From numerous structure studies by diffraction methods and structure sensitive physical properties measurements follows that structural units are formed preferentially on the base of like kind atoms. The main reason of such structure is a significant difference between atomic radii of constituent atoms and their small electronegativity difference.

On that reason we focused our attention on analysis of temperature dependence of structure parameters in various kinds of eutectic systems: simple eutectics, eutectics with large solubility limits and eutectics with envelope point in liquidus curve. Temperature dependencies of structure parameters have been estimated from structure factors and pair correlation functions.

It was shown that most of structure parameters reveal envelope point in their temperature dependences. This feature is supposed to be caused by transition from structure on the base of clusters to the structure close to random atomic distribution.

# Influence of ageing processes on the structure and physical properties of amorphous-crystalline films of gd-fe system

Prysyazhnyuk V.I., Mykolaychuk O.G.

*Ivan Franko National University of Lviv, Ukraine*

Thin films of binary compounds of Gd-Fe system were obtained by means of a thermal vacuum evaporation of polycrystal mix material of a corresponding composition. The films with by thickness of 50-60 nanometers were evaporated on splitting of NaCl, then NaCl dissolved in water. The part of films was picked up at once on copper electron diffraction grids. The second series of films transplanted on copper grids, prestressly coated thin collodion supports and in such way was maintained 3 years. Then recurring researches were carried out. For electrophysical measurings the films are condensed on glassceramics substrates. The thickness of films changed within 100-200 nanometers. The temperature of substrates had two values 300 and 500 K. For structural investigation the electron microscope UEMV-100K and high-temperature attachment PRON-2 were used. Angle dependence of atomic factors of electron scattering was considered by atoms of gadolinium and iron. All measurements were repeated in 3 years after the first stage of measurings.

Results of structural researches of  $GdFe_2$  films compounds are already studied in [1,2]. Films of  $GdFe_2$  compounds condensed in structural type  $MgCu_2$ . This structural type is also in structure of massive samples.  $Gd_2Fe_{17}$  films which condensed at temperature of a substrate  $T_s = 500K$  consisted of an intermixture of three compounds – hexagonal  $Gd_2Fe_{17}$  with structural type  $Th_2Ni_{17}$ , rhombohedral  $Gd_2Fe_{17}$  with structural type  $Th_2Zn_{17}$  and hexagonal  $GdFe_5$  with structural type  $CaCu_5$

Positions of diffraction peaks has not changed. It testifies that the generated structures have not changed in due course, and also oxidizing process is not observed. If to compare intensity of maximums it is possible to observe insignificant disproportionation of phases content. The content of hexagonal  $Gd_2Fe_{17}$  compound with structural type  $Th_2Ni_{17}$  has decreased (60%→50%). The content of rhombohedral  $Gd_2Fe_{17}$  compound with structural type  $Th_2Zn_{17}$  it was reduced (30%→40%). The only phase which has not changed the percentage is hexagonal  $GdFe_5$  with structural type  $CaCu_5$  (10%).

As a whole, the trend to the further crystallization of is amorphous-polycrystalline films is observed. Electron diffraction studies confirm the suggestion (peaks become of higher resolution).

1. V.Prysyazhnyuk, O.Mykolaychuk. Structure formation in Gd-Fe thin films. *Journal of Non-Crystalline Solids*. -2006. -Vol.352. -P.4299-4302.
2. V.Prysyazhnyuk, O.Mykolaychuk. *Stability and phase changes in thin layers of rare-earth metals/iron and other binary compounds*. *Journal of Non-Crystalline Solids*. -2008. -Vol.354. -P.4458-4460.

# Nanocomposite materials based on nanostructured carbon and III-VI layered semiconductors

Bakhtinov A.P.<sup>1</sup>, Vodopyanov V.M.<sup>1</sup>, Kudrynskyi Z.R.<sup>1</sup>, Kovalyuk Z.D.<sup>1</sup>,  
Netyaga V.V.<sup>1</sup>, Karbivskyy V.L.<sup>2</sup>, Vishniak V.V.<sup>2</sup> and Lytvyn O.S.<sup>3</sup>

<sup>1</sup> *Frantsevich Institute for Problems of Materials Science, NASU, Chernivtsi Ukraine*

<sup>2</sup> *Kurdyumov Institute of Metallophysics, NASU, Kyiv, Ukraine*

<sup>3</sup> *Lashkaryov Institute of Semiconductor Physics, NASU, Kyiv, Ukraine*

Future applications of nanostructured carbon materials in nanoelectronics require understanding the structure and the growth mechanisms of these materials on various substrates. In this work the morphology and composition of nanostructures formed on the basis of nickel and carbon on atomically smooth van der Waals (0001) GaSe surface by evaporation from a liquid ion source in vacuum were investigated.

The present study illustrates the possibility to form nanostructures with chemically and structurally abrupt defect-free interfaces on a van der Waals (vdW) surface, which contain thin carbon layers and carbon-encapsulated magnetic Ni nanoparticles. The self-organization of the (Ni–C) nanocomposite structures on the vdW surface of semiconductor layered crystal occurs as a result of electrostatic interaction between the charged liquid droplets and this surface, van der Waals and dipole-dipole electric and magnetic interaction between the nanoparticles (NPs). The morphology of the structures depends on technological conditions of growth, composition of evaporated material and surface state of the substrate. It was established that continuous thin layers of the Ga<sub>2</sub>O<sub>3</sub> wide-band-gap oxide with surface roughness of less 0.3 nm can be grown on a (0001) GaSe surface under intensive UV irradiation. Using this oxidation technique we fabricated nanostructures, in which the magnetic nickel–filled carbon nanocapsules (Ni @ CNCs) embedded into the Ga<sub>2</sub>O<sub>3</sub> oxide form chains and nanoscale rings. It was found that the phase separation occurs in nanocomposite (Ni–C) thin films grown on an oxidized (0001) GaSe surface with a large number of dangling bonds (oxygen vacancies).

The developed technology was used to fabricate a vertical metal oxide semiconductor (MOS) hybrid structure, which contains layered semiconductor GaSe, ferromagnetic metal Ni layer, core-shell Ni @ CNCs and (Ni–C) nanocomposite thin film. The peculiarities in the current-voltage characteristics of this structure are associated with a spin accumulation, which takes place at spin-dependent electron tunneling through barriers in the Coulomb blockade mode and spin-polarized electric current interactions with magnetic NPs [1].

1. J. Barnas, I. Weymann. Spin effects in single-electron tunnelling // J. Phys : Condens. Matter. – 2008. – Vol. 20. – P. 423202(1)- 423202(2).

## **ZnO nanowires with p-type conductivity as a material to create a vacuum pressure sensor**

Kapustianyuk V.B., Panasyuk M.R., Turko B.I., Dubov Yu.G., Vas'kiv A.P.

*Ivan Franko National University of Lviv, Ukraine*

ZnO is one of the earliest-discovered and well-known gas sensing oxides, which has been widely studied for detection of inflammable and toxic gases, such as nitrogen dioxide, ethanol, carbon monoxide, hydrogen. This material attracts great attention because of high sensitivity, chemical hardness, safety and low price. The small-scale gas sensors based on ZnO nanostructures possess higher sensitivity and smaller response time comparing to the thin film ones. A larger work area is one of the reasons of sensors sensibilization based on ZnO nanostructures. The effective use of modern microelectronics industry gauge to monitor the vacuum level is excluded due to their large sizes. Therefore, the vacuum technique can be considered as potential consumers of gas sensors based on the zinc oxide nanostructures [1-3]. Recently, several researchers reported the data concerning the properties of gauges based on ZnO nanostructures with *n*-type conductivity [1-3].

For the first time a vacuum pressure sensor based on the ZnO nanowires with a *p*-type conductivity is reported. The nanowires were grown by electrodeposition from an aqueous solution in the electrochemical cell with two electrodes [4]. The observed *p*-type conductivity in nanowires was supposed to be caused by the zinc vacancies. The created vacuum pressure sensor is based on the mechanism of chemisorption-desorption oxygen process on the ZnO nanostructure surface. It is shown that the current flowing through the ZnO nanostructures with *p*-type conductivity in the manufactured vacuum pressure sensor increases linearly with increase of pressure in the semilogarithmic coordinates.

1. S.J.Chang, T.J.Hsueh. A ZnO nanowire vacuum pressure sensor// Nanotechnology. -2008. -Vol.19. -P.095505.
2. L.Wu, F.F.Song. A practical vacuum sensor based on a ZnO nanowire array// Nanotechnology. -2010. -Vol.21. -P.475502.
3. X.J.Zheng, X.C.Cao. A vacuum pressure sensor based on ZnO nanobelt film// Nanotechnology. -2011. -Vol.22. -P.435501.
4. G.O.Lubochkova, B.I.Turko. Method of obtaining ZnO nanostructured material with p-type conductivity, UA Patent 78485, March 25, 2013.

## LED based on *p*-type ZnO nanostructures

Kapustianyk V.B.<sup>1</sup>, Turko B.I.<sup>1</sup>, Rudyk V.P.<sup>1</sup>, Tsybulskiy V.S.<sup>1</sup>, Luzinov I.<sup>2</sup>,  
Malynych S.<sup>2</sup>, Savchak M.<sup>2</sup>

<sup>1</sup>*Ivan Franko National University of Lviv, Ukraine*

<sup>2</sup>*Clemson university, United States of America*

ZnO is of great potential for development of white-light-emitting sources. The most challenging problem of ZnO based photonic devices is the lack of stable and reliable *p*-type doping; mainly due to the self compensation property of ZnO. In the past few years, rapid progress has been made in research of *p*-type ZnO doping. Some successful work has been done using group I and V elements as acceptors and deviations from stoichiometry [1].

The ZnO nanostructures with *p*-type conductivity on a glass substrate coated with indium tin oxide (ITO) were synthesized by electrodeposition from an aqueous solution in the electrochemical cell with two electrodes [2]. To produce LED's, array nanowires partially covered with an insulator layer of photoresist or photoresist and the hole-conducting polymer poly (3,4-ethylenedioxythiophene)-poly (styrene-sulfonate) PEDOT/PSS was then deposited on the structure by spin coating. This was followed by thermal evaporation of Au as the top electrode. As the photoresist-insulator used liquid photo-positive resist based on o-naphto-chinon-diazide and novolack (a type of phenol-formaldehyde resin) "Positive 20" KONTAKT CHEMIE. Using the AvaSpec-ULS2048-UA-50 spectrometer, we obtained electroluminescence spectrum of this LED's, recording emission through the glass substrate. The I-V characteristics for ITO/*n*-ZnO/*p*-ZnO/photoresist/Au heterostructures was investigated. Transmission spectra of glass/ITO/PEDOT:PSS, ITO/*n*-ZnO/*p*-ZnO/photoresist/PEDOT:PSS and ITO/*n*-ZnO/*p*-ZnO/photoresist heterostructures were investigated. Our LEDs (ITO/*n*-ZnO/*p*-ZnO/photoresist/PEDOT:PSS/Au and ITO/*n*-ZnO/*p*-ZnO/photoresist/Au) emit at wavelengths 480-498 nm, 569 nm, 650-670 nm and 458-460 nm, 560 nm, respectively. According to the literature data the defects responsible for occurrence of the blue band are  $Zn_i$  and  $V_{Zn}$ ; green band -  $Zn_i$ ,  $V_{Zn}$  and  $V_o$ ; red band -  $Zn_i$  and  $O_i$  [3].

1. M.Sun, Q.Zhang, J.Wu. Electrical and electroluminescence properties of As-doped *p*-type ZnO nanorod arrays// J. Phys. D: Appl. Phys. -2007. - Vol.40. -P.3798-3802.
2. G.O.Lubochkova, B.I.Turko, Method of obtaining ZnO nanostructured material with *p*-type conductivity, UA Patent 78485, March 25, 2013.
3. M.Willander, O.Nur. Luminescence from zinc oxide nanostructures and polymers and their hybrid devices// Materials. -2010. -Vol.3. -P.2643-2667.

# **Switching of the magnetic nanofilms with laser radiation and data recording using the spin current**

Krupa M.M.

*Institute of Magnetism National Academy of Science of Ukraine, Kiev, Ukraine*

Spintronic belongs to one of the most the quickly developing area of science and technology, which is based on the control by processes of transfer of spin current between the elements of electronic devices. Multilayer magnetic nanofilms are the basic material for spintronics elements and recording medium. The elements of spintronics based on such metallic nanostructures are compared to the semiconductor elements of microelectronics more low noise, high thermal stability factor and can be used in a higher frequency range.

For spin current control in spintronics devices it is necessary to change the state of magnetization of spin filter elements. Study the dynamics of the spin relaxation processes in solids and development of methods for active control of spin spin-polarized current in solid-state circuits constitute the main directions of the spintronics. Usually magnetic reversal of magnetic films is realized with the help of itself magnetic field of the electric current flowing through special electrodes. However in such simple way it is difficult to create a considerable high-frequency magnetic field in small micro- and nanoarea. Determination of maximum speed magnetic reversal of magnetic films is one of the fundamental problems of the physics of magnetism, which is important in the development of high-speed spintronic elements and systems magnetic recording media.

This article presents the results of experimental studies of the physical mechanisms and dynamics of magnetization reversal of films with one or two the magnetic nanolayers under an irradiation picosecond and femtosecond laser pulses and also the experimental samples of spin transistors and data recording devices on the spin storage medium are described.

# The Technology, Properties and Application of Thermoelectric Nanomaterials and Nanocomposites

Freik D.M., Klanichka V.M., Mezhylovska L.Yo.

*Vasyl Stefanyk Precarpatian National University, Ivano-Frankivsk, Ukraine*

The environment is filled with a large number of so-called gratuitous energy that is still not effectively used by humanity. The fact that a very urgent need is to improve the efficiency of its conversion into electricity using primarily solid-state thermoelectric modules based on semiconductor materials.. The main thermoelectric parameter is the dimensionless thermoelectric figure of merit  $ZT$  ( $ZT = S^2\sigma/\chi$ ,  $T$  -absolute temperature). Practical sense are the materials characterized by  $ZT \approx 1$  (efficiency = 3-6%). If  $ZT = 2 \div 3$  (efficiency: 20%), it would have led to a sharp increase in their use, while at  $ZT = 3 \div 4$  thermoelectric converters could compete with conventional electric generators. In this connection it is important to continue to search for efficient thermoelectric materials.

Note, that the Seebeck coefficient (thermoelectric power) ( $S$ ) and electrical conductivity ( $\sigma$ ) are defined only by electronic subsystem of the crystal, and thermal conductivity ( $\chi$ ) in the first approximation – by phonon and electron subsystems ( $\chi = \chi_l + \chi_e$ ). So, to maximize thermoefficiency  $Z$  of material it is needed the thermal conductivity to be minimal at maximum electrical conductivity. It takes material such as "phonon glass" and "electronic metal"?!

Recent advances in nanotechnology give some perspective to solve assigned problems [1,2]. It is believed now that the main direction of improvement of thermoelectric properties of materials is the use of spatially inhomogeneous structures with dimensions comparable to the characteristics wavelength of electrons and phonons, that are in nanoscale area. These systems should include quantum dots, wire and wells and created on the basis superlattice of quantum dots, wires and nanocomposites.

Potential impact on electronic and phonon subsystems of new structures by one more parameter – size – significantly expands ways to improve the thermoelectric figure of merit. In such structures there have been two main strategies (using quantum-size effects to enhance the Seebeck coefficient  $S$  and to control  $S$  and the conductivity  $\sigma$  somewhat independently; the introduction of numerous boundaries that scatter phonons more effectively than electrons and also scatter mainly those phonons which have the greatest contribution to the thermal conductivity) and three conceptions of their future development ("carrier-pocket" engineering, filtering energy, transition semimetal-semiconductor (SMSC-transition)).

The spatial place among nanothermoelectric materials is occupied by composites. This is because the introduction of many surfaces in the host material can significantly reduce the thermal conductivity, and the filtering of

carriers and quantum size effects (QSE) increase  $S$ , which leads to increase  $ZT$ . In particular, nanoparticles of  $\sim 10$  nm greatly reduce the amount of thermal conductivity. It is crucial that the shortwave phonons in nanocomposites are dispersed by point defects, while medium and long-wave – on the nanoparticles. It was revealed a marked dispersion (scattering coefficient  $\sim 3$ ) which is the characteristic of PbTe with metal particles ErAs (increase of  $ZT$  by 2 times)  $\chi = (5-6) \text{ W m}^{-1} \text{ K}^0$ .

It was defined the strategy for further development of new nanocomposite materials among which are the following: modulation of doping compared with uniform doping, coherent nano-inclusion compared to incoherent; ordered limits compared with random; modified grain compared with unmodified grains, spherical cavities in comparison with column. The idea of ordered nanocomposites is a new concept with a variety of well-organized nanostructures to repair electronic transport channel, unlike the most conventional nanocomposites with individual nanostructures.

In connection with said above the thermoelectricity is facing to following problems: the creation of new materials with low thermal conductivity and high thermoelectric figure of merit  $ZT$ ; development of theory and technology of spatially inhomogeneous materials: composites and quantum-dimensional structures based on superlattices, quantum wells, quantum wires, quantum dots, promoting of thermoelectricity as a promising form of alternative energy.

