<u>DMS – RE 2015</u>

The twenty-five joint seminar

DEVELOPMENT OF MATERIALS SCIENCE IN RESEARCH AND EDUCATION

BOOK OF ABSTRACTS OF THE 25th JOINT SEMINAR

31 August – 4 September, 2015 Kežmarské Žľaby

DMS – RE 2015

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DEVELOPMENT OF MATERIALS SCIENCE IN RESEARCH AND EDUCATION

31 August – 4 September, 2015 Kežmarské Žľaby

Organized by

Slovak Expert Group of Solid State Chemistry and Physics Czech and Slovak Association for Crystal Growth Faculty of Chemical and Food Technology STU Faculty of Materials Science and Technology STU Crystallographic Society Slovak Society for Industrial Chemistry Regional Committee of Czech and Slovak Crystallographers

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FOREWORD

The seminar "Development of Materials Science in Research and Education" is already the twenty fifth in the series started at Gabčíkovo in 1991 by the initiative of the Czech and Slovak Association for Crystal Growth and the Slovak Expert Group of Solid State Chemistry and Physics.

The objective of this meeting is to offer an opportunity to Czech and Slovak teachers and scientists as well as guests from other countries who are working in the field of Materials Science to present their recent results and experience and to exchange new ideas and information.

The scientific session will cover the following topics on materials science:

- Trends in development of materials research
- Education of materials science at the universities
- Information about the research programmes of individual institutions
- Information about equipment for preparation and characterisation of materials
- Results of materials research

This workshop is aimed at creation of a stimulating atmosphere of cooperation and at the support of patient dissemination of scientific idea s and propagation of materials science in education.

Organizers

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PROGRAM

Monday, 31 August 2015

12:00	_	14:00	Registration Location: Hotel Langue
13:00	_	13:40	Lunch Location: Lunchroom
14:00	_	14:10	Opening Location: Lecture Hall
14:10	_	15:50	Monday Session I Location: Lecture Hall (chairperson: B. Papánková)
14:10	_	14:30:	Karel Nitsch:
14:30	_	14:50:	The Origins of the Institutions for Crystal Growth Zdeněk Kožíšek: Growth rate of nuclei
14:50	-	15:10:	Pavel Ctibor: Dielectric properties through-thickness mapping on extremely thick
15:10	_	15:30:	plasma sprayed TiO2 Dana Mikolášová: Use of polyvinylpyrrolidone in the LiNbO3 thin films deposition
15:30	_	15:50:	Jiří A. Mareš: Scintillation properties of LuAG:Ce ceramic and single crystal ma- terials
15:50	_	16:20	Coffee break Location: Hotel Langue

16:20	_	17:20	Monday Session II
			Location: Lecture Hall
			(chairperson: Z. Kožíšek)
16:20	_	16:40:	Juraj Černák:
			The 90-year-old story of nickel benzoate
16:40	_	17:00:	Lucia Váhovská:
			<i>Co(II) complexes with pseudohalide anions: crystal structures and magnetic properties.</i>
17:00	_	17:20:	Ivan Potočňák:
			cis- $Pd(II)$ complexes with quinolin-8-ol derivatives and dimethylam- monium, K^+ , Cs^+ or quinolinium-8-ol cations as materials for phar- macological research
18:10	_	18:40	Dinner
19:30	-	22:00	Welcom party Location: Lecture Hall

Tuesday, 1 September 2015

08:00	_	8:40	Breakfast
09:00	_	10:00	Tuesday Session I
			Location: Lecture Hall
			(chairperson: M. Koman)
09:00	_	09:20:	Petr Mošner:
			Structure and properties of magnesium phosphate glasses modified by Fe_2O_3
09:20	—	09:40:	Antonín Račický:
			Lead phosphate glasses modified by additions of gallium(III) oxide
09:40	_	10:00:	Pavlína Ruleová:
			Preparation and transport properties of Bi _{2-x} Cr _x Se ₃
10:00	_	10:30	Coffee break
			Location: Hotel Langue

10:30	_	11:50	Tuesday Session II
			Location: Lecture Hall
			(chairperson: J. Černák)
10:30	_	10:50:	Blažena Papánková:
			Synthesis, structural and magnetic properties of mono- and trinuc- lear Co(II) complexes.
10:50	_	11:10:	Ľubor Dlháň:
			Application of the multivariety statistical methods in analysing the spin crossover behaviour
11:10	_	11:30:	Vladimír Jorík:
			The crystal structure - what information actually provides?
11:30	_	11:50:	M. Koman:
			The vector analysis of complexes type $Cu_4OX_6L_4$
12:30	_	13:00	Lunch
			Location: Lunchroom

14:00	_	15:40	Tuesday Session III
			Location: Lecture Hall
			(chairperson: P. Mošner)
14:00	_	14:20:	Maria Behulova:
			Numerical simulation of the resistance spot welding of parts from the AISI 304 steel
14:20	_	14:40:	Máté Nagy:
			Mechanical properties of Al weld joints prepared by friction stir wel- ding
14:40	_	15:00:	Maroš Martinkovič:
			The characteristics of the microstructure anisotropy of the plastically deformed material
15:00	_	15:20:	Marián Palcut:
			Corrosion behavior of Al-TM complex metallic alloys
15:20	_	15:40:	Jaromír Drápala:
			Segregation phenomena of cerium and selected elements at crystal- lization of 42CrMo4 steel
15:40	_	16:10	Coffee break
			Location: Hotel Langue

16:10	_	17:30	Tuesday Session IV
			Location: Lecture Hall
			(chairperson: J. Drápala)
16:10	_	16:30:	Michal Havrlík:
			Determination of structure of polymer nanotextiles
16:30	_	16:50:	Iveta Klicmanová:
			Interaction with nanotextiles
16:50	_	17:10:	Lukáš Válek:
			Novel applications of and solutions in the SOI technology
17:10	_	17:30:	David Lysáček:
			Gettering techniques for SOI wafers
18:00	_	18:40	Dinner
			Location: Lunchroom

Wednesday, 2 September 2015

08:00	_	8:40	Breakfast
			Location: Lunchroom
09:00	_	16:30	Joint meeting of the Slovak expert group of solid state physics and CSACG

Thursday, 3 September 2015

- 08:00 8:40 Breakfast
- 09:00 10:00 **Thursday Session I** Location: Lecture Hall (chairperson: Ĺ. Dĺháň)
- 09:00 09:20: Martin Klejch: New method to grow large core free YAG crystals

09:20	—	09:40:	Michal Horký:
			Ion-beam-induced magnetic transformation of metastable fcc iron- nickel films grown on Si(100) substrates
09:40	—	10:00:	Robert Král:
			Development of micro-pulling-down method for growth of oxide and halide single crystals
10:00	_	10:30	Coffee break

Location: Hotel Langue

10:30	_	12:30	Thursday Session II
			Location: Lecture Hall
			(chairperson: K. Nitsch)
10:30	_	10:50:	Jozef Dobrovodský:
			The current state of new ion beam and plasma facility for material synthesis, modification and analysis
10:50	_	11:10:	Kateřina Dragounová:
			Photoluminescence and Raman analysis of CVD diamond films
11:10	_	11:30:	Petra Zemenová:
			Study of glass by thermal analyses
11:30	_	11:50:	Vladimír Kucek:
			Thermoelectric properties of Ni-doped CuInTe ₂
11:50	_	12:10:	Jan Šik:
			Benefits of cooperation of industrial and university research and development of semiconductor materials and devices
12:10	_	12:30:	Jan Kulveit:
			Nucleation on surface with heterogeneous surface energy in Ising model
12:40	_	13:20	Lunch
			Location: Lunchroom
19:00	_	22:30	Farewell party

Location: Lecture Hall

ABSTRACTS

Numerical simulation of the resistance spot welding of parts from the AISI 304 steel

Maria Behulova and Máté Nagy

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Resistance spot welding (RSW) belongs to the highly effective methods of production weld joints. It is applied with many advantages such as high productivity, low cost, reliability, easy to operate and automate, predominantly in automotive industry [1]. The weld quality is usually affected by several welding and technological parameters: the current intensity, welding time, the force applied by electrodes, contact resistance, the size of electrodes, etc. [2]. Numerical analysis of RSW represents complex problem which involves multi-physics coupling of thermal, fluid, metallurgical and mechanical phenomena [3]. Despite the complexity and difficulty of modeling these coupled phenomena, numerical simulation of RSW processes can provide valuable information on nugget formation and the influence of different parameters on the weld properties [4].

