ADVATEC Meeting

Date: 12.12.2008

Location: Seminar Room, Villa, August-Bebel-Str. 55, Rostock

Presentations: 20 min talk + 10 min discussion

11.00 – 11.15	Introduction + Presentation of the ADVATEC webpage
11.15 – 11.45	**Subject:** Formation and characterization of quasicrystalline Al alloys **Lecturer:** Carmen Mihoc **Abstract:** Since the discovery of icosahedral phases in rapidly-quenched Al-Mn alloys [1], quasicrystals (QCs) were observed in over 100 alloy systems. Among them, the ternary Al–Cu–Fe alloy is most interesting [2-4], thanks to excellent properties, such as the low electrical and thermal conductivity, high hardness, low friction and wear, and good oxidation resistance. The synthesis of single-phase Al–Cu–Fe QC's by conventional casting is difficult, due to their very narrow composition domain [5]. Recent research efforts were devoted to the mechanosynthesis of quasicrystalline Al–Cu-Fe powders by powder metallurgy (P/M) routes [6-10]. The synthesis and investigation of the phase formation of icosahedral Al-Cu-Fe alloy powders has been studied. Nanocrystalline (nc-) Al–Cu–Fe powders were prepared by mechanical alloying (MA) in a planetary ball mill (RETSCH PM400). The chemical homogeneity and microstructure of the powders were investigated using scanning electron microscopy (SEM/EDX). The sequences of solid-state phase transformation were examined by in situ high-temperature synchrotron radiation diffraction (HTXRD) at HASYLAB/DESY. [1] D. Shechtmann, I. Blech, D. Gratias, J.W. Cahn, Phys. Rev. Lett. 53 (1984) 1951. [2] A.I. Salimon et al, Acta Mater. 49, 2001, 1821. [3] V. Srinivas, P. Barua, B.S. Murty, Mater. Sci. Eng. 294-296, 2000, 65-67. [4] H-R. Trebin (Ed.), Quasicrystals, Wiley-VCH, Weinheim, 2003. [5] R. Lück, L. Zhang, in Ref. [2], 2003, 26–44. [6] B.S. Murty, P. Barua, V. Srinivas, J. Eckert, J. Non-Cryst. Solids 334–335, 2004, 44–47. [7] R. Nicula et al., J. Alloys Compd. 434-435, 2007, 319-323. [8] F. Schurack, J. Eckert, L. Schulz, in: H.-R. Trebin (Ed.), Quasicrystals, Wiley-VCH, Weinheim,

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[10] X. Yong, I.T. Chang, I.P. Jones, J. Alloys Compd. 387, 2005, 128–133.

11.45 - 12.15

Subject: Surface Improvement: Coatings from Cluster Materials

Lecturer: Ester Sala Bosch

Abstract: Since the beginning of the study of the cluster chemistry,[1] increasing interest has been dedicated to group 5 elements and their capability to form metal clusters.[2-4] Besides, some studies on the properties of clusters on inert surfaces as heterogeneous catalysts have been performed.[5,6] In the case of Nb and Ta, the experiments performed by Kamiguchi et al.[7] showed that crushed crystals of halide clusters of these elements can be used to catalyze the production of some organic compounds.
On other terms, it is well known that the metals in these groups have refractive properties such as high melting point, hardness and tensile strength. In this work novel uses of the niobium cluster halides as precursors to obtain elemental niobium particles on metallic and non-metallic surfaces are studied. This niobium coating is intended to modify the properties of the bulk material used as substrate, especially mechanical properties (hardening coatings) and thermal properties (thermo barrier coatings).
The deposition of the metal on the surface takes place in two phases. In the first phase, the cluster material from the solution is deposited on the substrate. Several deposition techniques are used for this purpose, but the most promising ones are the direct spreading of the solution on the surface and the submersion of the pieces in the solution in a sealed tube under vacuum. In the second phase, the cluster bonds are broken in order to obtain elemental niobium particles on the surface, which must be done with the help of energy.