*The work supported by an integrated project of MES of Ukraine (N 0113U000185) and by projects of FRSS State Agency for Innovation and Informatization of Ukraine. (Contracts: R54, F53, 3), NAS of Ukraine (N 0110U006281).*

1. Freik D.M. Nanostructured thermoelectric materials: challenges, technologies, properties // *Physics and Chemistry of Solids* **14**(2) P.280-299 (2013).
2. Dresselhaus M.S., Chen G., Tang M.I., Yang R., Lee H., Wang D., Ren Z., Fleurial J-P., Gogna P. New Directions tar Low-Dimensional Thermoelectric Materials // *Adv. Mater* **19** pp. 1043-1053 (2007).

# Nanocomposite Materials Based on PbTe with Nano-inclusions

Gorichok<sup>1</sup> I.V., Krynytsky<sup>2</sup> O.S., Matkivsky<sup>1</sup> O.M.

<sup>1</sup>*Vasyl Stefanyk Precarpatian National University, Ivano-Frankivsk, Ukraine*

<sup>2</sup>*Ivano-Frankivsk National Technical University Oil and Gas, Ivano-Frankivsk, Ukraine*

During recent years, thermoelectric phenomena became an increasingly practical application for the direct conversion from thermal energy into electrical energy, the efficiency of which depends strongly on the properties of materials which are used in thermoelectric modules. They should have high values of conductivity ( $\sigma$ ), Seebeck coefficient ( $S$ ) and low thermal conductivity ( $\chi$ ), provided that certain values of the thermoelectric figure of merit ( $Z$ ) ( $ZT = S^2\sigma/\chi$ ,  $T$ -absolute temperature) [1].

Lead telluride (PbTe) is a good thermoelectric material. Typically it has a maximum value of  $ZT$  close to 1 at a temperature of about 650 K. PbTe crystallizes with the NaCl crystal structure (Fm3m) with Pb atoms occupying cationic positions and Te in anionic lattice positions. Lattice thermal conductivity for PbTe is about 2,2 W / m • K at room temperature and decreases at higher temperatures [2]. The authors of [3] have shown that in PbTe nanocomposites with combined nano-inclusions Ag and Sb, Pb and Sb are a filtration media that is causing the increase of  $S$  leads to a significant increase of  $ZT = 1,4$  at (650-700) K compared with  $ZT = 0.8 - 1.0$  for pure PbTe [4]. Also it was concluded that the inclusion of PbTe, PbS matrix without formation of solid solution effectively reduces the lattice thermal conductivity without significant effect on the electronic subsystem. Sufficiently high value of  $ZT = 1,5$  at 650K due to the fact that the interface beans PbS and PbTe crystal structure is totally ordered by the formation of inconsistent dislocations [5].

*The work supported by an integrated project of MES of Ukraine (N 0113U000185).*

1. Freik D.M., Galuschak M.O., Krynytsky O.S, Matkivskiy O.M. New Nanocomposite Thermoelectric Materials (Review) // Physics and chemistry of solid state 14, (2) p. 300-316 (2013).
2. Hsu KF, Loo S, Guo F, Chen W, Dyck JS, Uher C, Hogan T, Polychroniadis EK, Kanatzidis MG (2004) Science 303(5659):818.
3. Ma Y., Heijl R., Palmqvist A. E. C. Composite thermoelectric materials with embedded nanoparticles // J. Mater. Sci 48:2767–2778 (2013).
4. Sootsman JR, Kong H, Uher C, D'Angelo JJ, Wu C-I, Hogan TP, Caillat T, Kanatzidis MG (2008) Angew Chem Int Ed 47(45):8618
5. Androulakis J, Lin C-H, Kong H-J, Uher C, Wu C-I, Hogan T, Cook BA, Caillat T, Paraskevopoulos KM, Kanatzidis MG (2007) J Am Chem Soc 129(31):9780.

# The structure modeling and *ab initio* calculation of the thermodynamic parameters of zinc chalcogenides crystals

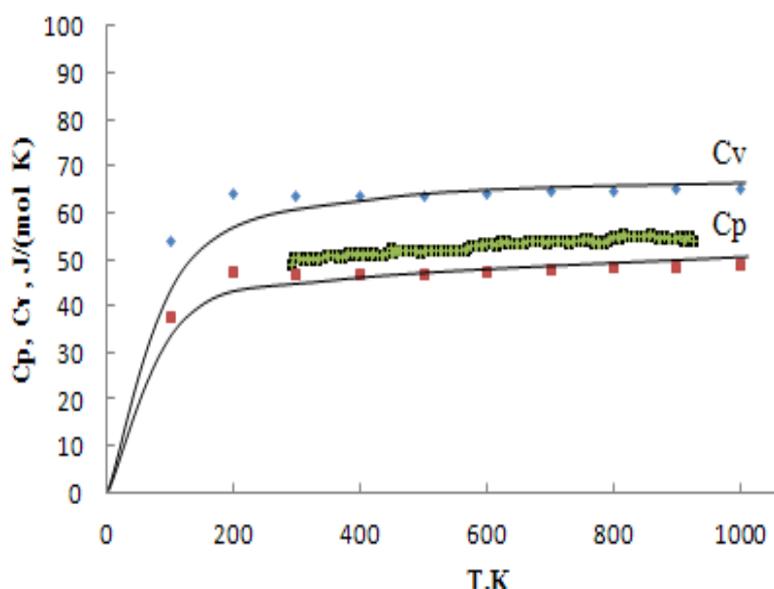
Freik D.M., Parashchuk T.O., Chobanyuk V.M. Gorichok I.V.

*Vasyl Stefanyk Precarpathian National University, Ivano-Frankivsk, Ukraine*

Zinc chalcogenides are promising materials for both techniques and scientific models. However, the practical application of ZnS, ZnSe, ZnTe are needed the reliable information about their crystal structure.

For the calculation of the thermodynamic parameters we used the cluster approach. The calculations were performed using the software package Firefly within the limited Hartree-Fock approximation, using the valence basis set SBKJC, which includes the skeleton of the effective potential. Visualization of spatial structures was carried out using Chemcraft.

As a result of the calculation were obtained formation energies  $\Delta E$ , formation enthalpy  $\Delta H$ , entropy  $\Delta S$ , Gibbs energy  $\Delta G$  and the specific heats at constant pressure  $C_p$  and at constant volume  $C_v$  of ZnS, ZnSe, ZnTe crystals.



**Fig.** Temperature dependence of the specific heats of ZnTe crystals at constant pressure  $C_p$  and constant volume  $C_v$  respectively; lines – is the approximation line of computer calculations points, points line is the experimental date.

The obtained values of the specific heats at constant pressure  $C_p$  and at constant volume  $C_v$  at different temperatures are shown in the Fig. We can see that our results of quantum-chemical calculations satisfactorily describe the experimental date taking from another work. In particular, the values of  $C_p$  and  $C_v$  are increases throughout the temperature in all presented range. At low temperatures there is a rapid increase in the value of the specific heats according to the theory of

Debye and at higher - growth trend becomes weaker and close to the Dulong-Petit limit.

*The work supported by an integrated project of MES of Ukraine (N 0113U000185).*

# **X-rays diffractometry for structure peculiarities of polymer-based nanocomposites investigations**

Gomza Yu.P., Klepko V.V

*Institute of Macromolecular Chemistry of the NASU, Kyiv, Ukraine*

The most of organic-inorganic polymer-based composites at the short-range ordering level (0.1-10 nm) are amorphous materials and at long-range ordering level (1 – 100 nm) are characterized by nearly random distribution of nanosized filler particles. The such systems are as a rule a weak-ordered ones and are characterized by hierarchy of structural levels. Conventional X-rays diffractometry as developed for determination of crystalline structure peculiarities for high-ordering mono- and polycrystalline materials are non-effective in above mentioned cases. That is why investigation of such systems demands of appropriate adaptation of the experimental X-rays diffraction methods and the data interpretation. In this report we represent the examples of application of wide angle (WAXS) and small angle (SAXS) X-rays diffractometry for structure peculiarities investigation of organic-inorganic nanocomposites.

The method of interpreting X-ray scattering data in general is based on the analysis of the scattering curve, which shows the dependence of the scattering intensity,  $I$ , on the scattering angle,  $\theta$ , or the wave vector,  $q$ .

The wide-angle X-rays scattering was used by as for primary estimation of short-ordering level – i.e. are the investigated material amorphous or partial crystalline. The second main application of WAXS for nanocomposites is the establishing of different stages of organoclay dispersion in polymeric matrix – i.e. differentiated the three canonical cases: i) phase separation; ii) intercalation, iii) exfoliation of primary inorganic sheets in polymeric matrix.

But the most informative for structure peculiarities determination for nanocomposites is the small-angle X-rays scattering. The method enables the structure peculiarities determination in the range of structural elements sizes from 1-2 to 100-200 nm. The character of the SAXS scattering curve enables us to differentiated the space-ordered nanoscale structures (the presence of discrete maxima) from disordered and fractal-like ordered (diffuse character of scattering) ones. The integral SAXS intensity in all cases of ordering is the measure of degree of microphase separation of investigated material at nanoscale level.

This approach has been successfully used for studying the structure peculiarities of the nano-sized powders-, clay minerals- and carbon nanotubes and polymer-based nanocomposites filled by them. It was established the correlation of functional characteristics of such materials (i.e. ionic conductivity and catalytic activity levels etc) and their structure peculiarities.

## Structural transformations and magnetic properties of amorphous films of Gd-Fe system

Gomza Yu.P.<sup>1</sup>, Dzyazko Yu.S.<sup>2</sup>, Ponomareva L.N.<sup>2</sup>, Nesin S.D.<sup>1</sup>, Volkovich Yu.M.<sup>3</sup>, Sosenkin V.E.<sup>3</sup>, Trachevskii V.V.<sup>4</sup>, Scherbatyuk N.N.<sup>5</sup>

<sup>1</sup> Institute of Macromolecular Chemistry of the NASU, Kyiv, Ukraine

<sup>2</sup> V.I. Vernadskii Institute of General & Inorganic Chemistry of the NASU, Kyiv, Ukraine

<sup>3</sup> A.N. Frumkin Institute of Physical Chemistry & Electrochemistry of the RAS, Moscow, Russia

<sup>4</sup> G.V. Kurdyumov Institute of Metal Physics of the NASU, Kyiv, Ukraine

<sup>5</sup> N.N. Kholodnii Institute of botany of the NASU, Kyiv, Ukraine

Organic-inorganic ion-exchangers have been obtained by means of modification of strongly acidic gel-like ion-exchange resin with zirconium hydrophosphate. The materials were investigated with methods of scanning and transmission electron microscopy, NMR <sup>35</sup>P spectroscopy, standard contact porosimetry, as well as small angle X-ray scattering. It was shown that the ion-exchangers contain non-aggregated nanoparticles of inorganic constituent and their aggregates or only aggregates. The first type of the ion-exchangers can be related to nanocomposites. Average size of the non-homogeneities in a dry polymer has been found to reach up to 16 nm [1], this is in agreement with data obtained for the swollen polymer [2]. A size of primary nanoparticles has been estimated as 18-19 nm from the dependence of natural logarithm of scattering intensity on square of wave vector. Single nanoparticles are located in clusters of the polymer matrix, which are formed from the non-homogeneities during swelling of the polymer. The aggregates, which size is up to several microns, are placed mainly in the structure defects. Composition of the inorganic particles has been determined, the highest P:Zr molar ratio as well as ratio of dihydro- and hydrophosphate groups have been found for the samples containing the aggregates. Influence of particle location on functional properties of the composites (swelling, electrical conductivity, selectivity towards Ni<sup>2+</sup>, Cd<sup>2+</sup> and Cu<sup>2+</sup> ions has been determined.

1. Yu.S. Dzyazko, L.N. Ponomareva, Yu.M. Volkovich, V. E. Sosenkin. Effect of the porous structure of polymer on the kinetics of Ni<sup>2+</sup> exchange on hybrid inorganic-organic ionites // *Russ. J. Phys. Chem. A.* – 2012. – Vol. 86. – P. 913-919.
2. L.N. Ponomareva, Yu.S. Dzyazko, Yu.P. Gomza, S.D. Nesin, T.E.Mitchenko. Structure and ion-exchange properties of organic-inorganic ion-exchangers containing nanoparticles of zirconium hydrophosphate // *Polymernii Journal.* – 2012. – Vol. 34. – P. 336-344.

## Structure peculiarities nanocomposites materials based on organic-inorganic interpenetrating polymer networks

Alekseeva T.T., Martyniuk I.S., Gomza Yu.P., Klepko V.V., Nesin S.D.

*Institute of Macromolecular Chemistry NASU, Kiev, Ukraine*

In the last decade scientific and practical interest is caused by the problem of creation of organic-inorganic hybrid materials with the use sol-gel of synthesis. The special attention is attracted by interpenetrating polymeric networks (IPN) based on different modifications of poly (titanium oxide) in connection with their unique electric, optical and chemical properties.

Structure peculiarities of simultaneous IPNs based on crosslinked polyurethane (PU) and organic-inorganic copolymer based on 2-Hydroxyethylmethacrylate (HEMA) and titanium-tetraisopropoxide ( $\text{Ti}(\text{O}^i\text{Pr})_4$ ) have been studied by SAXS method. The ratio polymer components PU/PHEMA in the initial and organic-inorganic IPN was 50/50 mass % and the molar ratio HEMA/  $\text{Ti}(\text{O}^i\text{Pr})_4$  – 4/1, 8/1, 12/1.

In SAXS curve of initial IPN (Fig., curve 1) is not observed any interference effects. Introduction of the minimal amount of  $\text{Ti}(\text{O}^i\text{Pr})_4$  leads to rise of interference peak corresponding of spatial periodicity at 9.7 nm in curve SAXS (curve 2). It is in agreement with the model of structure, where separate ( $-\text{TiO}_2-$ ) fragments were uniformly distributed on polymer matrix with formation of the space-ordered structure.

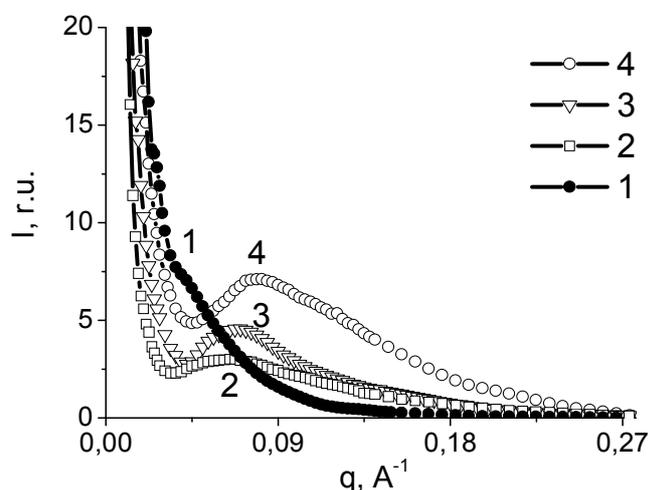


Fig. Scattered intensity  $I$  vs  $q$  for organic-inorganic IPN at variation of  $\text{TiO}_2$  content

Increasing of the Ti-component content ( $\text{TiO}_2$  – 3.4 mass %) (curve 3) caused its partially segregation, that lead to decrease spatial periodicity to 9.0 nm. At the molar ratio HEMA/ $\text{Ti}(\text{O}^i\text{Pr})_4$  – 4/1 ( $\text{TiO}_2$  – 5.6 mass %) (curve 4) enhanced the segregation processes of the ( $-\text{TiO}_2-$ ) fragments in a polymeric chain of PHEMA. As a result the spatial periodicity decreases to 7.9 nm and total level of scattered intensity rise. Such structure peculiarities are connected with crosslinking effect of the ( $-\text{TiO}_2-$ ) fragments in polymer system.

This has been confirmed by the methods of dynamic mechanical analysis and thermogravimetric analysis.

# The processes of self-organization and growth mechanisms of vapor-phase condensates based on CdTe, SnTe and PbTe

Freik D.M., Bylina I.S., Sokolov O.L. Lishchynsky I.M., Potyak V.Yu.

*Vasyl Stefanyk Precarpathian National University, Ivano-Frankivsk, Ukraine*

The processes of structure formation in the vapor-phase condensates CdTe, SnTe and PbTe attracted much attention of researchers due to the vast possibilities of their use in opto- and nanoelectronics, such as detectors hard radiation and LEDs in the visible light spectrum [1-3]. In particular PbTe is a basic semiconductor material to create active elements infrared technology and thermoelectric devices [4]. In recent years, interest has increased dramatically because of the new features that are associated with the transition of the material in the area of micro- and nanoscale. Cadmium telluride is a promising material for producing highly efficient solar cells.