The paper deals with the FEM simulation of the RSW of two sheet parts from the austenitic stainless steel AISI 304. To analyze the process of resistance spot welding, the simulation model considering geometrical characteristics of welded parts, temperature dependent material properties, the initial conditions, thermal, electrical and mechanical boundary conditions and loadings was developed and validated by the realization of real experiments of RSW of two sheet samples from the AISI 304 steel. Using the simulation model of RSW, the effect of chosen welding parameters on the characteristics of weld joints was evaluated by the numerical experiments in the program code ANSYS.

As it follows from obtained results, the welding current is the most important factor influencing the size of molten zone as well as the dimensions of heat affected zone. The welding time and the contact resistance as an indirect process parameter are the less significant factors. However, the correct setting of the contact electrical resistance and its dependence on the contact pressure is very important. Finally, based on the results of numerical simulations, the Lobe diagram enabling to find optimal process window for RSW was predicted. This diagram can help the process engineers to propose suitable welding parameters for production of high quality weld joints.

The research has been supported by the Scientific Grant Agency of the Slovak Republic (VEGA) within the project No. 1/1041/11 and the project ITMS 26220120048 under the Research & Development Operational Programme funded by the ERDF.

- [1] N. T. Williams, J. D. Parker: Int. Mater. Rev. 49, 2 (2004) 45 75.
- [2] M. Eshraghi et al.: Mater. Des. 56 (2014) 387–397.
- [3] E. Feulvarch, V. Robin, J. M. Bergheau: J. Mater. Process. Technol. 153–154 (2004) 436–441.
- [4] H. Moshayedi, I. Sattari-Far: J. Mater. Process. Technol. 212 (2012) 347–354.

The 90-year-old story of nickel benzoate

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The synthesis of nickel benzoate trihydrate, Ni(Bz)₂.3H₂O was first published by Ephraim and Pfister [1] and by Pfeiffer and Müllenheim [2] in 1925 and 1933, respectively. Later, in 1971 Pavkovic studied its IR spectrum and suggested the presence of coordinated and uncoordinated benzoate groups in the structure [3]. The anhydrous complex Ni(Bz)₂ was synthesized in microcrystalline form [4] and Balarew et al. studied the thermal properties of the nickel benzoate tetrahydrate [5]. In 2009 the crystal structure of the dinuclear "paddle wheel" type complex [Ni₂(μ_2 -Bz)₄(HBz)₂], formed incidentally under solvothermal conditions beginning with nickel(II) nitrate, sodium benzoate and bipyridine, was reported [6]. More recently, we were successful in preparing Ni(Bz)₂.3H₂O in single crystal form. The results of a crystal structure analysis led to the reformulation of the trihydrate as ([Ni(Bz)(H₂O)₂](Bz).H₂O)_n; its crystal structure is comprised of positively charged chains [Ni(Bz)(H₂O)₂]_nⁿ⁺, benzoate anions and one water solvate molecule per formula unit. Within the chains hexacoordinated Ni(II) atoms are triply bridged by two aqua ligands and one syn-syn benzoato ligand. The results will be discussed.

This work was supported by the Projects VEGA 1/0075/13, APVV-0132-11 and MAT2011-27233-C02-01 (Spain).

- [1] F. Ephraim, A. Pfister, Helv. Chim. Acta, 1925, 8, 369.
- [2] P. Pfeiffer and S. V. Müllenheim, J. Prak. Chem. 137 (1933) 9.
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- [5] C. Balarew, D. Stoilova, R. Krasteva, Thermochim. Acta 92 (1985) 719.
- [6] J. H. Deng, Y. P. Yi, Z. X. Xiong, L. Yuan, G. Q. Mei, Acta Crystallogr. E65 (2009) m1484.

Dielectric properties through-thickness mapping on extremely thick plasma sprayed TiO2

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Plasma spraying of self-supporting plates (SSP), tubes and variously shaped ceramic parts is performed by WSP process for a long time. First results were published nearly 20 years ago, when Al2O3, ZrO2, mullite and zircon ZrSiO4 were tested as the first materials. Later, various other materials as garnets, basalt, forsterite or diopside were tested. TiO2 was applied for thick wall tubes production as well as for thinner coatings for photocatalytic tests. This material is relatively insensitive to spray torch parameters, and when sprayed using a natural rutile feedstock, is it also inexpensive. The difference in thermal expansion between substrate and coating materials is most typically used for thick self-supporting plates production.

Rutile TiO2 received as a natural mineral was sieved to obtain feedstock powder for spraying (size 100-170 μ m^{''}). Plates were sprayed using the water-stabilized plasma spray system WSP 500 (IPP ASCR, Prague, Czech Republic). For the described experiments the voltage 320 V and current 480 A were set. The powder was fed in through two injectors and thickness of the produced coatings was as high as 15 mm. Massive aluminum blocks were used as substrates. To restore the stoichiometry, thermal post-treatment (annealing) was applied. The samples were heated in a laboratory furnace in the air atmosphere with heating and cooling rates 6 °C/min and with the dwell time of 3 hours on the maximum temperature 1100 °C. Such a temperature is high enough for a stoichiometry restoration and also for substantial changes in the microstructure, and in dielectric properties. Annealing changed the character of porosity. After annealing the porosity is higher but the mean size of pores is smaller. Correspondingly, the number of pores per square millimeter is higher. The pores are less flat and more globular as the annealed microstructure is approaching a sintered microstructure.

The extremely high coating thickness enables us to cut the SSP into three parallel "horizontal" slices (i.e. cuts were perpendicular to the spray direction): one was close the substrate, second one in the middle and the third one close to the surface. This sectioning was performed on as-sprayed deposit as well as on annealed one. Usually the low coating thickness does not allow such a slicing. The layers close to the surface of the annealed SSP exhibited dielectric relaxation at frequency 100 kHz while the central slice and the layers close to the substrate exhibited tendency to relax at frequencies over 1 MHz. Typical relative permittivity of the annealed material was around 150 and loss tangent around 0,05. The volume resistivity in the order 109 Ω m and the surface resistance of the individual slices in the order 1012 Ω were measured. Before the annealing the volume resistivity was in order of only 1 Ω m. This conductive character of the sample was due to the plasma-induced reduction of the TiO2 ceramics into TiO2-x, as reported by the authors in the past. For the restoration of stoichiometry and giving the dielectric character to the material, the thermal annealing is necessary.

Application of the multivariety statistical methods in analysing the spin crossover behaviour

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In a series of hexacoordinate Fe(III) complexes of the $[Fe^{III}L^5X]$ type, where L^5 stands for a pentadentate Schiff-base ligand and X⁻ is an unidentate (pseudo)halide coligand, the structural and thermodynamic characteristics of the spin crossover have been analyzed. Multivariety statistical methods have been applied such as Cluster Analysis, Principal Component Analysis, and pair Correlation Analysis.

The structural characteristics in the first group of complexes show a grouping into two clusters according to the spin state of the complexes (low-spin and/or high-spin) at the temperature of the X-ray experiment. Within the FeN₂N'O₂X chromophore, the bond lengths Fe-Nim, Fe-Nam and Fe-O display a tight mutual correlation along with the angle Σ (overall deviation for the octahedral pattern).

In the second group of the spin crossover complexes the thermodynamic characteristics, such as enthalpy and entropy of the spin transition, transition temperature, and the solid state cooperativeness have been assessed. The tight correlation shows $T_{1/2}$ and ΔH and this proceeds according to a straight line: $T_{1/2}$ [K] = 76 [K] + 38[K kJ⁻¹ mol]* ΔH [kJ mol⁻¹]. On the other side, the theory of the spin transition predicts $T_{1/2} = \Delta H / \Delta S$ because this is an entropy driven unimolecular reaction.