References:
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[2] A. Simon, H. G. Schnering, H. Wöhrle, H. Schäfer, *Z. Anorg. Allg. Chem.* 1965, *339*, 155-170.
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	153-163; (b) S. Kamiguchi, S. Takaku, M. Kodomari, T. Chihara, *J. Molec. Cat. A* 2006, *260*, 43-48.
12.15 – 12.45	**Subject:** Solidification of Polymers at Controlled High Cooling Rates. Differential Fast Scanning Calorimeter. **Lecturer:** Evgeny Zhuravlev **Abstract:** We present the capabilities of a new calorimeter device, positioned between DSC and ultrafast scanning techniques regarding scanning rate range. A thin film low addenda heat capacity sensor was taken as measuring cell. Small measuring area and gas as cooling agent allow controlled heating and cooling at rates up to 10^6 K/s in single sensor ultra-fast scanning setup [1]. But the signal to noise ratio is decreasing at rates slower than 10^2 K/s. To improve sensitivity at lower rates we connect two of such sensors into a differential setup with power compensation. The new device is able to measure heat flow at controlled heating and cooling rates from 10 to 10^5 K/s. The 3 ms equilibrating time gives plenty of possibilities for programming of complex temperature profiles. Solidification of isotactic Polypropylene was studied by means of the newly developed method at cooling rates 40...10^4 K/s within the temperature range 170...500 K. At rates faster than 400 K/s iPP does not crystallize on cooling, that allows to investigate isothermal crystallization at any temperature between glass transition and melting temperature. [1] Minakov AA, Schick C., Rev Sci Instr 2007:78(7):073902-073910. [2] De Santis, F.; Adamovsky, S.; Titomanlio, G.; Schick, C., Macromolecules 40 (2007) 9026 - 9031 Keywords: polypropylene crystallization, fast cooling, thin-film scanning calorimeter, power compensated DSC.

12.45 – 13.00 Break + Photo shooting (picture of the ADVATEC group + Supervisors)

13.00 – 13.30	**Subject:** Study of magnetic Nanoparticles with Potential use for Cancer Hyperthermia Treatment **Lecturer:** Karina Porath **Abstract:** The potential of hyperthermia and thermal ablation in cancer therapy has been well noted. Temperatures between 42°C and 46°C lead to inactivation of normal cellular processes, whereas above

46°C, extensive necrosis occurs. The inability to deposit effective doses of heat in a tumor without applying similar heat on surrounding tissues has prevented widespread clinical use. Magnetic nanoparticles responding to alternating magnetic fields provide a novel approach for the direct thermal ablation of tumor cells [4-5].

When exposed to alternating magnetic fields from kHz to GHz frequencies, the nanoparticles generate heat due to Brown and Neel relaxation phenomena. For a better understanding of the heat transfer between the suspension of the nanopatricles and the cancer tissue we employ full 3D electromagnetic simulations using finite integration technique (FIT). The magnetic properties of the nanoparticles are numerical studied with the finite element method micromagnetics.

In this work, we compare the experimental results of heating of with the nanoparticles to obtained simulation results [1-3]. The results of experiments and simulations are in good agreement with existing theories of the behaviour of the magnetic nanoparticles in alternating magnetic field.

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[5] D.-H. Kim et al., J. Magn. Magn. Mater. 320 (2008) 2390-2396

13.30 – 14.00

Subject: Full 3D Electromagnetic Simulations of Sintering of the Metallic and Ceramic Powders

Lecturer: Tomasz Galek

Abstract: The use of microwaves in ceramic processing is an established method for few decades. Microwaves can be applied effectively to heat and sinter ceramic objects. The most recent development in microwave applications is in sintering of metallic powders, a surprising application, in view of the fact that bulk metals reflect microwaves. It was reported in 1999 by R. Roy and coworkers that porous metal powder compacts heat when subjected to microwave radiation. The effective permittivity and permeability of the powdered material can be described by means of an analytical mixing law. The Maxwell-Garnet theory (MGT) or the effective medium approximation (EMA) can be used for example. The effective permittivity and permeability can also be retrieved from the electromagnetic simulations from the reflection and transmission data. The electromagnetic finite integration technique (FIT) simulations in combination with the extraction of the effective material properties method can be used to determine microwave properties of such materials as metallic and ceramic powders, multilayer systems and inhomogeneous mixtures. The full 3D

	electromagnetic simulations are performed with cutting-edge FIT simulation software CST Microwave Studio (CST MWS).The extracted effective properties are further used in finite element method (FEM) COMSOL Multiphysics software to model heating and sintering under microwave irradiation. The knowledge of the effective properties can be helpful for understanding the basic physical phenomena as well as for further modelling and optimization of the microwave sintering process.
14.00 – 14.30	**Subject:** Re-Inventing Non-Pneumatic Wheel **Speaker:** Kundan Kumar **Abstract:** Poor ride quality is a critical bottleneck of non-pneumatic wheel design. This research is focused on developing a non-pneumatic wheel which has pneumatic-like performance. Concepts of a flexible non-pneumatic structure and a ride-enhancing tread-band have been developed to improve the ride quality. Extensive finite element simulations have been carried out in the pre-development phase. Elaborate material characterization (laboratory) testing are being presently carried out to develop the prototypes for real-world performance.
14.30 – 14.40	Conclusion remarks

15.00 - ... Christmassy get-together (villa winter garden)