For nanostructures IV-VI compounds are widely used vapor-phase vacuum technology, with particular attention was attracted by the condensation of steam quasi closed volume. Thin-film nanostructures CdTe, SnTe and PbTe obtained from the vapor phase using the "hot wall" and open evaporation in a vacuum. The process of deposition occurred on substrates of glass, ceramics, mica. The thickness of the obtained films was determined by an optical method (with optical interference pattern reflection spectra). These thin-film structures were investigated by atomic force microscopy (AFM) Nanoscope 3a Dimension 3000 (Digital Instruments USA) in the periodic contact. According to the AFM studies in addition to surface morphology and profilogram the program Gwyddion by size of nanocrystals in the lateral direction and height. The processes of self-organization and growth mechanisms.

*The work supported by an integrated project of MES of Ukraine (N 0113U000185) and by projects of FRSF State Agency for Innovation and Informatization of Ukraine. (Contracts: R54, F53, 3), NAS of Ukraine (N 0110U003689).*

1. С.А. Медведев. *Физика и химия соединений  $A^{II}B^{VI}$* . Мир, М. 624 с. (1970).
2. С.А. Колосов, Ю.В. Клевков, А.Ф. Плотников. Транспортные явления в крупнозернистых поликристаллах CdTe // *Физика и техника полупроводников*, 38(3), сс. 305-309(2004).
3. И.П. Калинин, В.Б. Алесковский, А.В. Симашкевич. *Эпитаксиальные слои соединений  $A^{II}B^{VI}$* . Изд-во ЛГУ, Л. (1978).
4. Равич Ю. И., Ефимова Б. А., Смирнов И. А. *Методы исследования полупроводников в применении к халькогенидам свинца PbTe, PbSe и PbS*. Наука, М. 384 с. (1968).

# Oscillation of thermoelectric parameters in quantum-dimensional structures of compounds IV-VI

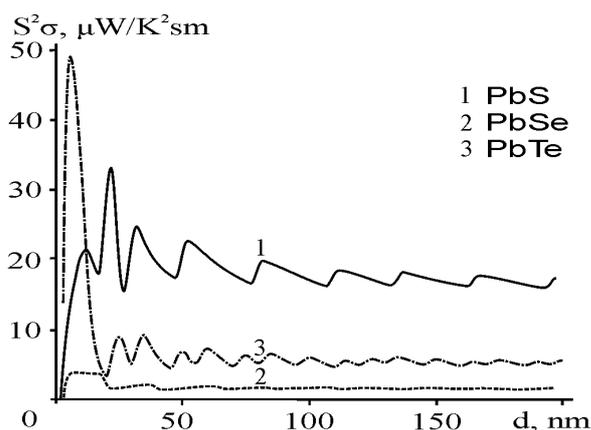
Freik D.M., Yurchyshyn I.K., Chobaniuk V.M., Potyak V.Yu.

*PreCarpathian National University, Ivano-Frankivsk, Ukraine*

The paper presents an analysis of new approaches to improve the thermoelectric parameters of nanostructures based compounds IV-VI.

Oscillation character of the thickness dependences of kinetic parameters quantum wells superlattices suggests that this behavior is due to quantum size effects associated with the restriction of movement of the main type carrier. Definition of oscillation period yielded the energy parameters of corresponding nanostructures.

Consideration of  $d$ -dependence of the Fermi energy  $E_F$  and  $z$ -component of the effective mass allowed us to obtain the corresponding dependences of the Seebeck coefficient  $S$  and electrical conductivity  $\sigma$  on the well width for nanofilms of lead chalcogenides (Fig. 1).



**Fig. 1** – Theoretical dependences of the TE power factor  $S^2\sigma$  on the width of QW for films PbS (1), PbSe (2), PbTe (3) in the model of infinitely deep potential well at  $T = 300$  K.

The number of levels below the Fermi energy is determined by  $d$ -dependence of the effective mass and actually by  $E_F$ , as well as by the well width  $d$ . The calculations take into account the change of the Fermi energy, and the change of the number of levels below it, depending on the well width. Calculating the electrical conductivity  $\sigma$  it was assumed that  $m_x^* = m_y^*$ . In the theoretical model the quantum well width was considered to be equal to the thickness of the condensate in the experimental dependences of relevant parameters. The calculation was carried out in the approximation of constant concentration and carrier mobility across all the range of well width. The values of the last were selected basing on the relevant experimental measurements. The resulting dependences of TE coefficients on the width of lead chalcogenides QW are characterized by nonmonotonic oscillating behavior (Fig. 1), what is in a good coordination with the experimental results.

## **Influence of inter-phase boundaries on charge carriers scattering mechanisms in lead chalcogenide films**

B.S. Dzundza, Ya.S. Yavorsky, A.I. Tkachuk, O.B. Kostyuk

*Vasyl Stefanyk Precarpathian National University, Ivano-Frankivsk, Ukraine*

There are executed the divide contribution of different charge carriers scattering mechanisms in the kinetic phenomena of lead chalcogenide thin films of different structural completeness on the basis of complex experimental researches and theoretical calculations.

The rules in the directed heterogeneities of the profiles of electric parameters both in annealing in vacuum and oxygen atmosphere, and grown lead chalcogenide films are define and determine. Within the framework of two-layers Petrits model the kinetic parameters of surface layers are determine [1,2].

On the base of electrical-technical conductive of poly-crystalline films model there are set the rules of time-dependence of the change of crystalline linear size in PbTe films and transport phenomena mechanisms by inter-grain boundaries that relation on thermal-electron emission.

The influence of diffuse and mirror scattering mechanisms on inter-phase boundaries, and also charge carrier scattering on the inter-grain boundaries, and dislocations of disparities was received. The surface density and dislocation radius was determine [3-5].

1. Petritz R.L. Theory of an experiment for measuring the mobility and density of carriers in the space-charge region of a semiconductor. // Physical review. – 1958. – V. 110, № 6. – P. 1254–1256.
2. Zemel J.N., Jensen J.D., Schoolar R.R. Electrical and Optical Properties of Epitaxial Films of PbS, PbSe, PbTe, and SnTe // Physical review. – 1965. – V. 140, № 1A. – C. 330–342.
3. Novoselova A.V., Zlomanov V.P. Thermodynamics and imperfections in lead chalcogenides // Current topics in material science. – 1981. – V. 7. – P. 643–710.
4. Jensen J.D., Schoolar R.B. Surfase charge transport in  $PbS_xSe_{1-x}$  and  $Pb_{1-y}SnySe$  epitaxial films // J. Vac. Sci. Technol. – 1976. – T. 13, № 4. – P. 920–925.
5. Rogacheva E.I., Tavrina T.V., Nashchekina O.N. Quantum size effect in PbSe quantum wells // Applied physics letters. – 2002. – V. 80, № 15. – P. 2690–2692.

*Work is executed within the framework of the themes of Ministry of education and science of Ukraine, №0113U000185.*

# **Magnetoplasma waves on the surface of a semiconductor nanotube with a longitudinal superlattice**

A. M. Ermolaev, G. I. Rashba

*V.N.Karazin National University of Kharkiv, Ukraine*

A two-dimensional electron gas on the nanotube surface is a convenient object for approbation of the idea that electron resonance transitions between energy levels under alternating field are accompanied by branches of collective excitation spectrum of the system. It has been shown that on a nanotube there are new modes near the frequencies of resonance electron orbital transitions. The spectra of magnetoplasma waves are related to peculiarities of the energy spectrum of electrons on a tube. The singularities of density of states on the subband boundaries are similar to those on the Landau levels in a magnetic field. So it is naturally to assume the existence of collective excitation branches spectra in the vicinity of frequencies of electron transitions between subbands, as well as oscillations of excitation spectrum reminiscent of de Haas-van Alphen oscillations. The electron energy spectrum peculiarities become manifest by the fact of their existing also without a magnetic field. The magnetic field results in Aharonov-Bohm type oscillations caused by nonconnectivity of the area occupied by electrons. The character of the energy spectrum is also manifested by the fact that with increasing the number of electron groups in different subbands the number of collective excitation spectrum branches increases.

Besides the planar superlattices, the semiconductor superlattices with a cylindrical symmetry gain widespread acceptance. The superlattices can be radial or longitudinal. These systems with an artificial periodicity along the cylindrical axis offer an opportunity to control the energy spectrum of the conduction electrons. Modern experimental techniques allow fabrication of coaxial rings made of different materials on a nanotube surface hence creating a set of potential barriers and wells. The magnetoplasma wave spectra oscillations of de Haas-van Alphen and Aharonov-Bohm types remain also in the presence of a longitudinal superlattice on the nanotube surface. The oscillation character is determined by the ratio of Fermi energy to the miniband width. At high value of this ratio, the beats are revealed on the plot of wave frequency versus tube parameters. If the ratio is small, the beats are absent.

The results given in this report allow determination of electron effective mass, tube parameters, and fundamental universal constants. Experimental observing the wave spectrum beats gives an possibility to obtain the ratio of Fermi energy to miniband width. The peculiarities of magnetoplasmon spectrum can be observed experimentally using light or electron scattering by the nanotubes with a superlattice in magnetic field.

# Production of nano-crystalline materials in hydrogen

Basaraba Yu.B.<sup>1</sup>, Zasadnyy T.M.<sup>2</sup>

<sup>1</sup> *Ivano-Frankivsk National Technical University of Oil and Gas, Ukraine*

<sup>2</sup> *Karpenko Physico-Mechanical Institute of the NASU, Lviv, Ukraine*

Nano-crystalline metallic materials have been recognized as perspective materials for a wide range of modern technologies due to their unique properties, occurring because of their mainly structural parameters, which are comparable with the interatomic distances. Among nano-crystalline materials, the investigation of which have proceed rapidly for the last two decades, hydrogen storage, in particular, metal hydrides for NiMH battery applications on the base of  $ZrCr_2$  Laves phase alloy, materials occupy an important place [1, 2].

Among the most widespread methods of obtaining metal hydride materials in the nano-crystalline state (crystallization of vapors of components of the used alloy, pouring out of the molten alloy onto a copper water-cooled rotating drum and synthesis in various mechanical mills) using hydrogen medium to obtain nano-crystalline state looks very promising.

This work presents study on the possibility of obtaining of nano-structured state in  $ZrCr_2$  metal hydride alloy using treatment in a hydrogen atmosphere. Treatment was carried out in autoclave at the hydrogen pressure of 30 atm and heating to 900°C. X-ray phase analysis was performed using diffractograms recorded on a HZG-4A diffractometer ( $CuK_{\alpha}$  – radiation). The crystallite sizes were evaluated by the broadening of peaks of X-ray powder pattern. The dimensions of domains of X-rays coherent scattering were determined by the method of approximations with the use of standard [3].

The X-ray phase analysis of  $ZrCr_2$  alloy indicates that the major phase of this alloy is hexagonal  $MgZn_2$  (C14) type Laves phase structure. After heating in hydrogen to 900°C and holding for 3 h the initial phase decomposes into a zirconium hydride ( $ZrH_2$ ) and chromium (Cr). After heating in vacuum to 900°C  $ZrCr_2$  alloy crystallizes with cubic  $MgCu_2$  (C15) type Laves phase structure. Using the approximation method was determined that the average crystallites size of 30 nm.

1. J.H. Woo, Ch.B. Jung, J.H. Lee, K.S. Lee Electrochemical characteristics of nanocrystalline  $ZrCr_2$  and  $Mg_2Ni$  type metal hydrides prepared by mechanical alloying // *J. Alloys and Compounds*. -1999.-Vol.293-295.-P.556-563.
2. M. U. Niemann, S. S. Srinivasan, A. R. Phani, A. Kumar, D. Y. Goswami, E. K. Stefanakos. Nanomaterials for Hydrogen Storage Applications: A Review // *J. of Nanomaterials*. – 2008. – Vol. 2008. – P. 1-9
3. I.I.Bulyk, Yu.B.Basaraba, V.I.Markovych. Production of functional nanocrystalline materials in hydrogen // *Materials Science*. – 2003. – Vol. 39. – P. 841 – 848.

## **Structure and electrooptical properties of 5CB liquid crystal – organomodified montmorillonite nanocomposites**

Bezrodna T.V., Chashechnikova I.T., Nesprava V.V.

*Institute of Physics NASU, Kyiv, Ukraine*

One of the actual trends in modern physics is investigations of physical properties of different heterocomposites, based on liquid crystals doped by inorganic nanoparticles of various chemical contents and geometrical shapes. These materials are used at the development of optoelectronic devices, sensor fast-response electrodes etc. The advantage of anisometric fillers (carbon nanotubes (NT), montmorillonite (MMT) clay particles) over the spherical ones is large area of contacting surface with organic media, which provides their good penetration into the liquid crystal matrix and easy reorientation under external field influence. To make the surface organophilic, MMT particles are treated with surface-active substances, which chemical contents determine affinity between components in the composites and affect their electrooptical properties. NT forms large clusters in liquid crystal media, not allowing to produce homogeneous systems. We have developed a method of simultaneous modification of the MMT surface by a surfactant and nanotubes and demonstrated that the composite of 5CB, doped with such hybrid particles possesses homogeneous structure.

Our present work deals with the investigations of composite materials based on 5CB, doped with organomodified MMT (OM) taken from three deposits, namely, Askan (OMa), Pyzhevsk (OMp) and Cherkassy (OMc). These MMT clay minerals differ one from another by dopant contents and physico-chemical properties. Cetyltrimethylammonium bromide (CTAB) is used as a surface-active substance. According to the IR-spectroscopy data, Van-der-Waals interactions are realized in all studied samples, being the strongest ones in the system with OMa particles. The affinity degree affects structure formation processes. Electrooptical parameters (memory, optical transmission) have their maximum values also in the composite with OMa. NT doping causes worsening of electrooptical properties for all composites, but increases significantly their electroconductivity. The degree of this growth depends on the MMT type. The highest electroconductivity is observed the 5CB+OMa-NT system due to the formation of a single percolation conducting network, as seen on the microphotographs from a polarizing microscope.

To summarize, the component interaction strength in the heterosystems is shown to be affected by changing not only surface-active substances, but also MMT type. This allows to obtain materials with desired electrooptical and electroconductive characteristics.

*The work has been carried out under NASU financial support (N153 and VC157 Projects).*

## Getting and some physical properties of nanoparticles of cadmium compounds

Danilevschaya N. B., Nechiporuk B.D., Yukhymchuk V. O.

*Rivne State Humanitarian University, Ukraine  
Institute of Semiconductor Physics V.S. Lashkarov NASU, Kiev, Ukraine*

Development of highly efficient methods for metallic and oxide nanoparticles becomes important in connection with the prospects of their use in the metallurgy, microelectronics and chemistry [1]. Among nanostructured cadmium compounds is particularly interesting cadmium hydroxide, which is highly stable cathode material and nanostructural forms can be used for cadmium sulfide and cadmium oxide [2].

Fine powders of cadmium compounds were obtained in a glass electrolytic electrochemical method. As a electrolyte solution used salt in distilled water (NaCl concentration value was 500 mg/l). Electrodes were made of cadmium of «ЧДА». To powder the electrolytic cell used stabilized constant voltage source. Electrolyte temperature during the experiment was 98 °C and current density  $2,75 \cdot 10^{-2} \text{ A/cm}^2$ .

After electrolysis the optical absorption spectra by spectrophotometer Carry-50 were investigated at room temperature. From the absorption spectra calculated dependence of  $(\alpha h\nu)^2$ , where  $\alpha$  – absorption coefficient, of the photon energy  $h\nu$ . Last dependency contains several straight sections indicating a mixture of compounds.

X-ray studies were carried out on a X-ray powder diffractometer ДРОН – 4 using Cu  $K_\alpha$  radiation at room temperature. They showed that these compounds were obtained cadmium: cadmium hydroxides hexagonal ( $\beta$ -Cd(OH)<sub>2</sub>) and monoclinic modifications ( $\gamma$ -Cd(OH)<sub>2</sub>) and cadmium carbonate the size of the order of 19 nm for  $\gamma$ -Cd(OH)<sub>2</sub>, 21 nm for  $\beta$ -Cd(OH)<sub>2</sub> and 22 nm for CdCO<sub>3</sub>.

Differential thermal analysis (DTA) was carried out at the facility which consist of heating furnace “Termodent” unit computer desk, power amplification thermocouple (Pt/Pt-Rh) made to basic "И-102" precision the thermostat to draw. A heating rate of  $10 \text{ }^\circ\text{C min}^{-1}$  were used. DTA a conclusion about the possibility of cadmium oxide during annealing at temperature above 600 °C. X-ray studies CdO given the size of the resulting nanocrystals above 40 nm.

1. Ф.Г. Рутберг, В.В. Гусаров, В.А. Коликов, И.П. Воскресенская, В.Н. Снегов В.Н., А.Ю. Стогов, И.А. Черепкова ЖТФ. 2012. Т. 82. вып. 12. С.33.
2. А.С. Ворох, Н.С. Кожевникова Доклады академии наук. 2008. Т.419. №1. С.58.

## Wagner-Vengrenovich distribution

Ivanskii B.V., Stasyk M.O., Yarema S.V., Panko I.I.  
*Yuriy Fedkovych Chernivtsi National University, Ukraine*

The Ostwald's ripening (OR) is the final stage of formation of a new phase as a result of phase transformation, such as decay of oversaturated solid solutions. Nanoclusters or nanocrystals (NC) of new phase having different sizes interact through the Gibbs-Thomson effect that results in dissolution of small NC and growth of large ones.