This work was supported by Slovak grant agencies (VEGA 1/0522/14, 1/0233/12, APVV-14-0078).

The current state of new ion beam and plasma facility for material synthesis, modification and analysis

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The new ion beam and plasma laboratories for advanced materials research are currently in the phase of finalization at the Faculty of Materials Science and Technology STU in Trnava. They are built within the project Üniversity Park Campus MTF STU -CAMBO"funded by European Regional Development Fund - Research and Development Operational Programme. The new technologies create conditions for the implementation of basic and applied research in the physical and material engineering including nanotechnology research, as they enable e.g. synthesis, modification and analysis of surface, subsurface and thin layers of solid states. The key technologies and facilities are briefly described, including some typical and/or possible examples of their applications.

The Ion Beam Laboratory is equipped by 6 MV Tandetron - tandem ion accelerator and by 500 kV ion implanter: a/ Two end stations of the 6 MV Tandetron are designed for ion implantation and ion beam analysis, respectively. The energy range from 600 keV up to 50 MeV for heavy multi-charged ions can be reached. Ion Beam Analysis (RBS, channeling, ERDA, PIXE, NRA) can provide for instance depth profile of elemental composition in the range from the surface to the depth of few microns of the samples, trace element analyses, etc.. b/ The 500 kV ion implanter has two end stations for ion implantation and experimental work as well.

The main systems of the Plasma Laboratory are the following: c/ Plasma-immersed ionimplantation apparatus for vacuum deposition and ion implantation with 20 kV bias for flat substrates. d/ Plasma-immersed ion implantation apparatus for plasma-immersion ion implantation and deposition with 40 kV bias system for material treatment and hard coatings of 3D-substrates. e/ DC pulsed magnetron sputtering system three magnetrons, conventional 1 kW DC. f/ Pulsed DC sources RF sputtering system with substrate bias, magnetrons with RF sources. Plasma immersion ion implantation PIII can be applied for synthesis of silicon on insulator, for shallow junction formation by plasma doping, trench doping, as well as for plasma doping and plasma surface modification of biomaterials and diamond-like carbon materials, etc.

The current state of mentioned facilities installation is presented. The completion of laboratories will be by the end of 2015.

This work was supported by the ERDF - Research and Development Operational Programme under the project Üniversity Scientific Park Campus MTF STU - CAMBOÏTMS: 26220220179 and by H2020-EU.4.a. project No. 664526, WIDESPREAD-1-2014 – Teaming: Slovak Centre of Excellence in Ion Beam and Plasma Technologies for Materials Engineering and Nanotechnology – SlovakION.

Photoluminescence and Raman analysis of CVD diamond films

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In recent years, individual colour centres in diamond attract great attention due to interesting potential applications, such as fluorescent markers for bio-imaging based on if they are incorporated in diamond nanoparticles. Recently, the nitrogen vacancy colour centre, in particular negatively charged complex of substitutional nitrogen atom with vacancy in neighbour position (NV⁻) was considered as a convenient candidate, because of pronounced room-temperature emission at 638 nm [1] accompanied with more intensive phonon sideband, which is its major disadvantage. As a promising alternative, it seems to be use of silicon vacancy (SiV) colour centres, with silicon atom incorporated between two vacant lattice positions. A main merit of these centres is the possibility to excite their luminescence by red light and narrow emission in IR/NIR spectral range, falling into the transmission window of biological tissues. Namely, at room temperature, spectrum consists of zero-phonon line (ZPL) at vicinity of 738 nm [2] and weak, practically insensible phonon sideband. Therefore, large effort is devoted to the development of controlled and reproducible methods for fabrication of SiV centres in synthetic diamond.

In this contribution, we focus on steady-state photoluminescence of diamond thin films grown using microwave plasma assisted CVD together with Raman spectroscopy. SEM was used to characterize the film morphology. The film quality was characterized by Raman spectroscopy and correlated by photoluminescence measurements. To recognize optimal preparation conditions, the systematic study on a number of samples series was performed. We investigated influences of gas composition (addition of CO_2 and N_2 in the range 0-4.5 vol. % and 0.5-6.0 vol. %, respectively), substrate temperature in the range 350–1100 °C, and substrate type (Si, quartz, Al₂O₃, and Mo). Our measurements suggest optimal substrate temperature around 800 °C, optical activity independent on substrate material and substantial suppression of luminescence intensity with rising content of CO_2 and N_2 in the gas mixture.

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Segregation phenomena of cerium and selected elements at crystallization of 42CrMo4 steel

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It is known that rare-earth metals (REM) are powerful deoxidising and desulphurising agents in steels. They are particularly attractive because they have boiling points that are high enough to allow their retention in solution in liquid steel to react with oxygen and sulphur according to thermodynamic and kinetic considerations. The influence of cerium, praseodymium and calcium addition on solidification structure of the low-carbon 42CrMo4 steel was investigated. Alloys were prepared by means of a centrifugal casting. The addition of this elements in amount about 0.1 wt.

This work was solved in the frame of the project TA CR No. TA03010161: Experimental development of non-ferrous metals utilization for microstructure refinement in the production of steel ingots for forgings in the specific work and project No. LO1203: Regional Materials Science and Technology Centre – Feasibility Program.

Determination of structure of polymer nanotextiles

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Before nanotextiles can find their place in civil engineering applications their properties must be carefully studied. Since these properties depend on the structure of the material, the determination of this structure becomes a vital task.

For our study we have chosen nanotextiles made of four polymers: PVDF (polyvinylidene fluoride), PUR (polyurethane), PAN (polyacrylonitrile), and PVB (polyvinyl butyral). Each of these polymers has some properties that can be interesting for civil engineering applications. The nanotextiles were produced at Czech Technical University in Liberec by NS 4S1000U device using Nanospider technology. For each polymer several samples have been produced with different speed of motion of supporting fabrics (10 - 50 mm/min).

In the first series of experiments we measured the surface density of our samples and have found its linear dependence on the speed of motion of supporting textile. This result is in a good agreement with theoretical modelling. That means, that if certain application requires nanotextile with a specific surface density, it is possible to predict the corresponding speed of motion of supporting textile.

In the next set of experiments the microstructure of the samples have been studied on SEM Tescan Maia 3. By the analysis of the obtained photos we found a number of important structural parameters: nanofibers and holes size distributions, their orientation. These results can be used to produce a numerical 3D model of the nanotextiles. The common model of a nanotextile structure consists of multiple 2D layers separated by certain distance [1]. Thus, it is important to determine the planar structure of each layer and the separation distance such that the resulting model serves as the best approximation to the real 3D structure.

In order to understand the internal structure of the material we have made blade cuts and studied the surface of the cuts by SEM. While we failed to get as detailed photos of the cuts as the planar structure, we were still able to determine the thickness of the cut and its basic structure. The cut looks almost exactly like the surface of the textile – a network of fibers with random orientations. We devised two different methods to determine the optimal set of parameters for the multilayered model, which give the best approximation to the observed structure of the material. The first method is based on measurement of thickness of the cut and analysis of the photos of the surface of the textile. The second method additionally takes into account the observed similarity of the cut structure to the planar one. The both methods produce close results.

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Ion-beam-induced magnetic transformation of metastable fcc iron-nickel films grown on Si(100) substrates

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Ultrathin fcc Fe films on Cu(100) have been studied for their unique capability of magnetic (paramagnetic to ferromagnetic) and structural (fcc to bcc) transformation upon ion beam irradiation. However, pure fcc Fe films undergo a spontaneous transformation when their thickness exceeds 10 ML (2 nm) [1]. We have shown that it is possible to grow fcc transformable Fe₇₈Ni₂₂ films on Cu(100) single crystal without a limit in thickness [2].

Because single crystals are expensive and inconvenient for industrial applications, we investigate growth of Fe-Ni films on Si(100).