Diffusion growth of NC under matrix of volume diffusion (*ls*-mechanism) has been firstly studied by Lifshitz and Slyozov [1]. Wagner has showed later [2] that beside of diffusion mechanism, another mechanism of NC growth is possible, which is governed by the rate of formation of chemical connections (chemical reaction) at NC surface. The theory developed in the cited papers is referred to as the *LSW* theory. Practical verification of this theory shows that in many cases it is proper for description of experimental data on temporal behavior of the mean NC size and the NC size distribution function, while in other cases the *LSW* theory must be refined. In this connection, NC growth is considered in papers [3] as a result of combined action of two growing mechanisms, diffusion and Wagner's ones.

However, in presence in a matrix of free dislocations interacting with elastic fields of NCs, or in presence of NCs located at dislocation network, just dislocation diffusion predominates rather than matrix one.

In the paper [4] we studied the process of coarsening of nanoclusters or nanocrystals (NC) is investigated for the case when cluster growth (dissolution) is governed simultaneously by both diffusion along dislocation pipes and the rate of formation of chemical connections (chemical reaction) at cluster surface, *viz.* the Wagner's growing mechanism [4]. For that, the total flow of atoms to (from) a cluster is represented by two parts, *viz.* diffusion part and Wagner (kinetic) one. The dependence of the rate of growth of NC on the ratio of the parts of the total flow has been determined as well as the NC's size distribution function referred to as the Wagner-Vengrenovich distribution. Computed distribution is compared with experimentally obtained histograms.

1. I.M. Lifshitz and V.V. Slyozov. On kinetics of diffusion decay of oversaturated solid solutions// JETP. -1958. –Vol.35. –P.479-492.
2. C. Wagner. Theorie der Alterung von Niederschlagen durch Umlösen (Ostwald Reifung)// Zs. Electrochem. -1961. -Vol.65. -P.581-591.
3. R.D. Vengrenovich, B.V. Ivanskii, A.V. Moskalyuk. Generalized Lifshitz-Slyozov-Wagner distribution// JETP. -2007. -Vol.131. -P.1040-1047.
4. Bohdan V. Ivanskii, Anatolii V. Moskalyuk, Sergey V. Yarema, Igor I. Panko, and Miroslav O. Stasyk. Wagner-Vengrenovich Distribution// ISRN Nanomaterials. -2013. -Vol.2013. -651576 (8 pages)

# Mechanism and kinetic of formation of ZnO nanocrystals from supersaturated solution

Vengrenovich R.D., Panko I.I.

*Yuriy Fedkovych Chernivtsi National University, Ukraine*

A generalized Lifshits-Slezov-Wagner distribution [1] for nanoclusters or nanocrystals growth according to two parallel mechanisms (Wagner and diffusion) has been used to explain a series of experimental histograms, which cannot be correctly related to the Wagner or the Lifshits-Slezov distribution separately. A process of the nanoclusters growth at the Ostwald ripening stage of the phase transformation in the solid systems can be correctly described using the generalized distribution of Lifshits-Slezov-Wagner.

The Ostwald ripening stage is also present in a process of formation of a new semiconducting nanoclusters phase (phase transformation of the first type) during chemical synthesis of nanoclusters in the liquid medium. That is why the Lifshits-Slezov-Wagner theory can be used for analysis of the mechanism and kinetics of the *ZnO* nanoclusters formation from supersaturated solutions. The theory should be modified taking into account possible joined influences of both (Wagner and diffusion) mechanisms on the process of the growth of the nanoclusters.

A metal oxide semiconductor *ZnO* has been chosen as a model for investigation of the mechanism and kinetics of NCs formation from supersaturated solutions based on the information from. It is one of the most universal and multipurpose semiconductors with optoelectronic properties, which is widely used in designing of some optoelectronic devices.

As a result, the growth of the *ZnO* nanoclusters can be controlled by any of the Wagner's or diffusion mechanisms.

The growth rate constants were estimated by means of comparison between experimental and theoretically calculated temporal changes in the average radii or average diameters of nanoclusters. These constants can be used to optimize technological conditions for synthesis of nanoclusters from supersaturated solutions.

A method of evaluation of an important energetic parameter – specific surface energy on the nanocluster/solvent interface is also proposed in the paper.

1. R.D. Vengrenovich, B.V. Ivanskii, A.V. Moskalyuk. Generalized Lifshitz-Slyozov-Wagner distribution// JETP. -2007. -Vol.131. -P.1040-1047.
2. Roman Vengrenovich, Bohdan Ivanskii, Igor Panko, and Miroslav Stasyk. Size Distribution of Nanoparticles of ZnO and SnS in the Frame of Lifshits-Slezov-Wagner Modified Theory// J. Phys. Chem. C. -2013. – Vol.117. –P. 13681-13687.

## To the derivation of Thomson's equation

Vengrenovich R.D., Ivanskii B.V., Yarema S.V., Stasyk M.O.

*Yuriy Fedkovych Chernivtsi National University, Ukraine*

Pressure of saturated gas at flat surface of a liquid,  $P_\infty$ , and solubility (concentration),  $C_\infty$ , are connected to each other by the relation:

$$\frac{P_\infty}{C_\infty} = kT. \quad (1)$$

Pressure of saturated gas above curved (in part convex) surface,  $P_r$ , is larger than above flat one ( $P_r > P_\infty$ ). For that, relation (1) between  $P_r$  and  $C_r$  is conserved:

$$\frac{P_r}{C_r} = kT. \quad (2)$$

Bending of liquid surface of itself takes place due to action of additional Laplace pressure,  $\Delta P$ , directed inwards liquid. Work  $\Delta A$  on bending one mole of liquid,  $V_\mu$ , is equal to:

$$\Delta A = V_\mu \cdot \Delta P. \quad (3)$$

This work may be determined through the work of isothermal expansion of one mole of saturated gas from pressure  $P_\infty$  to pressure  $P_r$ :

$$\Delta A = RT \ln \frac{P_r}{P_\infty}, \quad (4)$$

or:

$$V_\mu \cdot \Delta P = RT \ln \frac{P_r}{P_\infty}, \quad (5)$$

so that one has:

$$C_r = C_\infty \ell^{\frac{v_m \cdot \Delta P}{kT}}, \quad (6)$$

where:  $C_r = \frac{P_r}{kT}$ ,  $C_\infty = \frac{P_\infty}{kT}$ ,  $V_\mu = N_A \cdot v_m$ ,  $k = \frac{R}{N_A}$ ,  $R$  – the gas constant,  $N_A$  – the Avogadro number,  $v_m$  – volume of an atom, and  $C_r$  – concentration of saturated vapour above curved surface of liquid.

Eq. (6) is the generalized form of the Thomson's formula that can be applied to determine of solubility (concentration)  $C_r$  of atoms of solved matter at the interface cluster-matrix (cluster-substrate).

We obtained Thompson formula for the spherical clusters, segment-like and pyramidal-like islands.

# Ellipsometry study of nanocomposite materials based on Co-Fe-B

Polianska O.P., Stashchuk V.S.

*Taras Shevchenko National University of Kyiv, Ukraine*

The nanocomposite's optical properties were studied in this paper. The composite samples:  $(\text{Co}_{41}\text{Fe}_{39}\text{B}_{20})_x+(\text{SiO}_2)_{100-x}$  ( $x = 100\%$ ,  $56\%$ ,  $41\%$  and  $33\%$  at.) are amorphous metal alloy inclusions sized approximately 10 nm, distributed chaotically in an amorphous dielectric substrate. Ion-beam sputtering were used to obtain the metal alloy – dielectric composite nanostructures. The angular dependences of the samples' optical properties were carried out in a range of angles of incidence  $\varphi = 50\div 80$ , that includes the principal angle of incidence. A JIT-56 He-Ne laser was used as source of radiation ( $\lambda = 632.8$  nm).

Based on the obtained data it was shown that the principal angle of the studied samples depends on the metal content of the composite. Optical properties calculated basing on these data was found to depend strongly on the angle of incidence, which was attributed to the influence of the surface layer, removed afterwards by chemical etching. A 15% water solution of sulphuric acid was used for these samples. The ellipsometric parameters  $\Delta$  and  $\psi$  measurements have shown that the optimal etching time for these composites was 7 seconds. In this case the dependences of optical properties, such as the refraction and absorption indices  $n$  and  $\chi$ , dielectric permittivity  $\varepsilon$  and optical conductivity  $\sigma$ , on the incidence angle  $\varphi$  are described by smoother curves than the original samples. It indicates a notable improvement in composites' structure near the optical surface. The ellipsometric parameters'  $\Delta$  and  $\psi$  dependences on the incidence angle  $\varphi$  were studied for  $(\text{Co}_{41}\text{Fe}_{39}\text{B}_{20})_x+(\text{SiO}_2)_{100-x}$  nanocomposite structures in amorphous state with different contents of the metallic component has revealed that such dependences are described by smooth curves for all samples. With the decrease in the metallic component content in the composite the principal angle of incidence increases greatly due to a gradual transition from electron tunneling to the hopping mechanism of electronic conduction.

# Synthesis and electronic structure of the nanodispersed calcium hydroxyapatite

V.L. Karbivskyy, N.A. Kurgan

*G.V. Kurdyumov Institute for Metal Physics NASU, Kiev, Ukraine*

This paper presents the results of study of the electronic structure and morphology of nanodispersed calcium apatite - chemical analogue of bone mineral substances obtained using biogenic synthesis with varying of the synthesis parameters. For varying sizes of nanoparticles the obtained calcium hydroxyapatite powders at the last stage of synthesis washed in different organic substances: water, ethanol, acetone, glycerol, isopropanol. In addition, samples were annealing at various temperatures (500 °C, 700 °C, 900 °C, 1000 °C),

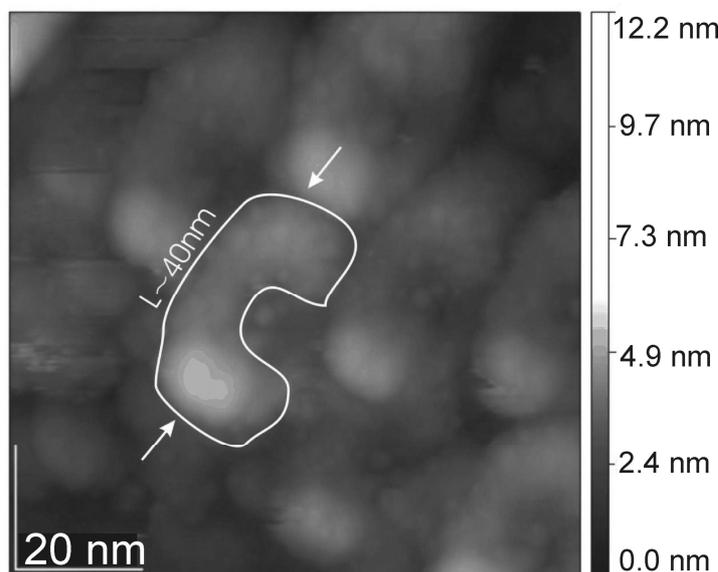


Fig. 1. AFM image of the HAP

which allowed to explore the complete formation process of the calcium hydroxyapatite nanoparticles and nanoagglomerates. Specimens diagnostic was carry out using X-ray diffraction, atomic force microscopy, and XPS spectroscopy. Study of electronic structure and morphology showed the dependence of particle size calcium hydroxyapatite powders on the synthesis parameters. Analysis of XPS spectra showed significant changes in an oxygen environment of calcium and phosphorus atoms by changing the apatite particle size, which shown in decrease of binding energy  $1s$  electrons of oxygen atoms. Particle size, when used water in the final stage of apatite synthesis and annealing at 700 °C for 2 h was 40 nm (Fig. 1). The sizes of apatite particles were very close to those in natural bone. However, the particles in natural bone have needle shape, and the “horseshoe” shape was due to the drying in the synthesis process. The ends of the particles were not fixed, which was caused by the surface tension. For example, by drying the particles in acetic acid remained needle-shaped.

# Local negative permeability and detection of nonlinear excitations in nanomagnetic metamaterials

Charkina O.V., Bogdan M.M.

*B.Verkin Institute for Low Temperature Physics and Engineering of NASU, Kharkiv, Ukraine*

Recently it has been shown theoretically and experimentally that novel magnetic metamaterials can demonstrate unique properties including the negative magnetic permeability. Electromagnetic excitations in one- or two-dimensional systems of the inductively-connected split ring resonators with nonlinear elements (diodes) are described by discrete equations which possess oscillating localized solutions, the discrete breathers [1]. It has been numerically found that in a small region of a few constants of the superlattice, where the discrete breather is excited, the magnetic response can be negative. Unfortunately an analytical description of nonlinear excitations in this highly discrete case meets evident difficulties and is not consistent with continuum definition of the magnetic permeability.

In the present contribution we propose the modification of the low-dimensional nanomagnetic metamaterials by including the additional capacitance connection between the nearest-neighbouring split ring resonators. Then the array of coupled split ring resonators can be consequently described in the long-wave limit by the regularized dispersive nonlinear Klein-Gordon equation [2] for the charge variable. It is found that in such nanosystems the high-frequency magnetic field excites dynamic solitons on the "pedestal", stable breathers, oscillating in opposite phase with respect to the background of uniform oscillations, that means the existence of finite regions with the negative magnetic permeability in the system. Using numerical simulations the values of the amplitude and frequency of the external pumping and physical parameters of the system are determined at which regimes of breather oscillations become stable and the effect of the local negative permeability in the metamaterial takes place. Supplemented by a medium with the negative permittivity such a system constitutes a "left-handed" metamaterial in which the regions with the breather excitations are transparent to electromagnetic radiation. Due to this effect the breather excitations can be detected and visualized in nonlinear metamaterials.

*This work was supported by the NASU project №4/13-H "Quantum phenomena in nanosystems and nanomaterials at low temperatures".*

1. N.Lazarides, M.Eleftheriou, G.P.Tsironis. Discrete breathers in nonlinear magnetic metamaterials// Phys.Rev.Lett. -2006. -Vol.97. -P.157406-1-157406-4.
2. M.M.Bogdan, O.V.Charkina. Dynamics of bound soliton states in regularized dispersive equations// Low Temp.Phys. -2008. -Vol.34. -P.564-570.

## ***Effect of carbon concentration on the crystallinity of polymer matrix in fluoroplastic/polyethylene-carbon composites***

Revo S.L., Lozovyi F.V, Ivanenko K.O.<sup>1</sup>, Sementsov Yu.I.<sup>2</sup>, Dong Zhanmin<sup>3</sup>

<sup>1</sup> *Taras Schevchenko National University of Kyiv, Ukraine*

<sup>2</sup> *O. O. Chuiko Institute of Surface Chemistry of NASU, Kyiv, Ukraine*

<sup>3</sup> *Tsinghua University Beijing, China*

The crystallinity degree ( $\chi$ ) of polymers and, thereafter, their mechanical and electrical characteristics depend on many factors. The most substantial factor, is the cooling rate of material after its sintering. The composite density varies from 1,57 to 2,27 g/cm<sup>3</sup> upon different cooling rates.

Here, the effect of thermally exfoliated graphite (TEG) and multiwall carbon nanotubes (MWNT) on the crystallization processes in polymer matrix of nanocomposites (NC) has been investigated. It was shown that the sintering of the NC with the subsequent cooling under pressure ( $P$ ) < 40MPa provides the increasing of crystallinity degree of fluoroplastic matrix up to 90%. The filler content poorly influences the fluoroplastic matrix crystallinity below the percolation threshold ( $C = 4$  vol.%). The value of  $\chi$  at low pressure ( $P = 1,5$  MPa) is much lower, e.g.  $\chi = 55\%$  at  $C = 5,5$  vol.%.

The crystallinity degree of polymer matrix in NC FP-TEG-MWNT is twice as lower as for NC FP-TEG under the similar sintering conditions. In case of NC polyethylene (PE)-TEG the crystallinity degree of polymer matrix monotonically increases from 86 to 89% with TEG content increasing up to 7 vol.%.

The crystallinity degree of polymer matrix depends on several factors such as the method of manufacturing, the character of filler distribution in a bulk of the composite, the adhesion between matrix and filler. For example the crystallinity degree of PE in NC PE-MWNT manufactured by sintering in the vacuum mold decreases from 0,85 to 0,80 vol.%, while for the same composite produced by hot extrusion it increases from 0,65 to 0,70 vol.% at the same filler content.

*Financial support from State fund for fundamental researches (Grant №M/76-2013) is gratefully acknowledged.*

## ***On the Nanoclusters Formation in Metallic Systems***

N.A. Korynevskii<sup>a,b,c</sup>, V.B. Solovyan<sup>a</sup>

<sup>a</sup>*Institute for Condensed Matter Physics, NASU, Lviv, Ukraine*

<sup>b</sup>*Lviv Polytechnic National University, Ukraine*

<sup>c</sup>*Institute of Physics, University of Szczecin, Poland*

The problem of theoretical and experimental study of nanosystems is one of the most topical both due to its fundamental role in the modern condensed matter physics investigations as well as the possible base of different technical applications [1]. Nanosystems are a prominent example of a low dimensional objects where a size effects (difference between bulk and surface properties play an essential role) are important.

The goal of the present paper is to demonstrate the possibility of some statistical model for nanoparticle system description. The model is based on the taking into account the particle-particle interactions and the external medium influence only. For the ground thermodynamic potential calculation the Ising-type Hamiltonian and the lattice gas model are exploited. The analytical description of the finite size metal nanoparticles formation in the homogeneous “infinite” phase is proposed. The finite size nanoparticles had appeared only due to the interaction of surface particles with the environment.

For experimentally observed physical systems description [2] the proposed theory used only one fitting parameter, which is responsible for temperature of nanoparticle state appearing. The stability of nanoparticle phase state is proved by the comparison of its specific energy with that of homogeneous state. The problem of relatively small (in order of few metal atom radius) of nanoparticles and its physical properties in this case will be a subject of the next investigations.

1. G. Schmidt, *Nanoparticles: From theory to application*, John Wiley and Sons, 2011, 500p.
2. D. Pomogailo, A.S. Rozenberg, I.E. Ufland, *Metal nanoparticles in polymers*, Chemistry, Moskow, 2000, 672 p. (in Russian).

# Luminescence and structural studies of CdI<sub>2</sub> crystals with nanocrystalline PbI<sub>2</sub> inclusions under high-energy excitation

I. M. Bolesta<sup>1</sup>, N. V. Gloskovska<sup>2</sup>, I. M. Rovetskyj<sup>1</sup>

<sup>1</sup> *Ivan Franko Lviv National University, Lviv, Ukraine*

<sup>2</sup> *Bogolyubov Institute for Theoretical Physics, NASU, Kyiv, Ukraine*

In the recent years layered crystals of cadmium iodide with isomorphic lead iodide inclusions have been the subject of intensive investigation as nanocrystalline ionizing radiation dosimeters.

Luminescence properties of CdI<sub>2</sub>-PbI<sub>2</sub> crystals obtained by diffusion from the gas phase and grown from the melt by Bridgman-Stockbarger method under synchrotron excitation at 9 K are examined in the present work. Surface structure of the crystals was analyzed using atomic force microscopy (AFM). Besides, nuclear quadrupole resonance (NQR) study of <sup>127</sup>I isotope of these crystals was undertaken.

PbI<sub>2</sub>-containing CdI<sub>2</sub> crystals, grown from the melt, exhibit luminescence peaks at 3.39, 2.39, 2.14, 1.87 and 1.69 eV. In the crystals, synthesized by the method of diffusion, 3.39, 2.14 and 1.69 eV bands are absent. Comparison of these spectra with photoluminescence characteristics of the crystals and the results of the AFM and NQR, has allowed to establish, that the structure of crystals grown from the melt is more perfect. Nanocrystalline PbI<sub>2</sub> inclusions in the synthesized from the gas phase CdI<sub>2</sub> crystals possess primarily 2H-polytype modification and crystals, grown from a melt, are of 4H. The possible models of luminescence centers are discussed.

## Research of diffusive processes is in the polymeric nanocomposites

Kolupaev B.B., Klepko V.V., Lebedev E.V., Gud V.M.

*Institute of Macromolecular Chemistry of the NASU, Kyiv, Ukraine*

Considerable scientific interest represents research of absorption of water steam by linear flexible polymers and heterogeneous systems (HGS).

In this case to describe diffusion by Fick's classical laws not absolutely correctly. In this case it is necessary to consider abnormal process of change of coefficient of diffusion ( $D$ ) in the form of "conditional Fick" interactions.

The diffusion equation for the systems, created on the basis of flexible polymers, in a look is considered:

$$\frac{dD}{dx} + P(x)D = Q(x), \quad (1)$$

where  $C$  - concentration of water steam;  $P(x) = \left( \frac{\partial^2 C}{\partial x^2} \right) / \left( \frac{\partial C}{\partial x} \right)$ ;

$$Q(x) = \frac{\partial C}{\partial t} / \frac{\partial C}{\partial x}.$$

The task (1) for an unlimited plate is solved under entry  $C(x,0) = 0$  and limit conditions on its surface  $C(h,t) = C(-h,t) = C_0 = \text{const}(t > 0)$ . It is as a result shown that:

$$C(x,t) / C_0 = 1 - \sum_{i=1}^{\infty} A_i \cos a_i \frac{x}{h} \exp(-a_i^2 F), \quad (2)$$

where  $A_i = \frac{2}{a_i} (-1)^{i+1}$ ;  $a_i = (2i - 1) \frac{\pi}{2}$ ;  $F = Dt/h^2$  - Fourier's criterion.

It is found out that  $D$  of water steam in HGS is described by the equation:

$$D_i = D_0 \exp \left( - \int_{h_i}^{h_{i+1}} P(x) dx \right) + \exp \left( - \int_{h_i}^{h_{i+1}} P(x) dx \right) \left( \int_{h_i}^{h_{i+1}} \left( \frac{\partial C}{\partial t} \right) / \left( \frac{\partial C}{\partial x} \right) \exp \left( - \int_{h_i}^{h_{i+1}} P(x) dx \right) dx \right) \quad (3)$$

where  $C_i; C_{(i+1)}$  - concentration of water steam in a point  $i$  and  $(i+1)$  respectively at any moment  $t$  with  $C_i \approx C_{(i+1)} = C(x,t)$ .

The analysis (3) for PVC-systems which are filled nanodisperse powders of copper is carried out. Powders are received by a method of electric explosion of the conductor. Maintenance of a naponitel (0 ÷ 0,10) vol.%, with  $\varphi = 13$  nm. Change of size of  $D(x,t)$  with  $h$ ,  $C$  indicates abnormal diffusion of water steam in HGS. These changes are caused by structural changes of a composite in the course of diffusion.

# Position dependent effective mass of carriers and energy states of periodic nanoscale heterosystems

Voznyak O.M.

*Vasyl Stefanyk Precarpathian National University, Ivano-Frankivsk, Ukraine*

The practical availability of the semiconductor's heterostructures, superlattices, systems of quantum wells, etc. stimulates the consideration of problems of physical systems, where effective mass of carriers is the function of their coordinates. Except a purely practical significance, there are also important common physical issues appearing during the consideration of the systems with position dependent mass, which is associated with ordering of coordinate and momentum operators in the Hamiltonian, because the mass depending on coordinates does not commutes with momentum operator in the kinetic energy. The proposed option (see work [1]) for constructing such Hamiltonian assumes that Hamiltonian is the product of four consecutive functions, which are represented via square root of function of the mass and two momentum operators. We shall use it for one-dimensional case when both the wave function and mass depends only on one coordinate. Some models for describe of nanoscale heterosystems was investigated in paper [2], where both mass and potential functions are considering as piecewise functions of coordinates.

In present paper we use the method based on factorization of the Hamiltonian, i.e. representation of Hamiltonian as the product of the momentum operator and some operator which is referred as superpotential for the studying the systems, where effective mass of the electrons depends on the coordinates. Using the superpotential for generating periodic potentials, a few cases have been found, where for a given mass depends on the coordinates exists exact solutions. We examined the case of non-singular periodic potentials of the particle with position dependent mass, which are periodic function of the coordinates too on the base of different superpotentials and functions for describe of mass dependence on the coordinate. The exact solutions were found for the case of non-singular superpotential, and for the case of singular superpotential with poles of the first order only. It is interesting that function for describing mass dependence on the coordinates always has smooth behavior. Also we have considered the case of constant potential and have found the dependencies, which provide exact solutions. It was shown, that mass dependence on the coordinates provides existence of the delocalized states in the case of particle moving in the field of constant potential.

1. Levy-Leblond J. M., Position-dependent effective mass and Galilean invariance //Phys. Rev.A. – 1995. – v.52. – p.1845.
2. Levy-Leblond J. M., Elementary quantum models with position dependent mass// Eur.J. Phys. – 1992. – v.13. – p.215.

## Дослідження акустичних властивостей наноінаповнених гнучкоіанцюгових полімерних систем

Левчук В.В., Колупаєв Б.С., Максимцев Ю.Р.

*Рівненський державний гуманітарний університет, Україна*

Комплекс унікальних властивостей композитів, які містять наночастинки, обумовлює інтенсивне їх дослідження та використання. При цьому, залишаються недослідженими системи на основі гнучкоіанцюгових полімерів, інаповнених нанодисперсними металами.

Досліджено концентраційну і температурну залежність величин швидкостей поширення поздовжньої ( $v_l$ ) та поперечної ( $v_t$ ) ультразвукових хвиль та відповідних їм коефіцієнтів поглинання ( $\alpha_l, \alpha_t$ ), дійсних та уявних величин в'язкопружних модулів деформацій ( $E', E''$ -модуль Юнга,  $\mu', \mu''$  - модуль зсуву,  $k', k''$  - модуль об'ємного стиску) наноінаповнених гнучкоіанцюгових систем.

Встановлено, що лінійної залежності між відповідними характеристиками акустичних та в'язкопружних властивостей систем (ПВХ, ПVB, ПС, ПММА) та вмістом нанорозмірних частинок Си в діапазоні концентрації  $0 < \varphi < 1$  об.% не спостерігається. При зростанні температури має місце зменшення величини в'язкопружних модулів деформацій. Максимальні зміни цих величин притаманні для металонаноккомпозитів із вмістом нанодисперсного інаповнювача 0,3 об.% та 0,5 об.% Си. Характерно, що величини в'язкопружних властивостей композицій, величини поздовжньої і поперечної ультразвукових хвиль, досліджені в широкій області температур ( $273 \text{ K} < T < T_g + 10 \text{ K}$ ), з підвищенням температури зменшуються. Однак для металонаноккомпозитів із вмістом інаповнювача 0,3 об.% та 0,5 об.% характерні максимальні значення швидкостей поширення поздовжньої та поперечної ультразвукових хвиль порівняно з полімерними системами із іншим вмістом інаповнювача. Показано, що між в'язкопружними та теплофізичними властивостями гетерогенних полімерних систем існує кореляційний взаємозв'язок. Аналіз температурної залежності  $\alpha_l, \alpha_t$  досліджених композицій показує, що максимум дисипативних втрат енергії елементами структури композицій спостерігається в області температурних  $\beta$ - та  $\alpha$ -переходів, положення та величину яких можна інапряму регулювати вмістом наноінаповнювача. Вказані шляхи практичного використання композитів як поглиначів акустичної енергії в широкому діапазоні частот ( $20 \div 10^6$  Гц).

## Thermal behavior of poly-3,4-ethylenedioxythiophene doped with inorganic nanoclusters

Konopelnyk O.I., Aksimentyeva O.I., Opaynych I.Ye., Horbenko Yu.Yu.

*Ivan Franko National University of Lviv, Ukraine*

The regularities of charge transport in hybrid nanocomposites of poly-3,4-ethylene dioxythiophene (PEDOT) doped with inorganic nanoclusters - multi-layer carbon nanotubes (MWCNT), ferric (III) chloride and ferricyanide  $K_3[Fe(CN)_6]$  have been studied. It is shown that in the temperature range of 293 - 373 K the conductivity of the composites has activated nature and is well described by an exponential equation. Doping of PEDOT with carbon nanotubes off their content of 1-2% leads to a decrease in the resistivity of the composite is almost an order of magnitude and activation energy of conductivity decreases with 1.5 times. For samples of PEDOT doped with ferric nanoclusters the increasing of energy barrier for charge transport was found. Parameters of conductivity calculated using the hopping model showed that  $T_0$  varied from  $22.2 \cdot 10^3$  K (PEDOT- $FeCl_3$ ) up  $15.1 \cdot 10^3$  K (undoped PEDOT) and  $8.26 \cdot 10^3$  K (PEDOT-MWCNT). The value of the activation energy of conductivity calculated using the band model, correlates well with the change of the parameter  $T_0$  and has the lowest value for the PEDOT composites with MWCNT. These facts can explain by lowering the energy barrier for charge transport for PEDOT chains and greater length of charge localization in the case of composites PEDOT -MWCNT.

The compact uniform nanofilms of PEDOT on the indium-tin-oxide (ITO) substrates obtained by layer-by-layer assembling [1] are characterized by absorption at 380-390 nm indicates the existence of localized polarons, and broad band at 700-800 nm attributed to vibronic coupling indicated the inter-chain  $\pi$ -stacking interaction of thiophene rings. Doping of the polymer with  $K_3Fe(CN)_6$  complex decreases the intensity of the absorption spectra. These films exhibit sensitivity to temperature. Exposure films at 323 K resulted in decrease in the intensity of both absorption bands of the spectrum, which can be explained by an increase in chain mobility leading to disturbances in the conjugation system. It is interesting that thermal-induced changes in coloring and absorption are reversible, but recovery of film lasts about 48 hours.

The influence of temperature on the parameters of conductivity and absorption spectra suggest that the charge transport occurs because dominated by hopping and phonon-induced delocalization in the disordered regions, or even tunneling between metallic islands. The thermo-optical characteristics of PEDOT have been depending on the morphology and the presence of inorganic nanoclusters in the polymer chain.

1. O.I. Konopelnyk, O.I. Aksimentyeva, V.P. Dyakonov, et al. // Functional Materials, 2013. Vol. 20, N 2. P. 248-252.

# Electronic properties of metals with disordered system cylindrical nanosized volume-filling defects

Marenkov V.I.

*Odessa National I.I. Mechnikov University, Ukraine*

Effect of system volume filling defect (SVFD) arising in a metal sample due to uncontrolled or purposeful action in the stage of its manufacture on the effective electronic properties is essential for a significant redistribution of carriers between the VFD-subsystem and base metal (BM) matrix. Investigation of functional dependencies effective Fermi level carriers in nano-structured metal samples is important for aerospace technology and create nanosensors based porous materials [1].

The paper proposes a new method for determining the effective medium volume electronic parameters of samples heat-resistant metals with nanoscale SVFD, based on a statistical approach plasma "quasi-neutral cells" [2]. The main point of the theory is the concept of instantaneous cell electroneutrality (CE) that its allocated simply connected element of the extremum surface electrostatic potential. Statistical cell electroneutrality in the base metal of the cylinder filling defect volume is at least averaged over the ensemble of realizations of the spatial domain of BM, which fully retains its own separate volume defect. By solving electrostatic problems for efficient local distribution of space charge and local self-consistent electrostatic potential in cylindrical filling defect volume distributed in disordered matrix BM derived analytical equations that relate these distributions with local parameters of electronic micro-inhomogeneous metal.

The dependence of the effective Fermi level carriers in inhomogeneous samples heat-resistant metal with a system of cylindrical filling defect volume on temperature, concentration and the geometric size of subsidiaries and dependent companies, electronic and dielectric characteristics of the metal. In computer experiments were obtained and analyzed data on functional dependencies electrochemical potential carriers of resistant metals with multiple filling defects cylindrical volume of nano- and mesoscopic dimensions of the defining parameters. It is noted good agreement between theory and data known from literature experiments.

1. Marenkov V.I. Local electrostatic field and carrier density in the heat-resistant metals with regular matrix of volume-filling nano-defects.-XIV ICPTTFN, 20-25 May, 2013 . - Materials. - Ivano-Frankivsk, Ukraine. - 2013 . - P 317 - 318.
2. Marenkov V.I. Manifestation of Polarization Effects in Dusty Plasma // Journal of Molecular Liquids. - 2005 , Vol. 120.- P.181 - 184.

# Electrochemical fabrication of Zinc oxide nanoparticles

<sup>1</sup>Gaevskiy V.R., <sup>2</sup>Nechyporuk B.D., <sup>2</sup>Novoselets'kyi N.YU. <sup>1</sup>Rudyk B.P.

<sup>1</sup>*National University of Water Management and Nature Resources Use of Rivne, Ukraine*  
<sup>2</sup>*State Humanitarian University of Rivne, Ukraine*

ZnO has a direct wide bandgap with energy of 3.37eV, which makes it transparent in visible light and gives an ability to create UV optical electronic devices. During the recent 20 years the research to develop methods of obtaining nanoparticles of zinc oxide has been conducted and different shapes of nanocrystals have been obtained. We used a hydrothermal electrolytic method of fabrication of zinc oxide nanoparticles which is given in [1]. The electrolysis was conducted using chemically pure Zn electrodes, as the electrolyte was a solution of NaCl (500mg/l) in deionized water. After the process, the white powder was obtained. XRD pattern corresponds to standard JCPDS 36-1451, and shows that this is a ZnO powder with the hexagonal wurtzite structure. The electrolyte opalesced after the long period of fabrication, so optical properties of an after process electrolyte were studied on spectrophotometer Carry-50 at room temperature. Results were predictable – electrolyte absorbs UV-light and transparent in visible light. It means that the electrolyte contains floating ZnO nanocrystals.

The shape and dimensions of the crystals were studied from SEM images. ZnO crystallized into the flower-like shape, which is typical for ZnO, when rods grow from one center, creating a ‘flower’. Average dimensions are: the diameter of the flower is 1.5 $\mu$ m, the rod has the diameter 0.23 $\mu$ m and length 0.77 $\mu$ m.

The room temperature PL spectra showed that ZnO has all well-known peaks UV (band gap) and visible (dopping band): green (500-530nm), yellow-orange (590-620nm) and very weak red (760-780nm) emission bands.