We present a study of deposition and transformation of 22 (4 nm) and 44 ML (8 nm) thick $Fe_{78}Ni_{22}$ films grown on Si(100) substrates. The growth of fcc paramagnetic $Fe_{78}Ni_{22}$ films directly on Si(100) substrate is impossible because of the lattice mismatch. Hence it is necessary to grow an epitaxial Cu(100) buffer layer [3]. Prepared films were transformed by irradiation with 2 keV Ar+ ion beam and the results of the transformation results were observed by Low Energy Electron Diffraction (LEED) and Surface Magneto-Optical Kerr Effect (SMOKE). The possibility of direct focused ion beam writing of ferromagnetic elements embedded in a paramagnetic thin film makes these $Fe_{78}Ni_{22}/Cu(100)/Si(100)$ films an ideal candidate for the fabrication of magnetic nanostructures.

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The crystal structure - what information actually provides?

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A crystal consists of a set of molecules or ions ordered by periodic manner such that the overall free energy of the system is minimum. Such an arrangement is determined by the force action among the atoms which is related to size, shape, charge, dipole moments and hydrophobicity of individual molecules or ions. Due to the existence of a polymorphism and allotropism of crystalline materials it is obvious that despite these general principles, the arrangement of basic building particles in a crystalline solid will also depend on other factors. The shape of crystal is considerably affected by the conditions of its creation - and undoubtedly affect its inner crystal structure, too. These include temperature, pressure, concentrations of starting materials, the sequence in which the components are added, the crystallization method, the homogeneity of the environment and time. Sometimes a change of the arrangement of basic building particles in the crystal needed a big change some of these factors, sometimes it's a subtle change. As a rule, the lattice parameters obtained from single crystal and polycrystalline sample of the same substance may significantly vary in size (the differences often exceed more than ten times standard deviation). A possible explanation lies precisely in the different conditions of their crystallization. Important role to play here time and associated other factors. The process of creation of single crystals of suitable quality for structural analysis can be lengthy, whereas the formation of polycrystalline materials can be extremely fast. With such rapid processes you can assume numerous occurrence of inhomogeneities in the crystallization environment. The crystal structure arising microcrystalline substance will not reach the status of a global free energy minimum. If the energy barrier for example between polymorphs is small, there arise a mixture. A similar effect can also cause an isomorphic substitution of the atoms or ions in the crystal structure of the substance. In polycrystalline form there is possible to prepare the substance with any"ratio of isomorphic atoms (ions), in the case of single crystal it is often practically impossible. The question then is whether there is a transition state of transformation from one polymorphic form to another, or there is always a mechanical combination thereof.

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New method to grow large core free YAG crystals

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A new crystal growth method CRIG (CRystal Improved Growth) has been developed to grow large (currently 125 mm in diameter) core-free single crystals of yttrium aluminum garnet (YAG). Using this method [1], crystals of unmatched quality are produced – size, homogeneity, low stress etc. The growth of 5 inch un-doped YAG for optical elements as well as YAG:Ce for scintillating screens and Yb:YAG for solid-state laser systems has been accomplished in CRYTUR spol. s r.o.

Two types of laser elements were cut and polished from these Yb:YAG crystals: disc of diameter 80 mm \times 8 mm thickness and square slab with dimensions $120 \times 100 \times 8$ mm. The wavefront distortion of laser-quality polished crystals was smaller than $\lambda/20$ (λ of HeNe laser = 633 nm) in its Peak/Valley value. This indicates very low level of internal stress in the optically perfect flat surface of the crystal. The laser surface finishing parameters measured on the smaller disc are: Scratches/Digs 10/5, parallelism ; 1' arc min. Such large laser slabs are being finalized in collaboration with ELI beamlines project (Extreme Light Infrastructure) in the Czech Republic.

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Interaction with nanotextiles

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Nanotextiles physical properties modelling has been a much discussed lately. Understanding their physical properties and process parameters for their production is very important for the future use of this type of material. To be able to adequately describe nano, it is also necessary to examine their various physical and mechanical interactions. Construction practice focuses on macro scale and thus neglects some interactions. Therefore it is necessary to deal with interactions at the micro and nano levels. Beyond a doubt Van der Waals forces or dipole moments affect this world. This article is a brief research describing the Van der Waals interactions, DLVO potential and the piezoelectric effect. These interactions can have a positive impact on changing the properties of nanotextiles and their subsequent use in practice.

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The vector analysis of complexes type Cu₄OX₆L₄

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The vector model of chemical structure is based on vector analyses of valence bonds, nonvalence interactions and selected interatomic distances in the structure of chemical compounds. The vector structural model is applied to known structures of coordination compounds of the type $Cu_4OX_6L_4$, X = Cl, Br; L = ligands with Cl, N, O donor atoms.

Vector analysis is applied to structures of $Cu_4OCl_6(3\text{-pyme})_4$ (3-pyme = 3-pyridylmetanol) [1] and $Cu_4OCl_6(3\text{-pyet})_4$ (3-pyet = 3-pyridyletanol) molecules [2]. Composition of these molecules differs very slightly in different ligand substituents -CH₂-OH and -CH₂-CH₂-OH. The consequences of the ligand difference for structures of both complexes are presented by means of vector analysis which provides for both structures the sets of quantitative vector parameters. These are compared with structures and corresponding vectors of $Cu_4OCl_6(OPPh_3)_4$ molecule (highest symmetry, lowest possible vector values) [3] and $Cu_4OCl_6(2\text{-Mepy})_4$ molecule (steric effects in low symmetry, very high vector values) [4].

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Growth rate of nuclei

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Lagragian approach to growth rate of nuclei considers growth of isolated clusters formed by collisions of monomers (molecules, atoms or growth units) with cluster surface. Growth rate is derived from attachment and detachment frequencies on cluster surface, respectively from volume changes of clusters [1]. Eulerian approach instead of observing the growth of specific cluster is based on the study of fluxes between two adjacent clusters [1]. We introduce new alternatively approach based on the growth of the largest nuclei within the standard nucleation theory.

The kinetic equations for formation of nuclei are solved numerically to determine the number of clusters, F_i , formed by *i* monomers. The maximum size of nuclei, i_{max} , in considered volume V, is determined from the condition $F_iV = 1$. Growth rate of nuclei is determined as time derivative of radius of the largest nucleus within system. It is shown that at low supercooling (or supersaturation) growth rate of nuclei in sufficiently large volume reaches the values, which are very close to Lagragian model. As system volume decreases, the supercooling needed to form nuclei is higher [2]. At low supersaturation the growth of nuclei will be stopped and only certain maximum nucleus size is reached. It is necessary to have sufficiently high supersaturation to enable growth of supercritical nuclei.

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Development of micro-pulling-down method for growth of oxide and halide single crystals

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The micro-pulling-down (μ -PD) technique is a new crystal growth method from the melt, which has been developed since 1992. The term "pulling-down" represents the direction of solidification and "micro" reflects the presence of microcapillary channel(s) about 0.2-2 mm in diameter at the bottom of the crucible [1]. The melt residing in a crucible is transported downward the microcapillary in the bottom of the crucible, where solidification and formation of the crystal-melt interface take place. Appropriate configuration of the crucible bottom and properly selected temperature gradient allow to control the crystal shape and the dimensions of the crystals cross section ranging from 0.1 to 10 mm. Yoon et al. [2] presented a first modern design of a resistively heated μ -PD apparatus created in Tohoku University, Japan, for the growth of LiNbO₃ thin-fiber crystals. Furthermore, a μ -PD prototype apparatus equipped with a radiofrequency inductive heat source for preparation of Si_{1-x}Ge_x mixed crystals was reported by Koh and Fukuda [3]. In 1999, Yoshikawa et al. [4] reported on crystal growth of Al₂O₃/Y₃Al₅O₁₂ eutectic fibers using μ -PD apparatus equipped with Ir crucible placed on Ir afterheater with two windows for real-time observation with CCD camera. Significant contribution on adaptation of μ -PD apparatus for crystal growth of fluoride materials (Ce:PrF₃) was presented by Yoshikawa et al. [5]. The μ -PD apparatus was equipped with tight vacuum chamber, allowing evacuation of the system down to 10⁻⁵ Torr before crystal growth, CaF₂ window for direct observation, and carbon crucible and afterheater surrounded by refractory carbon as heat shield. In 2010, Yokota et al. [6] presented a development of μ -PD apparatus for preparation of hygroscopic halide crystals by adding a removable chamber into the growth arrangement. This chamber allowed its transportation into an atmosphere controlled glove box where an experimental setting and handling of starting materials was held. This contribution presents a review of the development of the μ -PD method used for preparation of oxide crystal growth and growth of materials with more demanding experimental arrangement. Recent results of new material conceptions for applications as radiation detectors or mid-IR lasers will be discussed.

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Thermoelectric properties of Ni-doped CuInTe₂

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There is currently a boom in a search for alternative power resources. One of the alternatives is the usage of the thermoelectric effect. Research on thermoelectric (TE) materials is thus a very active field of research. Efficiency of a TE material is expressed in terms of a so-called dimensionless figure of merit, ZT, where $ZT = \alpha^2 \sigma T / \kappa$. In this formula, α , σ , T and κ are the Seebeck coefficient, electrical conductivity, absolute temperature and thermal conductivity, respectively [1].

Recently, a classes of ternary I-III-VI₂ (I = Cu, Ag, III = Al, Ga, In, and VI = S, Se, Te) and quaternary Cu₂-II-IV-VI₄ (II = Cd, Hg, IV = Sn, Ge, VI = Se, Te) copper-based compounds with diamond-like structures have been reported to show promising TE properties in the middle-temperature range. For example, the maximum ZT values are 0.77 for Ag_{0.95}GaTe₂ at 850 K [2], 1.4 for CuGaTe₂ at 950K [3], 1.18 for CuInTe₂ at 850 K [4].

Polycrystalline samples of composition $Cu_{1-x}Ni_xInTe_2$ (for x = 0 - 0.05) were synthesized from elements of 5N purity using a solid-state reaction. The phase purity of the products was verified by X-ray diffraction. Samples for measurement of the transport properties were prepared using hot-pressing. The samples were then characterized by the measurement of electrical conductivity, the Hall coefficient, the Seebeck coefficient, and the thermal conductivity over a temperature range of 300 - 675 K. All of the samples demonstrate p-type conductivity. We discuss the influence of Ni substitution on the free carrier concentration and the thermoelectric performance. The investigation of the thermoelectric properties shows an improvement up to 50 % improvement of ZT in the temperature range of 300 - 600 K.

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Nucleation on surface with heterogeneous surface energy in Ising model

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First order phase transitions begin with a stage of nucleation, when individual particles form small domains of the new phase within the metastable old phase. Basics of this process can be described using the classical nucleation theory, but is some more complex nucleation scenarios, necessary modifications of theory were often hard to test experimentally. In such cases computer simulations can be very useful.

We utilize Ising model to study a specific case of nucleation scenario: nucleation in the presence of an inhomogenuous surface energy. The results are obtained using Monte Carlo simulation in lattice Ising model with spin-flip dynamics, utilizing the Ümbrella samplingäs a method to overcome difficulties with simulation of rare events. We also utilize corrected cluster-counting algorithm, leading to different results from so called "geometrical cluster" count.

Several cases of inhomegeuouss surface energy were studied: array of regular bars of different energy, random noise, and a specific patterns designed in attempt to influence nucleation progress. Results mainly show that heterogenity of the surface energy helps the nucleation process.

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Gettering techniques for SOI wafers

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The Silicon-On-Insulator (SOI) wafer consists of a handle wafer and a device layer, both being separated by a dielectric isolation. The handle wafer usually serves as the supporting layer only with no influence to device parameters. The device layer (made from silicon single crystal) has the thickness ranging from less than one micrometer for "thin SOI" up to more than ten micrometers for "thick SOI". The electrical insulation is usually less than one micrometer thick silicon dioxide layer which helps to reduce parasitic capacitances, leakage currents and temperature dependent performance degradation. The SOI concept allows making the electronic devices and integrated circuits smaller, faster, and more powerful. On the other hand, solution of heat dissipation or impurity gettering is more complicated than for standard silicon wafers.

The presence of the buried oxide layer prevents diffusion of contaminants from the device layer to the bulk of the handle wafer and to the wafer backside. The gettering sinks are therefore preferentially placed between the buried oxide and the device layer or on the top of the device layer. However, the close proximity of the gettering sinks to the devices induces some restrictions and requirements to the gettering techniques used. The solution may vary for thin and thick SOI.

The overview of the gettering techniques used for SOI wafers will be presented and the need for novel solutions will be discussed.

Scintillation properties of LuAG:Ce ceramic and single crystal materials

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An intense studies and research of Ce^{3+} -doped heavy and fast lutetium based $Lu_3Al_5O_{12}$ (LuAG) garnet scintillation crystals started around year 2000 [1]. Detailed properties of LuAG:Ce single crystal were summarized by M. Nikl et al. in paper [2]. Besides LuAG:Ce scintillating crystal also LuAG:Ce ceramics were prepared and investigated from year 2005 [3,4]. LuAG:Ce ceramics are characterized with no antisite-based shallow electron traps which are present in the Czochralski grown LuAG:Ce single crystals [4]. Besides LuAG:Ce ceramics also LuAG:Pr ones were prepared [5].

In this talk we will present the newest results of scintillating properties of LuAG:Ce ceramic and single crystal materials including a comparison between them. Scintillating properties as light yield, energy resolution (both the photopeak ones and the photo-escape ones) and non-proportionality were measured by a HPMT photomultiplier under various radioisotope excitation [6]. Different LuAG:Ce ceramics were studies as (i) Mg co-doped ones, (ii) nonstoichiometric ones (with an excess of Lu) and an influence of annealing (both on ceramics and single crystals). The latest development of LuAG:Ce ceramics resulted in high performance materials with the same light yield 27000 ph/MeV as that of LuAG:Ce single crystals.

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The characteristics of the microstructure anisotropy of the plastically deformed material

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Final properties of formed steel or another alloy pieces are affected even by plastic deformation of material. Therefore it is needful to know detail structure changes of material under conditions of plastic deformation caused by forming, milling, turning, grinding, drilling etc. Estimation of the deformation based on its observable macroscopic effects doesn't correspond fully with microscopic structural changes in whole volume of deformed parts and such estimation is quite impossible in case if only surface layers are deformed. In case of plastic deformation a non deformed isometric structure will take an anisometric status. In the polycrystalline material (metal, alloy) the main microstructural parameter is grain boundary - surface interface between individual grains. In case of isotropic structure the grains have isometric dimension mean grain size or size distribution of grains is sufficient specific surface area of grain boundaries can be measured. In case of anisotropic structure the grains have anisometric dimension, it is necessary to describe their anisotropy [1]. Grains boundaries orientation is the same as direction of deformation and due to it in most of deformation processes prior knowledge of the axes of orientation are known. It allows scalar measurement of anisotropy - to determine degree of orientation. The anisotropic microstructure is decomposed into isotropic, planar and/or linear oriented components - specific surface area of grain boundaries and these parameters are measured using stereology [2]. Degree of grain boundary orientation can be used for estimation of local plastic deformation. Real state of grain shape is quit impossible to describe [3], therefore model of conversion of degree of grain boundary orientation to deformation based on an idealized shape of grains has been proposed. Our conversion model is independent on an initial grain size (as it is in another model [4]) – strain depends only on the shape of the grain and does not depend on its dimension. It allows experimental estimation of local plastic deformation by means of measurement of anisotropy of structure - grain boundary orientation in various areas of plastically deformed parts.

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Use of polyvinylpyrrolidone in the LiNbO₃ thin films deposition

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Lithium niobate belongs to the group of the most important crystalline materials. This ferroelectric material with the Currie temperature of $1150 \,^{\circ}$ C is mostly used in acusto-optic devices, optical waveguides, nonlinear optics and pyroelectric sensors. Its applications are extended using rare earth ions doping. LiNbO₃ is prepared in the form of monocrystals, optical fibers or thin films. The thin films are produced by various methods – e.g. ion implantation, liquid phase epitaxy (LPE), pulsed laser deposition (PLD), molecular beam epitaxy (MBE), chemical vapor deposition (CVD), physical vapor deposition (PVD) or a sol-gel technique. Due to the Er^{3+} ion luminescence, the doped LiNbO₃ can be used in the IR region for the amplification of optical signal in the third telecommunication window (1525 nm). The codoping of Er^{3+} and Yb³⁺ ions increases the intensity of the Er^{3+} luminescence due to energy transfer between the excited states of both ions.