After annealing PL showed blue-shift of the UV band and red-shift of the visible band with decrease of its halfwidth, the intensity of the peaks grows, and it depends on the annealing temperature, on 700°C intense of the UV band increased by 3 times.

Some of the samples were created with air pumping through the electrolyte during the fabrication. PL spectra shows lesser intense of visible emission and stronger UV emission compare to nonpumping samples. It can be explained by the decrease of oxygen vacancies which are centers of visible luminescence. After annealing PL emission considerably grows, and UV band shifts to shorter wavelengths.

1. Ю.П. Лаворик, Б.Д. Нечипорук, М.Ю. Новоселецький, Б.П. Рудик, В.В. Філоненко, О.В. Парасюк, Патент на винахід №92078, МПК С22В19/00, С01Г9/00, 2010.

# Діелектричні та оптичні властивості кристалів $Tl_4HgI_6$ і $Tl_4PbI_6$

Франів В. А., Кашуба А.

*ЛНУ ім. І. Франка, факультет електроніки, Львів, Україна*

Дослідження напівпровідникових кристалів  $Tl_4HgI_6$  і  $Tl_4PbI_6$  є актуальним завданням сьогодення оскільки на основі них передбачається створення нових пристроїв функціональної електроніки, інтегральної оптики та сенсорів температури і тиску [1]. Враховуючи результати попередніх робіт роботи [1,2] актуальним для даних об'єктів було проведення досліджень їх оптичних та діелектричних властивостей, з метою встановлення закономірностей температурної поведінки таких фізичних характеристик, як іонна провідність, діелектрична постійна, ширина забороненої зони та енергій активації центрів рекомбінації.

В зв'язку з цим в роботі приведено результати діелектричних досліджень залежностей питомої іонної провідності та залежність дійсної частини діелектричної проникності з температурою. Результати отримані за допомогою RLC-методики. Встановлено, що в кристалах  $Tl_4HgI_6$  в області температур  $500K > T > 450K$  в температурній поведінці  $\sigma(T)$  і  $\epsilon(T)$  спостерігається гістерезис, який задовільно корелює з результатами досліджень лінійного розширення  $\Delta L/L$  [3]. Аналогічні результати отримано для кристала  $Tl_4PbI_6$  з тією різницею, що температурна область гістерезисну знаходиться нижче кімнатної ( $77K < T < 300K$ ). Робота також містить результати оптико-спектральних досліджень кристалів  $Tl_4HgI_6$  і  $Tl_4PbI_6$  в області краю фундаментального поглинання та рекомбінаційних переходів. Визначено енергії зона – зонних переходів (ширина забороненої зони), проаналізовано природу центрів рекомбінації.

1. Д.В. Бадиков, В.В. Бадиков, Г.М. Кузьмичева, В.Л. Панютин, В.Б. Рыбаков, В.И. Чижиков, Г.С. Шевырдяева, Е.С. Щербакова. Вирощування та X-дослідження  $Tl_4HgI_6$  кристалів. Неорган. матер., **40**, 372 (2004).
2. Sreejith Nair, Yahya A.I., Agaf Ahvad. Ionic conductivity and dielectric constant of  $Tl_4CdI_6$ , Solid State Ionics, 88-86, 1996, 137-139.
3. M. Piasecki • G. Lakshminarayana • A. O. Fedorchuk • O. S. Kushnir • V. A. Franiv • A. V. Franiv • G. Myronchuk • K. J. Plucinski Temperature operated infrared nonlinear optical materials based on  $Tl_4HgI_6$  J Mater Sci: Mater Electron (2013) 24:p.1187–1193

# Specificity of luminescent aluminium selenide nanocrystals

Balitski O.O.

*Department of Electronics, Lviv Ivan Franko National University, Lviv, Ukraine*

Luminescent semiconductor fabricated in organic solvents have been thoroughly investigated for the last two decades. The majority of them belong to the II–VI family due to simplicity, safeness and cheapness of the synthesis procedures. The main goal of colloidal nanoparticles chemistry is to achieve a precise control of the composition, size, shape and properties at the same time. One of the ways to resolve such puzzle is an extending the number of materials fabricated in nanostructured form. Among colloidal nanoparticles members of III–VI family were less studied with only indium and gallium selenides underwent careful photophysical examination. In particular colloidal gallium selenide were then highlighted in a perspective describing directions towards excellence in nanocrystals optical properties. Aluminium selenide is to date one of the least described III–VI semiconductors, even as a bulk material.

The metalorganic synthesis of highly luminescent aluminium selenide nanoparticles in the trioctylphosphine solvent with decent size distribution and elucidates their structure and optical properties were carried out.

The nanoparticles with 6.8 nm diameter and decent size distribution are bright blue luminescent. The crystallinity of the nanoparticles was explored by XRD and TEM measurements. The synthesis and characterization of colloidal aluminium selenide nanoparticles using trioctylphosphine as a solvent was proposed. The obtained nanoparticles have several absorption bands in the spectral region 330–410 nm and are bright UV-blue luminescent, which is well demanded in light collecting and emitting devices, e.g. for tuning their spectral characteristics to higher energy solar photons.

# Structural aspects of liquid-solid reactions at formation of nanocomposite systems

Stepan Mudry, Ihor Shtablavyi

*Ivan Franko National University of Lviv, Ukraine*

A nanometer-sized materials attract more attention in the recent years. First of all this is related with the fact that the nanometer size scale brings substantial changes into physicochemical properties, in comparison with properties of bulk materials. In heterogeneous systems, size effects are influenced also by morphology of particles, their distribution, and interface interaction. Because of this, investigation of nano-sized heterogeneous systems can play an important role in the understanding of properties formation process at manufacturing of materials in nanosize regime. An example of such systems are metal matrix composites with nanosized metallic or non-metallic fillers.

Synthesis of metal matrix composites filled with metal nanoparticles confronted with the problem of chemical interaction between the matrix and metal particles. Such interaction may be useful in some cases, or vice versa. For example, chemical interaction of powdered metals and alloys with liquid metals is basic to diffusion-hardening solders or the so-called metal glues. In such multicomponent systems, several intermetallic phases form in parallel or in sequence, effecting the phase formation process and the properties of the synthesized material. Analysis of the literature indicates that this issue has not yet been addressed in sufficient detail. The formation sequence of intermetallic compounds in systems containing several intermetallics is unclear, and the factors governing this process are as yet not understood.

On the other hand, the chemical interaction is undesirable in the formation of magnetic fluids with a metal matrix.

On that reason the phase formation upon interaction of fine metal particles with metal matrix have been investigated in this work.

Composites were prepared by mechanical mixing method, followed by heat treatment at different temperatures for different duration. Phase analysis was performed based on X-ray powder diffraction data collected on an automatic diffractometer STOE STADI P (Cu  $K_{\alpha 1}$  radiation,  $\lambda = 1.5406 \text{ \AA}$ , in the angular range  $6 \leq 2\theta \leq 100^\circ$  with scan step  $0.015^\circ$  and scan time 250 s). Structure in liquid state was investigated by means of high temperature X-ray diffractometer at various temperatures.

As a one of the result of studies the formation of intermetallic compounds in the solid-liquid boundary has been found.

*This work was supported by a grant from Fundamental Researches State Fund of Ukraine (№ 0113U002789).*

# Luminescence of $\text{Eu}^{2+}$ -doped microcrystals embedded in KBr matrix

A.S. Pushak<sup>a</sup>, V.V. Vistovsky<sup>b</sup>, T.M. Demkiv<sup>b</sup>, Yu. Dacyuk<sup>b</sup>,  
A.V. Gektin<sup>c</sup>, A.S. Voloshinovskii<sup>b</sup>

<sup>a</sup>Ukrainian Academy of Printing, Lviv, Ukraine

<sup>b</sup>Ivan Franko National University of Lviv, Ukraine

<sup>c</sup>Institute for Scintillation Materials, NASU, Kharkiv, Ukraine

The  $\text{KBr-BaBr}_2(1 \text{ mol.}\%)\text{-EuBr}_3(0.01 \text{ mol.}\%)$  crystalline system is studied in this work with aim to detect the formation of  $\text{Eu}^{2+}$  doped barium containing microphases embedded in KBr matrix. The  $\text{KBr-BaBr}_2(1 \text{ mol.}\%)\text{-EuBr}_3(0.02 \text{ mol.}\%)$  crystals were grown in evacuated quartz ampoules using the Bridgman–Stockbarger technique. As-grown  $\text{KBr-BaBr}_2\text{-Eu}$  crystals were annealed at 200 °C during 150 h for an activation of aggregating processes. Time-resolved luminescent spectroscopy studies were performed at  $T=9\text{--}300 \text{ K}$  using the facility of SUPERLUMI station at HASYLAB.

The  $\text{KBa}_2\text{Br}_5$  microphases of 1–10  $\mu\text{m}$  size are revealed on the freshly cleaved surface of  $\text{KBr-BaBr}_2\text{-Eu}$  crystalline system by scanning electron microscopy.

Luminescent studies allow us to reveal the distribution of europium ions between  $\text{KBa}_2\text{Br}_5$  microcrystals and KBr matrix. The luminescence band peaked at 445 nm in the luminescence spectra of  $\text{KBr-BaBr}_2\text{-Eu}$  crystalline systems (Fig. 1) are attributed to the emission of  $\text{Eu}^{2+}$  ions in  $\text{KBa}_2\text{Br}_5$  microphases embedded in KBr matrix and luminescence band peaked at 418 nm corresponds to emission of europium ions in KBr matrix.

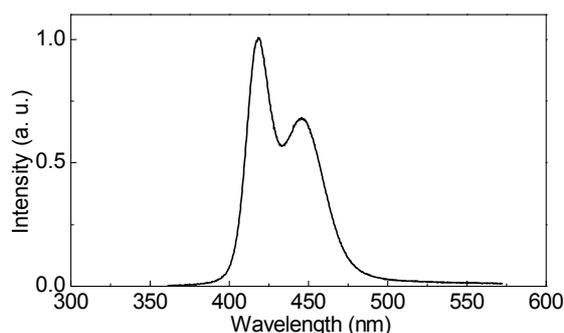


Figure 1: Luminescence spectra of  $\text{KBr-BaBr}_2\text{-Eu}$  crystalline system,  
 $\lambda_{\text{exc}} = 307 \text{ nm}$ ,  $T = 10 \text{ K}$ .

The dominance of 418 nm luminescence band indicates that the most of europium ions remains in the KBr matrix of  $\text{KBr-BaBr}_2\text{-Eu}$  system in comparison with previously studied of  $\text{KI-MeI}_2\text{-Eu}$  ( $\text{Me}=\text{Ca}, \text{Sr}, \text{Ba}$ ) crystalline systems where most of europium ions enters into embedded microcrystals.

*This work is supported by the 7<sup>th</sup> FP INCO.2010-6.1 grant agreement № 266531 (project acronym SUCCESS).*

## Energy transfer in LaPO<sub>4</sub>-Pr,Ce nanoparticles

T. Malyy<sup>1</sup>, V. Vistovskyi<sup>1</sup>, O. Shapoval<sup>2</sup>, N. Mitina<sup>2</sup>, A. Zaichenko<sup>2</sup>,  
O. Antonyak, A. Gektin<sup>3</sup>, A. Voloshinovskii<sup>1</sup>

<sup>1</sup>Ivan Franko National University, Lviv, Ukraine

<sup>2</sup>Lviv Polytechnic National University, Ukraine

<sup>3</sup>Institute for Scintillation Materials, NASU, Kharkiv, Ukraine

Optimal excitation energy transfer from the matrix to the emission centers is essential for high efficiency scintillation material. One of the possible ways to improve the efficiency of excitation energy transfer from the matrix to luminescent impurities such as Ce<sup>3+</sup>-ions is to use sensitizer that effectively capture the excitation energy. The use of Gd<sup>3+</sup>-Ce<sup>3+</sup> and Pr<sup>3+</sup>-Ce<sup>3+</sup> ion pairs [1,2] are examples of such approach.

In this work the luminescence properties of LaPO<sub>4</sub>-Pr,Ce nanoparticles with different mean size in range of 8-90 nm were studied. LaPO<sub>4</sub>-Pr,Ce nanoparticles upon excitation with energy quanta 4.0-50 eV reveal only emission inherent only for Ce<sup>3+</sup> ions (Fig.1, a). The emission of Pr<sup>3+</sup> ions in the range 210-280 nm corresponding to 5d-4f emission transfer was practically not observed. In the luminescence spectra of LaPO<sub>4</sub>-Pr,Ce nanoparticles with mean size 90 and 40 nm the position of cerium emission bands at 317 and 336 nm well correspond with their position in microcrystals LaPO<sub>4</sub>-Ce [3]. For nanoparticle with mean size 8 and 16 nm small shift to the low energy side (325 and 343 nm, respectively) is observed as a result of crystalline symmetry change of LaPO<sub>4</sub> matrix.

In the luminescence excitation spectra of LaPO<sub>4</sub>-Pr,Ce (Fig 2b) excitation bands corresponding to intracenter absorption of Ce<sup>3+</sup> ions (4,0-6,3 eV), intracenter absorption of Pr<sup>3+</sup> ions (6,3-8,0 eV), fundamental absorption of LaPO<sub>4</sub> matrix and the range of electronic excitation multiplication (E>16 eV).

The spectral overlap of 5d-4f emission range of praseodymium ions with the range of cerium ions absorption provides conditions for efficient transfer of excitation energy in Pr<sup>3+</sup>-Ce<sup>3+</sup> pair. Luminescence decay kinetics of praseodymium ions in LaPO<sub>4</sub>-Pr,Ce is significantly faster compared with that for LaPO<sub>4</sub>-Pr nanoparticles. The latter indicates that the mechanism of excitation energy transfer in Pr<sup>3+</sup>-Ce<sup>3+</sup> pair is nonradiative.

1. M. Nikl, A. Yoshikawa, T. Satonaga et. al. phys. stat. sol. (a). **201**, R108 (2004)
2. G. Stryganyuk, T. Shalapska, A. Voloshinovskii et al. J. Lumin. **131**, 2027 (2011)
3. G. Stryganyuk, J. Lumin. **128**, 355 (2008).

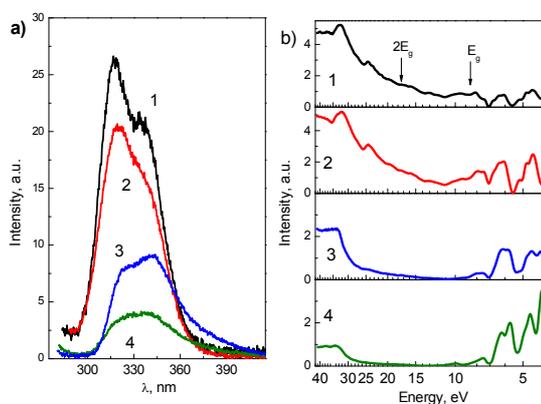


Fig 1. Emission (a) and luminescence excitation (b) spectra of LaPO<sub>4</sub>-Pr,Ce nanoparticles with different size. Curves: 1 – 90 nm, 2 – 40 nm, 3 – 16 nm, 4 – 8 nm.

## Luminescence Processes in SrF<sub>2</sub> Nanoparticles

Zhyshkovych A.V.<sup>1</sup>, Vistovskyy V.V.<sup>1</sup>, Bulyk L.-I.I.<sup>1</sup>, Pashuk I.P.<sup>1</sup>  
N.E. Mitina<sup>2</sup>, Zaichenko A.S.<sup>2</sup>, Voloshinovskii A.S.<sup>1</sup>

<sup>1</sup> *Ivan Franko National University of Lviv, Ukraine*

<sup>2</sup> *Lviv Polytechnic National University, Ukraine*

It is known that upon intracenter excitation the luminescence intensity depends on the nanoparticles size according to the rate of growth of surface-to-volume ratio. Such behavior can be explained as a result of surface defects influence. However, when the excitation energy exceeds another parameters possess the determinative influence on the luminescence intensity of nanoparticles. One of them is electron thermalization length. As it was shown for CaF<sub>2</sub> nanocrystals [1] the luminescence intensity upon band-to-band excitation is determined by the ratio between the thermalization length and the nanoparticle size. Therefore, it is advisable to study the dependence of luminescence intensity on the nanoparticles size upon the band-to-band excitation for experimental evaluation of electron thermalization length.

In the present work, the luminescence properties of SrF<sub>2</sub> nanoparticles (18-100 nm) have been studied using VUV synchrotron excitations on SUPERLUMI station (HASYLAB, DESY) in 9 – 35 eV range of excitation energies in order to identify the influence of commensurability of charge carrier mean free path and nanoparticle size on the luminescence of STE.

It was found that the intensity of STE luminescence is least sensitive to the nanoparticles size reduce upon the excitation quanta with energy of direct creation of excitons ( $h\nu > 2E_g$ ). On the other hand, the most sensitive to the nanoparticles size reduce is energy range  $E_g < h\nu < 2E_g$ , where the luminescence intensity decreases. In a case of X-ray quanta excitation, in the energy range  $E_g < h\nu < 2E_g$ , a similar situation is observed. In the range of electronic excitations multiplication ( $h\nu > 2E_g$ ), where the mean free path of photoelectrons is small due to the inelastic scattering on valence electrons, the dependence of the luminescence intensity on the nanoparticle size is similar to the case of the optical creation of excitons. The revealed regularities are discussed in terms of correlation between nanoparticle size and thermalization length of secondary electrons and the mean free path of primary photoelectrons.