This work presents the preparation of LiNbO₃ thin layers doped with 0.5 at % of Er^{3+} and 0.5 at % of Yb³⁺. The layers were deposited on a sapphire (0001) substrate by spin-coating. Used solutions were prepared by a non-aqueous sol-gel method using a 2-methoxyethoxide solution of present cations and polyvinylpyrrolidone (PVP). The influence of different PVP molar mass (29 000 or 360 000 g/mol) on the final microstructure was tested. Then the effect of different annealing of the deposited films (one- or two-step) was examined. Its influence on the film crystallinity, on the Er^{3+}/Yb^{3+} : LiNbO₃ luminescence and waveguiding properties was investigated. The thin films were characterized by the photoluminescence and transmittance spectroscopy, m-line spectroscopy, X-ray diffraction analysis, scanning electron microscopy, atomic force microscopy and thickness measurement.

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Structure and properties of magnesium phosphate glasses modified by Fe_2O_3

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Magnesium-iron phosphate glasses were studied in the compositional series $(40-x)MgO-xFe_2O_3-60P_2O_5$ within the concentration range of x=0-40 mol

Raman spectra showed that the structure of all glasses is formed mainly by metaphosphate (Q^2) and diphosphate (Q^1) structural units interconnected by P-O-P bonds. The replacement of MgO by Fe₂O₃ leads to the depolymerisation of the phosphate structural network and to the partial transformation of Q^2 units into Q^1 units and finally to the isolated Q^0 orthophosphate units. The incorporation of FeO_x structural units to the parent magnesium phosphate glass results in an increase of the density, molar volume, chemical durability and refractive index of glasses whereas their Abbe number nonlinearly decreases. The replacement of P-O-P bonds by P-O-Fe(II) or P-OFe(III) bonds with increasing Fe₂O₃ content leads also to changes in thermal properties of these glasses. Increasing Fe₂O₃ content in the glasses resulted in a gradual decrease of glass transition temperature and dilatometric softening temperature whereas thermal expansion coefficient does not change significantly. The DTA curves showed that all glasses crystallize on heating in the temperature decreases with increasing Fe₂O₃ content. The lowest thermal stability and therefore the highest tendency towards crystallization were found for the glass containing 40 mol

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Mechanical properties of Al weld joints prepared by friction stir welding

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The paper deals with the friction stir welding (FSW) of the EN AW 7075-T651 high strength aluminum alloy with the aim to analyze the influence of welding parameters on the mechanical properties of Al-weld joints. FSW represents relatively novel solid-state technology of material joining which can be successfully applied as well as for welding of several metallic alloys including the high-strength aluminum alloys that are hard to weld by conventional fusion welding processes [1,2].

In cooperation with VÚZ - PI SR Bratislava, nine experimental weld joints of samples with dimensions of $300 \times 150 \times 10$ mm were prepared using the welding machine of the FSW-LM-060 type and different parameters of welding – the welding speed from 60 to 120 mm/min. and the tool rotation rate from 600 to 1000 rpm in clockwise direction. The quality of weld joints was evaluated by X-ray testing. Subsequently, the static tensile tests and microhardness measurements of weld joints were performed.

According to obtained results of tensile testing, the average values of ultimate strength of weld joints are by 32.2 % lower comparing with the ultimate strength of the base material. On the other hand, the ductility increased by 7.2 %. By the tool rotation rate of 600 rpm, the decrease in ultimate strength and also in ductility with increasing welding speed was identified probably as a result of imperfect mixing the base materials. The highest microhardness of weld joints at the level of 129 HV was measured in thermo-mechanically affected zone on the retreating side.

Based on the attained result, the following parameters of friction stir welding for joining of sheets with the thickness of 10 mm from the investigated high strength aluminum alloy can be recommended: the welding speed of 60 mm/min. and the tool rotation rate of 600 rpm.

The research has been supported by the Program to support young researchers (NUM-KOM-FSW) 2015 STU Bratislava and by the Scientific Grant Agency of the Slovak Republic within the project VEGA No. 1/0470/14.

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The Origins of the Institutions for Crystal Growth

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The aim of this contribution is to inform participants of the 25th Joint Seminar DMSRE about the origins of the International Conferences on Crystal Growth and formation of the International and National Organizations on Crystal Growth and Journal of Crystal Growth.

International Conference on Crystal Growth held on 20 - 24 Juni 1966 Boston (MA), USA is labeled as the ICCG-1. Organizing such a conference was an idea of Michael M. Schieber, at that time a Research Fellow at the Imperial College at Harvard University. M. Schieber started to organize this conference in summer 1964 and for his thought he obtained such heavyweights in the field of crystal growth as were B. Chalmers, S. Peiser, R.A. Laudise, K. Jackson, J. Wenckus, R. Parker, D. Turnbull, K. Button (all from the USA), Ch. Frank, W. Bardsley (UK), R. Kern (France), I.N. Stranski, S. Haussuhl (Germany), H. Bethge (East Germany), I. Sunagawa (Japan). These crystal growers became later members of the Organizing Committee of the ICCG-1.

Organization of this conference was not simple because some American organizations, mainly those which have organized so far meetings dealing with crystals growth and their characterization, remonstrated against organization of Schieber's conference (for instance American Ceramic Society, Electrochemical Society, American Crystallographic Society, and International Union of Crystallography (IUCrys). The last one, according to the then President P.P. Ewald, was convinced, that both crystal growth and crystals preparation pertain to crystallography.

Another problem that the organizers had to solve was the Conference Proceedings edition. They should be only as Appendix of the Journal of Physics and Chemistry of Solids not distributed to all subscribers of the Journal. M. Schieber made a rapid action – to establish a new journal concerning only with crystal growth. B. Chalmers agreed to co-edit such a journal, K. Button accepted the position of principal editor and N. Cabrera joined the Editorial Board as a member.

The conference was a great success. It attracted some 625 participants presenting more than 160 contributions published in the Proceedings of an International Conference on Crystal Growth.

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Corrosion behavior of Al-TM complex metallic alloys

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Binary Al–TM alloys (TM = transition metal) belong to a recently discovered group of complex metallic alloys (CMA). These materials are composed of structurally complex intermetallic phases with large unit cells, inclusive of quasicrystals. Because of their complex crystal structure, the properties of these materials differ from traditional alloys. Corrosion studies of CMA are limited. Only few investigations have been conducted so far in spite of their significance for technological applications of these alloys.

In the current work, we studied the corrosion performance of Al-Co and Al-Pd alloys in saline solutions. Six Al-Co alloys and three Al-Pd alloys were prepared from high purity lumps of Al, Co and Pd by arc–melting. The as-cast alloys microstructure and phase occurrence were investigated by a combination of scanning electron microscopy and roomtemperature X–ray diffraction. The alloys were found to consist of several microstructure constituents with different chemical composition. Structurally complex intermetallic phases have been identified. The alloys phase occurrence has been discussed based on both previously published Al–TM phase diagrams and non–equilibrium processes taking place during casting.

The Al-Co and Al-Pd alloys were corrosion tested in aqueous NaCl solution (3.5 wt %) at 21 °C. The electrochemical polarization was conducted in a standard 3–electrode cell controlled by potentiostat. The corrosion potentials and corrosion current densities were determined by Tafel extrapolation of the experimental polarization curves. A pitting corrosion has observed on the alloy surfaces, with some of the phases being preferentially corroded. The effect of the phase chemical composition has been evaluated. The local nobility of individual intermetallic compounds is discussed. Finally, the conclusions for the alloys corrosion resistance in marine environments are provided.

Mr. Dušan Janičkovič is thanked for sample preparation. The project support from European Regional Development Fund via agreements ITMS:26220120014 and ITMS:26220120048; the Grant Agency VEGA via projects nos. 1/0018/15 and 1/0068/14; the Slovak Research and Development Agency via agreement no. APVV–0076–11 and the Slovak Academy of Sciences via "Centre of Excellence for functional multiphase materials" (FUN–MAT) are gratefully acknowledged.

Synthesis, structural and magnetic properties of mono- and trinuclear Co(II) complexes.

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Co(II) complexes are of particular interest for developing magnetic and optical materials because of (a) variable coordination geometries (i.e. octahedral, tetrahedral, etc.), (b) significant stability in the air, (c) two different spin states (s = 3/2 and 1/2) depending on the ligand field, (d) different electronic structures and color, and (e) large orbital moment through a spin orbit coupling in octahedral geometry.

Heterocyclic N-donor ligands are widely used in assembling complexes which exhibit interesting magnetic properties. Carboxylate groups display a variety of binding geometries, such as monodentate, terminal, chelating, bidentate bridging and monodentate bridging in coordination chemistry. The reactions of cobalt(II) acetate with 2-ethylbenzimidazole (2-etbz) or with 1,10 – phenathroline (phen) were observed at a ratio of 1:1 methanol – acetonitrile solution. Two kinds of complexes were isolated: mononuclear $[Co(2-etbz)_2(OAc)_2],(1)$ and linear trinuclear $[Co_3(phen)_2(OAc)_6]$, (2). The structures of complexes 1, 2 were determined by X-ray diffraction analysis. The complex 1 crystallizes in the monoclinic system and the centrosymmetric space group P21/n. The structure of complex 1 confirms a tetrahedral coordination with CoN₂O₂ chromophore. Several groups have reported cobalt(II) coordination compounds showing a similar stoichiometry $[Co(bz)_2X_2]$ (X⁻ = Cl, Br, I)[1]. In all cases, the geometry adopted by the metal ion is tetrahedral. The complex 2 crystallizes in the triclinic system and the space group P-1. The structure of 2 consist of linear trinuclear molecules; each pair of cobalt atoms are bridged by three acetate ligands to the central Co(2) atom, which is located at an inversion center. Two of them acting as a monoatomic bridge plus bidentate chelating mode, at a distance of 2.373 Å. The coordination environment of Co(2)is completed by two N atoms of phen ligand to form a distorted CoN2O4 octahedron and the Co(1) has a CoO_6 octahedral geometry. The $Co_3(OAc)_6$ core is similar to those found in $[Co_3(bipy)_2(OAc)_6].[2]$

The objectives of this contribution are high-spin Co(II) monomer and linear trimer in various coordination. Magnetic data, reported in literature, for the high-spin Co(II) complexes are reviewed. The investigation of high-spin Co(II) monomer in distorted tetrahedral coordination and distorted octahedral coordinated linear trimer is presented.

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cis-Pd(II) complexes with quinolin-8-ol derivatives and dimethylammonium, K⁺, Cs⁺ or quinolinium-8-ol cations as materials for pharmacological research

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NH₂(CH₃)₂[PdCl₂(XQ)] complexes (XQ are halogenderivatives of quinolin-8-ol (5-chloro-7-iodo-quinolin-8-ol (CQ), 5,7-dibromo-quinolin-8-ol (dBrQ) and 5,7-dichloro-quinolin-8ol (dClQ)) exhibit moderate anticancer activity tested on human ovarian carcinoma cell line A2780 and cisplatin resistant cell line A2780/CP [1]. Therefore we decided to prepare complexes with the same $[PdCl_2(XQ)]^-$ complex anions however with the cations which are more easily accepted by a human body. Trials to prepare such complexes with cations of alkali metals in direct syntheses have been unsuccessful, however complexes in powder form were prepared within cationic exchange between dimethylammonium and K⁺ or Cs⁺ cations. All six prepared complexes were characterized by IR spectroscopy which showed that ν (N–H) and ν (C–H) vibrations from NH₂(CH₃)₂⁺ cations were missing in K/Cs[PdCl₂(XQ)] complexes thus confirming successful cationic exchange. On the other hand, four HQH[PdCl₂(XQ)] crystalline complexes were prepared by direct syntheses (HQH is quinolinium-8-ol, while XQ are CQ, dBrQ, dClQ and 5-nitro-quinolin-8-ol). Their structures contain square-planar cis- $[PdCl_2(XQ)]^-$ complex anions in which XQ molecules are bidentately coordinated to Pd(II) atoms by nitrogen and oxygen atoms. Negative charges of the anions are balanced by uncoordinated planar HQH cations. The structures are stabilized by hydrogen bonds and π - π interactions. Anticancer and antimicrobial activities of the prepared compounds will be presented.

This work was supported by the Slovak Research and Development Agency under contract No. SK-SRB-2013-0004, by the VEGA grant 1/0598/14, and by the Ministry of Education, Science and Technological Development of the Republic of Serbia (grant No. 41010 and projects Nos. 175069 and 175103). S.A.D. thanks The National Scholarship Programme of the Slovak Republic for the financial support during his stay at P.J. Šafárik University in Košice.

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Lead phosphate glasses modified by additions of gallium(III) oxide

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Lead phosphate glasses doped with Ga_2O_3 were prepared and studied in the compositional series A: (50-x)PbO-xGa_2O_3-50P_2O_5 within the concentration range of x=0-15 mol

The structure of the glasses was studied by Raman spectroscopy. Optical properties were studied using critical angle method. Differential thermal analysis, thermodilatometry and heating microscopy have been used to study thermal behaviour of the glasses.

According to the Raman spectra, the glass structure consist of tetrahedral PO_4 metaphosphate (Q²) units and increasing Ga_2O_3 content leads to their transformation to Q¹ units. In the glasses with high Ga_2O_3 content we can see vibrational bands belonging to GaO_6 and GaO_4 structural units.

Index of refraction decreases and Abbe number increases with increasing Ga_2O_3 content in B series. DSC studies showed that all of glasses crystallize on heating within the temperature region of 365-800° C. Compounds formed by crystallization were $Ga(PO_3)_3$ and $GaPO_4$. Glass transition temperature and crystallization temperature increase with increasing Ga_2O_3 content. The thermal stability of glasses in A series has a maximum at 10 mol

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Preparation and transport properties of Bi_{2-x}Cr_xSe₃

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The objective of this work is the synthesis of single crystals Bi_2Se_3 with the greatest concentrations of chromium and determine its influence on the transport properties of Bi_2Se_3 . The use of chromium, according to our ideas should lead to a reduction in the concentration of free electrons due to the different value of electronegativity Cr and Bi, and thus positively influence the thermoelectric (TE) properties of Bi_2Se_3 . In addition to practical application in TE applications, Bi_2Se_3 is also examined with respect to magnetic or topological properties [1]. Another issue is the possible development of ferromagnetism or change in topological properties due to the presence of chromium substitution.

Own work describes both the preparation and characterization of single crystal Bi₂Se₃ doped with chromium [2]. Single crystals of the composition Bi_{2-x}Cr_xSe₃ where x = 0; 0.02; 0.03; 0.04 were grown from elements of high purity. The purity of the prepared samples was confirmed by X-ray diffraction, which was also used to measure the lattice parameters. Transport properties comprising the Seebeck coefficient S, Hall coefficient RH and the electrical conductivity σ were measured in the temperature range 80-470 K. The transport measurements suggest that the incorporation of chromium atoms in the crystal structure Bi₂Se₃ actually leads to a decrease in concentration of free charge carriers apparently due to increased activation energy of formation of native point defects in the crystal. From the data was calculated the value of the power factor σ S² and the estimated value of the figure of merit ZT at 370K.

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Benefits of cooperation of industrial and university research and development of semiconductor materials and devices

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Abstract was not sent.

Co(II) complexes with pseudohalide anions: crystal structures and magnetic properties.