1. V. V. Vistovskyy, A. V. Zhyshkovych, N. E. Mitina et.al., J. Appl. Phys. 12, 024325 (2012).

## Methods of micro- and formation nanocrystals in the CsI dielectric matrix

Voloshinovskii A.S.<sup>1</sup>, Myagkota S.V.<sup>2</sup>, Demkiv T.M.<sup>1</sup>, Pushak A.S.<sup>3</sup>,  
Dacyuk Y.R.<sup>1</sup>, Demkiv L.S.<sup>1</sup>

<sup>1</sup>*Ivan Franko National University of Lviv, Ukraine*

<sup>2</sup>*Lviv State Agrarian University, Ukraine*

<sup>3</sup>*Ukrainian Academy of Printing, Lviv, Ukraine*

Recently the development of new scintillation materials based on alkaline earth metal halides doped with rare-earth ions cause considerable interest. Materials with high specific light yield and short luminescence decay times are promising materials for fast nanosecond range scintillators.

However, the difficulty of obtaining homogeneous samples and their water absorption limit the potential use of these crystals as scintillators. The CsI, KCl and NaCl crystals doped with MeI<sub>2</sub>-Eu (Ba, Sr) were grown using Stockbarger growth technique. The obtained crystals underwent the annealing at 150-200 °C during 100 hours with the purpose forms microphase luminescent material in the crystalline matrix dispersed by volume and removes restrictions in use absorbent materials [1].

On the scanning electron microscope JEOL JSM-T220A with X-ray microanalyzer has been investigated the microstructure and microanalysis fluorescent microcrystals SrI<sub>2</sub>-Eu and BaCl<sub>2</sub>-Eu embedded in CsI host. The size distribution histogram of SrI<sub>2</sub>-Eu and BaCl<sub>2</sub>-Eu microparticles in the CsI dielectric matrix has been made. This histogram was compared with the generalized distribution Slezov-Lifshitz-Wagner.

Analysis of the histogram distribution of microcrystals dispersed in CsI matrix showed, that the probable mechanism of their formation is controlled by the rate of formation chemical bonds on the surface of microcrystals. Prolonged annealing of CsI-SrI<sub>2</sub>-Eu leads to a change in the mechanism of SrI<sub>2</sub>-Eu microcrystals formation in the CsI matrix: the mechanism of which is determined by the rate of chemical bonds formation on the microcrystals surface in a slight predominance of the diffusion mechanism of microcrystals growth.

1. Vistovskyy V. V. Luminescence of Ce doped LaCl<sub>3</sub> microcrystals incorporated into a single-crystalline NaCl host. / V. V. Vistovskyy, P. V. Savchyn, G. B. Stryganyuk, A. S. Voloshinovskii and M. S. Pidzyrailo. Journal of Physics: Condensed Matter – 2008. – Vol. 20. – P. 325218 – 325223

# Functional properties of supramolecular complexes

Grygorchak I.I., Venhryn B.Ya., Balaban O.V., Verkhola D.R.

*Lviv Polytechnic National University, Ukraine*

At present time, a variety of cathode materials are widely used in the energy industry field. Nevertheless according to requirements of the modern devices the qualitative characteristics of these materials are clearly not enough for their long-term and effective using. Some of currently used cathode materials are suitable only for the capacitive storage, while the others are suitable for the Faraday power generation. On that reason we proposed an approach that provides the possibility to combine these two mechanisms in a single device.

An activated carbon and expanded graphite were selected as initial materials for research. Crown-ether (18-crown-ether-6), which bind alkaline metals in the “lock-key” way was encapsulated in these materials. In the created structure the interaction of components occurs by the host-guest type. The thermal vacuum desorption was preceded by the encapsulation process. With thus obtained supramolecular complexes <carbon based material (CBM)<18-crown-ether-6>> (Fig. 1) a number of electrochemical measurements to determinate their specific characteristics and a possibility of combining in a single device above-mentioned mechanisms was conducted.

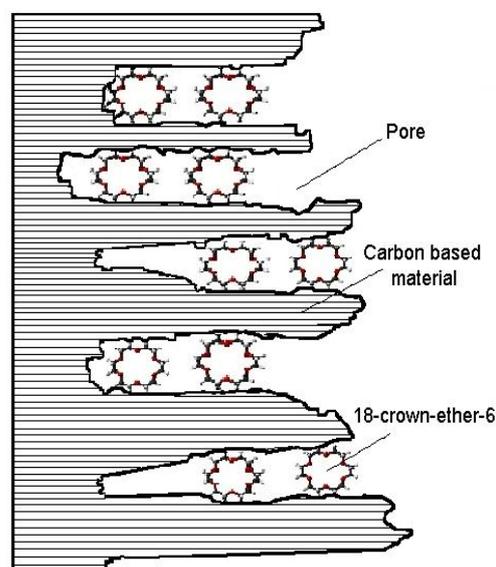


Fig. 1. Supramolecular complex <CBM<18-crown-ether-6>>.

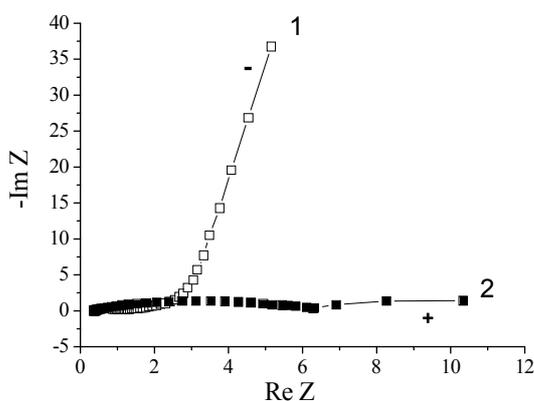


Fig. 2. Typical Nyquist diagrams for polarization processes in supramolecular complexes <CBM<18-crown-ether-6>> in anode (1) and cathode (2) regions.

Nyquist diagrams as the results of impedance measurements of investigated supramolecular complexes are shown in Fig. 2. The behavior of curve 1, indicated a capacitive accumulation in the anode region and curve 2, displayed the Faraday power generation in the cathode region. In turn, the charge-discharge galvanostatic cycles between potentials of 0.4 V and 1.24 V demonstrated the realization of the capacitive storage, and at lower than 0.4 V potentials they confirmed the Faraday energy generation.

## З М І С Т

<i>S.Mudry</i> : Fundamental importance of the Ya. Dutchak works in study of melts for modern nanophysics and nanotechnologies	4
<i>Романюк М.О.</i> : Професор Дутчак Я.Й. – знання і рішучість	5
<b>Секція 1</b>	6
<i>Markiv B., Vasylenko A., Tokarchuk M.</i> : Effect of ion polarization on transverse excitations in molten salts	7
<i>Terekhova Yu.V., Stefanovich L.I., Yurchenko V.M.</i> : Kinetics of spinodal decomposition in amorphous alloys	8
<i>Kostrobij P. P., Markovych B. M., Tokarchuk R. M., Chornomorets Yu., Tokarchuk M. V.</i> : Statistical theory of reaction-diffusion processes lithium ions in the system “electrolyte – electrode”	9
<i>Токарчук М., Марків Б., Омелян І.</i> : Узгоджений опис кінетики та гідродинаміки слабонерівноважних процесів у простих рідинах	10
<i>Bryk T., Ruocco G., Scopigno T.</i> : Coupling of longitudinal and transverse collective excitations in collective dynamics of liquid metals	11
<i>Agraval P.G., Dreval' L.O., Turchanin M.A.</i> : Characteristic features of the temperature and composition dependencies of the thermodynamic properties of liquid alloys of binary and ternary glass forming systems	12
<i>Agraval P.G., Dreval L.A., Turchanin M.A.</i> : Experimental investigation and modeling of the mixing enthalpies of liquid Co–Cu–Zr and Cu–Fe–Zr alloys	13
<i>Agraval P.G., Dreval' L.O., Turchanin M.A., Storchak-Fedyuk A.M.</i> : Chemical short-range order and composition range of amorphization of liquid Ni–Ti–Zr alloys	14
<i>Візнович О., Костробій П., Марків Б., Токарчук М.</i> : Узагальнені кінетичні рівняння для густих газів та рідин у статистиці Рені	15
<i>Shvets V. T.</i> : Effective Proton–Proton Interaction and Metallization of Hydrogen	16
<i>Shvets V. T.</i> : Equation of State of Liquid Metallic Helium	17
<i>Shvets V. T.</i> : Higher Order Perturbation Theory Effects in the Resistance of Simple Disordered Metals	18
<i>P.Kostrobij, B.Hnativ, I.Penyak, I.Ryzha</i> : Stabilization of temperature in models of catalytic CO oxidation on the surface	19
<i>Kostrobij P.P., Uchanska O.M.</i> : Influence of the memory function for diffusion dynamics of low-dimensional systems	20
<i>Kozlovskii M.P., Romanik R.V.</i> : A method for describing the phase behaviour of many-body systems	21
<i>Гуменюк Й.А., Токарчук М.В.</i> : Функції розсіяння кінетичної теорії для густих газових сумішей з багатосходиновою взаємодією між частинками	22

<i>A.L. Parakhonsky, M.V. Lebedev, A.A. Dremin, and I.V. Kukushkin:</i> Correlation analysis of giant optical fluctuations of 2D electrons	23
<i>Haysak M.I., Haysak I.I., Klenivskyi M.S.</i> Energies of affinity for metastable triplet states of the negative ion of hydrogen isotopes in a one-dimensional space in hyperspherical adiabatic approach	24
<i>Haysak M.I., Muchychka Yu.Yu., Onysko V.V.:</i> Binding energy of ground states of negative hydrogen ion and helium isotopes in two-dimensional space	25
<i>Haysak M.I., Yevych M.J., Yevych R.</i> Binding energy of odd quantum states of negative exciton ions for CdSe and Si semiconductors in a one-dimensional space	26
<i>A.V. Nazarenko</i> Directed random walk on the eight-branching cayley tree	27
<i>Yu.V. Slyusarenko, S.O. Nikolayenko:</i> On the role of correlations in systems of particles interacting with multiplying and capturing hydrodynamic media under external stochastic field	28
<i>Шугорін П.П., Дмитрук І.П., Головій В.М.:</i> Дисперсія звуку в бозе-газі за наявності конденсату	29
<i>Boichuk V.I., Bilynskyi I.V., Shevchuk I.S.:</i> Electron-hole pair-phonon interaction in semiconductor quantum dots	30
<i>Kuzmak A. R.:</i> Preparation of a Quantum States of Two Spin-1/2	31
<i>A. Rovenchak:</i> Fractional statistics in D dimensions: Thermodynamics of the harmonic oscillator system	32
<i>H. P. Laba, V. M Tkachuk:</i> Quantum mechanical analogy and supersymmetry of electromagnetic wave propagation in planar waveguides	33
<i>M. Samar:</i> Relativistic particle dynamics and deformed Poincaré symmetry	34
<i>Voznyak O.O., Tkachuk V. M.:</i> Supersymmetric approach for quasi-exactly solvable systems with a position-dependent mass	35
<i>Vakarchuk I. O., Panochko G.:</i> The impurity states in the liquid Helium – 4	36
<i>I.V. Stasyuk, O.V. Velychko:</i> The effect of the stage ordering in layered crystals on electron states	37
<i>Trokhimchuck P.P</i> Relaxed Optics: problems of development and application	38
<i>Kosynska O.L., Dorozhka T.N.</i> Investigation of the conditions of crystallization suppression by quenching from melt	39
<i>Saliy Y.P., Bylina I.S., Freik I.M.</i> Models of simple crystallographic forms of vapor-phase PbTe nanostructures on Sital	40
<i>M. Dudka, Yu. Holovatch:</i> Influence of different types of structural disorder on the critical properties of magnets	41
<i>Pursky O.I., Chastokolenko I.P.:</i> Molecular rotation and volume dependence of the thermal conductivity in liquid nitrogen	42

<i>Дон Н.Л.</i> : Моделювання структурних перетворень в кристалах класу $A_3^{\text{II}}B_2^{\text{V}}$	43
<i>V. Kartuzov, Y. Dmytrishyna</i> : Simulation of the structure of liquid aluminum using fractal theory	44
<i>Martemyanova J.A., Ivanov V.A., Paul W.</i> : The study of nanostructures in a single semiflexible macromolecule with inhomogeneous distribution of the chain stiffness by means of Monte Carlo simulation.	45
<i>Stashchuk V.S., Stukalenko V.V., Filipov Ya. V., Polianska O.P.</i> : The aluminium oxide thin film – cooper system's optical properties modeling.	46
<i>Paramonova E.V., Gevorkyan V.E., Avakyan L.A., Bystrov V.S.</i> : The modeling of biocompatible molecular ferroelectrics.	47
<i>Ferlat G., Seitsonen A.P., Lazzeri M., Mauri F.</i> : Vittrification of $B_2O_3$ : Role of hidden polymorphs revealed from molecular dynamics simulations	48
<i>Manyk T.O., Bilynskyj-Slotylo V.R.</i> : Modelling of thermoelectric modules for low-grade heat recovery	49
<i>Д.О.Харченко, В.О.Харченко, С.В. Кохан</i> : Моделювання процесів формування нано-островків конденсату у реакційно-дифузійних системах із пам'яттю	50
<i>Kharchenko V. O.</i> : Formation of nano-size structures on the Silicon surface induced by Argon ions sputtering	51
<i>Dvornichenko A.V.</i> : Formation of pyramidal islands during epitaxial growth: phase-field modeling	52
<i>Klevets I., Bryk T.</i> : Ab initio study of charge correlations in compressed liquid alkali metals	53
<i>Klym H., Balitska V., Brunner M., Shpotyuk O., Hadzaman I.</i> : Thermodegradation kinetics in monolithized spinel ceramics	54
<i>Stadnyk V.Yo., Kurlyak V.Yu., Romanyuk M.O., Brezvin R.S., Rudysh M.Ya.</i> : The influence of admixture on the optical properties of the crystals	55
<i>Луцишин Т.І., Шевчук О.В., Максимів М.М.</i> : Конфігураційна ентропія змішування розбавлених розчинів $Al_{1-x}Ni_x$ .	56
<i>P.M. Yakibchuk, O.V. Bovgyra, I.V. Kutsa</i> : Model pseudopotential calculations for the electronic structure of semiconductors	57
<i>O.V. Bovgyra, M.V. Kovalenko, R.V. Bovhyra</i> : Electronic structure and magnetism of 3d transition metal-doped ZnO nanostructures	58
<i>P. Yakibchuk, V. Patsahan and T. Patsahan</i> : Structure and dynamic properties of aluminium-copper alloys: a molecular dynamics study	59
<i>Chaplya Y.Y., Goncharuk V.Y., Dmytruk V.A. and Chernukha O.Y.</i> : Simulation of advective diffusion in horizontally periodical stratified structures	60
<i>Shopa Y.I., Ftomyn N.Y., Sokolyuk I.V.</i> : Optical activity of disordered gallogermanate crystals	61