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There is continuous and increasing research interest in the preparation of coordination compounds containing metal ions with an orbital contribution to the magnetic moment and thus to strong magnetic anisotropy, because of their potential use as magnetic materials. The first theoretical studies on the magnetic anisotropy of six-coordinated cobalt(II) complexes caused by axial distortion date to more than 40 years ago [1]. Among the ligands used, linear pseudohalides, such as cyanide, azide and thiocyanate, have long been studied.

The purpose of our work was to synthesize new mono-, binuclear or polymeric hexacoordinated Co(II) complexes with the CoN₆ chromophore containing linear (N₃, NCSe) and nonlinear [N(CN)₂ (dicyanamide, dca), C(CN)₃ (tricyanomethanide, tcm), ONC(CN)₂ (nitrosodicyanmethanide, ndcm), NO₂NCN (nitrocyanamide, nca), NC(CN)₂₂ (1,1,3,3-tetracyano-2azapropenide, tcap), NO₂C(CN)₂ (nitrodicyanomethanide, nodcm), C(CN)C(CN)₂₂ (1,1,2,3,3pentacyanopropenide, pcp)] pseudohalide anions and to investigate their magnetic properties, depending on the crystal structures.

From the Co(II)–L–X systems, where L= 2,2'-bipyridine, 1,10-phenanthroline, 4-amino-3,5-bis(2-pyridyl)-1,2,4-triazole and X = NCSe, N₃, dca, tcm, ndcm, nca, tcap, nodcm, pcp, 17 compounds have been isolated and structurally characterized. Magnetic properties of these compounds were studied, too [2, 3].

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Novel applications of and solutions in the SOI technology

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The Silicon-On-Insulator (SOI) wafer comprises a single crystal silicon layer (device layer) situated on the supporting silicon wafer (handle wafer), both being separated by a dielectric layer. The electrical insulation of the devices from the handle wafer reduces parasitic capacitances, leakage currents, temperature dependent performance degradation and occurrence of latchup. As the consequence, SOI has allowed making the electronic devices and integrated circuits smaller, faster, and more powerful for already a few decades. While typical applications utilize the insulating function of the oxide in the SOI structure, here we present a novel, alternative way of taking the advantage of SOI – utilizing the extraordinary accuracy of thickness control.

There are types of electronic devices whose performance strongly depend on the final thickness of the die. For example the device efficiency of IGBT technologies increases as the die gets thinner. In order to guarantee the performance stability, however, the thickness must be controlled within limits, which become tighter for thinner dies. The SOI approach offers the solution for new IGBT generations where standard manufacturing technologies are no longer sufficient.

The BGSOI technology (Direct Bond and Grind-back SOI) - the basic method of making SOI wafers – will do the trick for reasonable price. After wafer bonding and bond strengthening annealing, the material of the device wafer is removed by means of mechanical grinding and the surface of the final device layer is finished by polishing. The typically achievable uniformity of the device layer thickness is $\pm 0.5 \ \mu$ m. The material of the supporting wafer is removed by Taiko grinding and silicon etching and the buried oxide is removed by HF etching. The resulting die thickness keeps the exceptional thickness uniformity of BGSOI, which is an order of magnitude better compared to conventional variability of Taiko grinding $(\geq \pm 5.0 \ \mu$ m) used with conventional process of device manufacturing.

Novel solutions of aspects specific for SOI are discussed as well. These include gettering and stress engineering.

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Study of glass by thermal analyses

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Thermal analyses are widely used in the study of thermal properties such as glass transition (the reversible transition in amorphous materials) and crystallization (nucleation and growth of crystals). Thermal properties are studied by methods DTA (differential thermal analysis), DSC (differential scanning calorimetry), TMA (thermomechanical analysis), thermodilatometry, and optical thermomicroscopy. Samples are measured by both non-isothermal (constant heating rate) and isothermal modes (constant temperature). [1]

The result of measurements are curves, which show dependence of heat flow (DTA, DSC) or displacement ΔL (TMA, thermodilatometry) on the time or temperature. These curves provide information about the change of physical properties, physical and chemical phenomena that take place in the sample during its heating, cooling or isothermal soaking time. Thermal stability, kinetic parameters (i.e. activation energy, frequency factor, Avrami parameter) for both the glass transition and the crystallization are calculated from obtained data [1]. From TMA and thermodilatometry measurement the first and second order phase transition, the values of coefficient of thermal expansion, viscoelastic behaviour, and softening temperature are obtained [2, 3]. Crystallization of transparent glassy sample (formation of nuclei, their dimensions, and crystallization front movement) was studied by optical thermomicroscopy [4].

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SLOVALYTICAL & ME	ASURING & TESTING	ANAMET Slovakia s.r.o. 1.Mája 794/29, 900 01 Modra
A)	Materiálové analýzy (f	vzikálne a chemické metódy)
Kombinované technik Testovanie žiaruvzdor (RUL, CIC, HMOR).	Termická analýza TG, DTA, DSC, STA, TMA, DMA, DIL. y (TA-MS, TA-FTIR). ných materiálov	Objektívne hodnotenie farebnosti. Prenosné a stolné spektrofotometre, leskomery, receptovanie farieb. Analýza svetla a meranie obrazoviek.
Quantachrome INSTRUMENTS metria, He pyknometr	Meranie špec. povrchu a porozity, Hg porozi- ia , sorpcia vodnej pary .	Distribúcia veľkosti a tvaru častíc, Zeta potenciál, molekulová hmotnosť, Morfológia, rotačné viskozimetre a rheometre.
B) Aplik	ácia pre farmáciu, potr	avinárstvo, biochémiu, kozmetiku
Biotage	Mikrovlnné syntézy, flash ch syntetizátory peptidov	romatografia,
PRRTICLE MERSURING SYSTEMS	Čítače častic vo vzduchu (a monitorovanie čistých priest Biologické monitorovacie sy ISO 14698-1, cGMP, GAMP C) Materiálo	ž 100 l / min) a vo vodách, orov podľa ISO 14644-1 a USP 797, stémy v súlade s požiadavkami PR a farmakológie. vé skúšobníctvo
a vibračné komory (n vrátane shakeru TIRA	Klimatické, termostatické, šokové, vákuové, korózne nožnosť TURN KEY riešení I), ESS a HALT/HASS	Komory pre simuláciu poveternostných COFOMEGRA podmienok (UV a slnečné žiarenie, 100% vlhkosť, korózna atmosféra v soľnej hmle-Salt Spray,atď.)
Skúšanie materiálov Kalorimeti Spaľovaci bod vzpla	požiarnej odolnosti /. re (Bomb&Cone), e komory (horľavosť, nutia, toxicita atď.)	Univerzálne hydraulické a elektromechanické skúšobné stroje pre skúšky v ťahu, tlaku a ohybe, Charpyho kladivá, MFI-tavný index, dart drop impact testery, teplota priehybu pri zaťažení HDT, stanovenie odolnosti za tepla podľa Vicata, meranie tuhosti, torzné skúšobné stroje.
elementar	D) Analyf Spaľovacie elementárne an TOC/TN autosampler pre k Izotopová hmotnostná spek	ické techniky alyzátory C/H/N/S/O, Rapid N, vapaliny a pevné vzorky, troskopia.
	E) Analýza	a paliv a maziv
SETA Setta	IR stanovenie b	Analýza palív a mazív (bod vzplanutia, destilačná skúška, viskozita, cetanové číslo atď.) jozložky v palive, analýza biopalív HPLC.
www.anamet.cz		email: igor.culak@anamet.sk Tel: +421 905 249 664

pingo Mab

plynová chromatografia ICP-OES príprava vzorky elementárna ANALÝZA elektrochémiaSEA analýza povrchov separačné techniky **REOLOGIA** ATÓMOVÁ spektroskopia GC temperácia kvapalinová chromatografia **UV-VIS** spektrometria LIMS lyofilizatory B.E.T. GC-MS koncentrátory CHNSO analýza Hypercarb AAS hmotnostná HPLC centrifúgy spotrebný materiál SERVIS analýza **ICP-MS** termická **NMR** AIR monitoring TracePLOT XPS Kapilára Ramanovská **TFXTÚRA** spektroskopia automatické dávkovanie elektroforéza Orbitrap

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