<i>Yakibchuk P.M., Volkov O.V., Vakarchuk S.O.</i> : Compressed sensing and structure of multicomponent alloys	62
<i>Yakibchuk P.M., Volkov O.V., Vakarchuk S.O.</i> : Simulation of metallic alloy structure during melting process	63
<i>Yakibchuk P.M., Volkov O.V.</i> : Deterministic approach to construction of structure factors for metallic alloys	64
<i>Ya. Chornodolskyy, A. Gloskovskii, V. Vistovskyy, O. Shevchuk, O. Myagkota, S. Syrotyuk, A. Zaichenko, V. Voloshinovskii</i> : Calculation and experimental study of energy bands of LaPO <sub>4</sub> nanoparticles	65
<b>Секція 2</b>	66
<i>M.Krasnytska, B. Berche, Yu. Holovatch</i> : Scaling functions and critical amplitude ratios for the Potts model on scale-free networks	67
<i>Freik D.M., Mudry S.I., Kryskov C.A., Gorichok I.V., Lyuba T.S., Turovska L.V., Krynycky O.S., Matkivskyi O.M.</i> : Defect Subsystem of Solid Solutions PbTe-Sb <sub>2</sub> Te <sub>3</sub> and PbTe-Bi <sub>2</sub> Te <sub>3</sub>	68
<i>L. A. Avakyan, A. S. Manukyan, A. A. Mizarkhanyan, E. G. Sharoyan, Y. V. Zubavichus, A. L. Trigub, N.A. Kolpacheva, L. A. Bugaev</i> : The EXAFS and DFT Study of Doped Nickel Phthalocyanine as a Potential Room-Temperature Molecular Magnet	69
<i>Lytvynenko D.M., Slyusarenko Yu.V.</i> : Spatial periodic structures in the system of charged Fermi particles above the surface of liquid dielectrics	70
<i>V.M.Silonov, V.V.Chubarov</i> : Amorphization of the ice near melting point	71
<i>O. O. Davydenko, V. E. Sokolskii, I.O. Goncharov</i> : Calculation of the mass fraction of spinel MgAl <sub>2</sub> O <sub>4</sub> that formed at the operation with ceramic welding fluxes	72
<i>V. E. Sokol'skii, A.S. Roik, O.O. Davidenko, S.A. Fesenko, N.V. Faidyuk, and R. N. Savchuk</i> : X-Ray Diffraction Study of the NaF–LiF–NdF <sub>3</sub> and NaF–LiF–LaF <sub>3</sub> Eutectic in the Liquid and Solid States	73
<i>Roik O.S., Kazimirov V.P., Sokolskii V.E.</i> : Atomic structure of the binary and ternary Al-based liquid alloys	74
<i>Roik O.S., Muratov O.S., Kazimirov V.P.</i> : Origin of the shoulder on the high Q side of the main peak on the structure factors of liquid Si and Ge	75
<i>Nahusko O.T., Studenyak I.P.</i> : Compositional disordering in amorphous Ti <sub>1-x</sub> Zr <sub>x</sub> O <sub>2</sub> thin films	76
<i>I.D.Shcherba, M.V.Sacharevycz, A.O. Stosyk, L.O.Dobryanska, B.M.Jatsyk</i> : Electron structure and magnetic properties of the new ternary intermetallic compounds	77
<i>J. Dziejic, J. Rybicki</i> : Hybrid quantum-classical approach for dynamical simulations of metallic systems	78
<b>Lutsyk N.Yu., Balitska V.O., Mykolaychuk O.G.</b> : <i>Structure and conditions for forming amorphous films of the GaSb – Ge system</i>	79
<i>Chekaylo M.V., Akselrud L.G., Gladyshevskii R.E., Ilchuk H.A., Ukrainets V.O., Ukrainets N.A.</i> : Temperature investigations of the structure of β'- and γ-phases of Ag <sub>8</sub> SnSe <sub>6</sub> argyrodite	80

<i>S.Mudry, Yu.Kulyk, S.Zhovniruk</i> : The X-ray study of relaxation processes in amorphous Fe <sub>75</sub> Mo <sub>5</sub> Si <sub>6</sub> B <sub>14</sub> alloys	81
<i>Nykyruy Yu.</i> : Structure changes in laser irradiated iron and cobalt-based amorphous alloys.	82
<i>Koman B. P, Yuzevich V.M.</i> : Atomic structure of SiO <sub>2</sub> after alpha irradiation.	83
<i>A.Korolyshyn, V.Vus, M.Lytvyn, S.Mudry</i> : Structure of (PbTe) <sub>x</sub> (Bi <sub>2</sub> Te <sub>3</sub> ) <sub>1-x</sub> molten alloys	84
<i>S. Mudry, S. Prokhorenko, I. Bordun, V. Ptashnyk</i> : Heat flow researching in the fluid at the process of electrical activation arising	85
<i>Mazur Yu.P., Nosenko A.V., Semen'ko M.P., Zakharenko M.I.</i> : Influence of the temperature-temporal prehistory of the melts on crystallization kinetics of the Fe-Si-B amorphous alloys	86
<i>Semen'ko M.P.</i> : Correlation between electro-transport properties of the disordered systems and their electronic and atomic structures	87
<i>Zakharenko M.I.</i> : Physical properties, phases' stability and electronic structure parameters of the random metallic systems	88
<i>Yushchenko O.V., Yurko D.S.</i> : The synergetic theory of plastic deformation	89
<i>Neimet Yu.Yu., Studenyak I.P.</i> : Structural and dielectric studies of disordered solid electrolytes of Ag-As-S system	90
<i>A.Usseinov, E.A. Kotomin, Yu.F. Zhukovskii, J. Purans, A. Akilbekov, A.K. Dauletbekova</i> : Hydrogen adsorption on non-polar surfaces of ZnO: Ab initio calculations	91
<i>Lysov V.I., Tsaregradska T.L., Turkov O.V., Saenko G.V.</i> : The influence of thermocycling and cryotreatment on stability of amorphous alloys	92
<i>Krivchikov A. I., Vdovichenko G. A., Korolyuk O. A. Romantsova O. O.</i> : Thermal conductivity of molecular glass	93
<i>Myhal V.M., Derzhko O.V.</i> : Vapour-liquid phase diagram and surface tension for a fluid of two-level atoms with taking into account short-range order	94
<i>Ashcheulov A.A., Manyk O.M., Manyk T.O., Bilynskyj-Slotylo V.R.</i> : Dynamics of chemical bond formation in iron based materials	95
<i>V.L. Karbivskyy, O.I. Slukhovskyy, N.A. Kurgan</i> : Mathematical morphology and electronic structure of the amorphous metal alloy Fe <sub>77</sub> Si <sub>8</sub> B <sub>15</sub> surface at thermal effect	96
<i>Stupka A.A.</i> : Long-wave high-frequency plasma oscillations in alkali-halid liquid salts	97
<i>Poperenko L.V., Manko D.Yu., Yurgelevich I.V.</i> : Optical conductivity peculiarities and electronic parameters of Fe-rich amorphous metallic alloys	98
<i>Yakymovych A., Flandorfer H., Fürtauer S., and Ipser H.</i> : Influence of Co and Cu additions on the enthalpy of mixing of liquid Li-Sn alloys	99

<i>M. Shpotyuk, O. Shpotyuk, M. Vakiv, S. Kozyukhin: Radiation-induced defect formation in glassy As-S/Se</i>	100
<i>V. Boyko, V. Gurin, O. Shpotyuk, M. Vakiv: On the problem of self-organization effect in Ge-Se system</i>	101
<i>Мороз М.В., Миколайчук О.Г., Прохоренко М.В.: Електропровідність склоподібних сплавів системи <math>Ag_2S-GeS_2-AgBr</math></i>	102
<i>Balitska V.O., Golovchak R.Ya., Shpotyuk O.I.: Sigmoid tendencies in the kinetics of natural physical ageing in <math>As_{10}Se_{90}</math> glass</i>	103
<i>Shpotyuk O.I.: Notes on functional metastabilities in chalcogenide semiconductor glasses: the role of free-volume deviations as probed by positron annihilation</i>	104
<i>Romanyuk R.R. Mykolaychuk O.G.: The charge carriers transfer in amorphous <math>(GeS)_{1-x}Bi_x</math> films</i>	105
<i>Yu. Plevachuk, V. Sklyarchuk, A. Yakymovych, I. Kaban: Electrophysical and structure-sensitive properties of liquid Ag-Sb-Sn and Bi-Cu-Sn alloys</i>	106
<i>Yu. Plevachuk, V. Sklyarchuk, A. Yakymovych: Thermophysical properties of the liquid <math>Au_{15.9}Pb_{84.1}</math> eutectic alloy</i>	107
<i>V. Sklyarchuk, Yu. Plevachuk, S. Mudry, Yu. Kulyk, I. Shtablavyi, A. Korolyshyn: Structure and thermophysical properties of Au-Ag-based alloys</i>	108
<i>Popovich K.P., Holovey V.M., Prymak M.V., Birov M.M.: Effect of structural disordering on the optical properties of <math>Li_2B_4O_7:Cu</math></i>	109
<i>Onanko A.P., Lyashenko O.V., Kulish M.P., Prodayvoda G.T., Onanko Y.A., Lyashenko I.O.: Inelastic-elastic properties and defect nanostructure changing of amorphous MgBa alloys and automated system of ultrasonic anisotropy visualization</i>	110
<i>Puga P.P., Danyliuk P.S., Popovych K.P., Turok I.I., Krasylynec V.M., Birov M.M., Vuchkan V.I., Puga G.D., Chychura I.I.: X-Ray <math>Er^{3+}</math> Luminescence in the Glassy Lithium Tetraborate Matrix</i>	111
<i>Gurin V.S., Kislyakov E.F., Ratkevich S.V., Shpotyuk O.I., Boyko V.: DFT calculation of clusters within vitreous germanium selenide</i>	112
<i>Peleshchyshyn R., Sokolovskyi B., Vus V.: Electrophysical properties of Pb-Mg based eutectic melts</i>	113
<i>Pazdriy I. P.: Prospects for the use of low melting metal alloys</i>	114
<i>Kuzhel B.S., Salamakha L.P., Romaka L., Belan B.D.: Magnetoresistance of RE-M(Cu, Ni)-X(Si, Sn) ternary compounds</i>	115
<i>Kulyk Yu. Zhovneruk S., Mudry S.: Evolution of nanocrystalline structure in amorphous <math>Al_{86}Ni_8Ho_6</math> alloy.</i>	116
<i>Vus V., Yakymovych A., Mudry S., Plevachuk Yu.: The viscosity and electrical conductivity of liquid Bi-In alloys</i>	117
<i>Vus V., Shevernoga I., Mudry S., Korolyshyn A.: Structure of <math>Ni_{1-x}In_x</math> molten alloys within near-eutectic (<math>\zeta + \delta</math>) concentration region</i>	118

<i>Prysyazhnyuk V.I., Mykolaychuk O.G.:</i> Magnetic properties of Gd-Fe system (Films and Bulk)	119
<i>L. Bulavin, Yu. Plevachuk, V. Sklyarchuk, A. Omelchuk, N. Faidiuk, R. Savchuk, I. Shtablavyi, V. Vus:</i> Concentration dependence of physical properties of liquid NaF–LiF–NdF <sub>3</sub> alloys	120
<i>V. Klanichka, I. Shtablavyi, S. Mudry:</i> Temperature dependence of structure in eutectic melts	121
<i>Prysyazhnyuk V.I., Mykolaychuk O.G.:</i> Influence of ageing processes on the structure and physical properties of amorphous-crystalline films of gd-fe system	122
<i>Bakhtinov A.P., Vodopyanov V.M., Kudrynskyi Z.R., Kovalyuk Z.D., Netyaga V.V., Karbivskyy V.L., Vishniak V.V. and Lytvyn O.S.:</i> Nanocomposite materials based on nanostructured carbon and III-VI layered semiconductors	123
<i>Kapustianyk V.B., Panasyuk M.R., Turko B.I., Dubov Yu.G., Vas'kiv A.P.:</i> ZnO nanowires with p-type conductivity as a material to create a vacuum pressure sensor	124
<i>Kapustianyk V.B., Turko B.I., Rudyk V.P., Tsybulskyi V.S., Luzinov I., Malynych S., Savchak M.:</i> LED based on p-type ZnO nanostructures	125
<i>Krupa M.M.:</i> Switching of the magnetic nanofilms with laser radiation and data recording using the spin current	126
<i>Freik D.M., Klanichka V.M., Mezhylovska L.Yo.:</i> The Technology, Properties and Application of Thermoelectric Nanomaterials and Nanocomposites	127
<i>Gorichok I.V., Krynytsky O.S., Matkivsky O.M.:</i> Nanocomposite Materials Based on PbTe with Nano-inclusions	129
<i>Freik D.M., Parashchuk T.O., Chobanyuk V.M. Gorichok I.V.:</i> The structure modeling and ab initio calculation of the thermodynamic parameters of zinc chalcogenides crystals	130
<i>Gomza Yu.P., Klepko V.V.:</i> X-rays diffractometry for structure peculiarities of polymer-based nanocomposites investigations	131
<i>Gomza Yu.P., Dzyazko Yu.S., Ponomareva L.N., Nesin S.D., Vol'kovich Yu.M., Sosenkin V.E., Trachevskii V.V. Scherbatyuk N.N.:</i> Structural transformations and magnetic properties of amorphous films of Gd-Fe system	132
<i>Alekseeva T.T., Martyniuk I.S., Gomza Yu.P., Klepko V.V., Nesin S.D.:</i> Structure peculiarities nanocomposites materials based on organic-inorganic interpenetrating polymer networks	133
<i>Freik D.M., Bylina I.S., Sokolov O.L. Lishchynsky I.M., Potyak V.Yu.:</i> The processes of self-organization and growth mechanisms of vapor-phase condensates based on CdTe, SnTe and PbTe	134
<i>Freik D.M., Yurchyshyn I.K., Chobaniuk V.M., Potyak V.Yu.:</i> Oscillation of thermoelectric parameters in quantum-dimensional structures of compounds IV-VI	135

<i>B.S. Dzundza, Ya.S. Yavorsky, A.I. Tkachuk, O.B. Kostyuk:</i> Influence of inter-phase boundaries on charge carriers scattering mechanisms in lead chalcogenide films	136
<i>A. M. Ermolaev, G. I. Rashba:</i> Magnetoplasma waves on the surface of a semiconductor nanotube with a longitudinal superlattice	137
<i>Basaraba Yu.B., Zasadnyy T.M.:</i> Production of nano-crystalline materials in hydrogen	138
<i>Bezrodna T.V., Chashechnikova I.T., Nesprava V.V.:</i> Structure and electrooptical properties of 5CB liquid crystal – organomodified montmorillonite nanocomposites	139
<i>Danilevscaia N. B., Nechiporuk B.D., Yukhymchuk V. O.:</i> Getting and some physical properties of nanoparticles of cadmium compounds	140
<i>Ivanskii B.V., Stasyk M.O., Yarema S.V., Panko I.I.:</i> Wagner-Vengrenovich distribution	141
<i>Vengrenovich R.D., Panko I.I.:</i> Mechanism and kinetic of formation of ZnO nanocrystals from supersaturated solution	142
<i>Vengrenovich R.D., Ivanskii B.V., Yarema S.V., Stasyk M.O.:</i> To the derivation of Thomson's equation	143
<i>Polianska O.P., Stashchuk V.S.:</i> Ellipsometry study of nanocomposite materials based on Co-Fe-B	144
<i>V.L. Karbivskyy, N.A. Kurgan:</i> Synthesis and electronic structure of the nanodispersed calcium hydroxyapatite	145
<i>Charkina O.V., Bogdan M.M.:</i> Local negative permeability and detection of nonlinear excitations in nanomagnetic metamaterials	146
<i>Revo S.L., Lozovyi F.V., Ivanenko K.O., Sementsov Yu.I., Dong Zhanmin:</i> Effect of carbon concentration on the crystallinity of polymer matrix in fluoroplastic/polyethylene-carbon composites	147
<i>N.A. Korynevskii, V.B. Solovyan:</i> On the Nanoclusters Formation in Metallic Systems	148
<i>I. M. Bolesta, N. V. Gloskovska, I. M. Rovetskyj:</i> Luminescence and structural studies of CdI <sub>2</sub> crystals with nanocrystalline PbI <sub>2</sub> inclusions under high-energy excitation	149
<i>Kolupaev B.B., Klepko V.V., Lebedev E.V., Gud V.M.:</i> Research of diffusive processes in the polymeric nanocomposites	150
<i>Voznyak O.M.:</i> Position dependent effective mass of carriers and energy states of periodic nanoscale heterosystems	151
<i>Левчук В.В., Колупаєв Б.С., Максимцев Ю.Р.:</i> Дослідження акустичних властивостей нанопоповнених гнучколанцюгових полімерних систем	152
<i>Konopelnyk O.I., Aksimentyeva O.I., Opaunych I.Ye., Horbenko Yu.Yu.:</i> Thermal behavior of poly-3,4-ethylenedioxythiophene doped with inorganic nanoclusters	153
<i>Marenkov V.I.:</i> Electronic properties of metals with disordered system cylindrical nanosized volume-filling defects	154

<i>Gaevskiy V.R., Nechyporuk B.D., Novoselets'kiy N.YU. Rudyk B.P.:</i> Electrochemical fabrication of Zinc oxide nanoparticles	155
<i>Франів В. А., Каууба А.:</i> Діелектричні та оптичні властивості кристалів $Tl_4HgI_6$ і $Tl_4PbI_6$	156
<i>Balitski O.O.:</i> Specificity of luminescent aluminium selenide nanocrystals	157
<i>S. Mudry, I. Shtablavyi:</i> Structural aspects of liquid-solid reactions at formation of nanocomposite systems	158
<i>A.S. Pushak, V.V. Vistovskyy, T.M. Demkiv, Yu. Dacyuk, A.V. Gektin, A.S. Voloshinovskii:</i> Luminescence of $Eu^{2+}$ -doped microcrystals embedded in KBr matrix	159
<i>T. Malyu, V. Vistovskyy, O. Shapoval, N. Mitina, A. Zaichenko, O. Antonyak, A. Gektin, A. Voloshinovskii:</i> Energy transfer in $LaPO_4$ -Pr,Ce nanoparticles	160
<i>Zhyshkovych A.V., Vistovskyy V.V., Bulyk L.-I.I., Pashuk I.P., N.E. Mitina, Zaichenko A.S., Voloshinovskii A.S.:</i> Luminescence Processes in $SrF_2$ Nanoparticles	161
<i>Voloshinovskii A.S., Myagkota S.V., Demkiv T.M., Pushak A.S., Dacyuk Y.R., Demkiv L.S.:</i> Methods of micro- and formation nanocrystals in the CsI dielectric matrix	162
<i>Grygorchak I.I., Venhryn B.Ya., Balaban O.V., Verkhola D.R.:</i> Functional properties of supramolecular complexes	163