# MM 27: Transport I - Materials/Methods

Time: Tuesday 11:45–13:00 Location: IFW B

MM 27.1 Tue 11:45 IFW B

**Studying spatially resolved atomic diffusion processes using X-rays - atomic-scale X-ray photon correlation spectroscopy and its application to metallic alloys** — •Markus Stana[1], Michael Leintner[2], Manuel Ross[1], and Bogdan Sepiol[1] — [1]Universität Wien, Fakultät für Physik, Boltzmanngasse 5, 1090 Wien, Austria — [2]Technische Universität München, Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II), 85747 Garching, Germany

In the recent years our group succeeded in studying spatially resolved diffusion processes on the atomic scale by extending X-ray photon correlation spectroscopy (XPCS) to large scattering angles. In my talk I will give an overview of this new technique and present the results we achieved for binary metallic systems. Special attention will be given to solid solutions (Ni-Pt) and intermetalic phases like B2 (Fe-Al) and $L1_2$ (Cu-Au, Ni-Pt). I will conclude by briefly showing that this technique can also shed light on atomic motion in noncrystalline systems like glasses.

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MM 27.2 Tue 12:00 IFW B

**Diffusion of Atoms and Vacancies in Thin Nano Crystalline Platinum Films** — •Wolfgang Gruber[1], Johanna Rahn[1], Florian Strauss[1], Lars Dörrer[1], Erwin Hüger[1], Michael Horisberger[2], Thomas Geue[2], Jochen Stahn[2], Carsten Bähtz[3], Wolfram Leitenberger[4], and Harald Schmidt[1] — [1]TU Clausthal — [2]Paul Scherrer Institut — [3]Helmholtz-Zentrum Dresden-Rossendorf — [4]Universität Potsdam

An important characteristic of thin metal films deposited on substrates is the presence of a high number of defects in the metal film which is correlated to residual stress and strain. During heat treatment strain in the metal films relaxes. The relative changes of the film thickness and the interplanar distance are correlated to the change of the defect concentration during relaxation. In-situ X-ray diffraction and X-ray reflectometry using synchrotron radiation revealed that strain relaxation is accompanied by an increase of the vacancy concentration at the surface of the film [1]. In this work we present experimental results supporting the stress relaxation model outlined in [1]. To clarify the rate determining process for strain relaxation, grain boundary and volume self-diffusion of platinum is investigated. Samples enriched in the stable isotope 194Pt as tracer source were prepared and used for analysis with secondary ion mass spectrometry and neutron reflectometry. [1] W. Gruber, S. Chakravarty, C. Baehtz, W. Leitenberger, M. Bruns, A. Kobler, C. Kübel, H. Schmidt, Phys. Rev. Lett. 117 (2011) 265501.

MM 27.3 Tue 12:15 IFW B

**Conductance through itinerant geometrically frustrated electronic systems** — •Alexandre Lopes[1], Bruno António[2], and Ricardo Dias[2] — [1]Institute of Physics, University of Freiburg, Hermann-Herder-Straße 3, 79104 Freiburg, Germany — [2]Universidade de Aveiro, I3N, Campus Universitário de Santiago, Aveiro, Portugal

We study a two terminal electronic conductance through an $AB_2$ ring which is an example of the family of itinerant geometrically frustrated electronic systems. These systems are characterized by the existence of localized states with nodes in the probability density. We show that such states lead to distinct features in the conductance. For zero magnetic flux, the localized states act as a filter of the zero frequency conductance peak, if the contact sites have hopping probability to sites which are not nodes of the localized states. For finite flux, and in a chosen orthonormal basis, the localized states have extensions ranging from two unit cells to the complete ring, except for very particular values of magnetic flux. The conductance exhibits a zero frequency peak with a dip which is a distinct fingerprint of the variable extension of these localized states.

MM 27.4 Tue 12:30 IFW B

**Conductivity and Dielectric Properties of $Li_xNa_{2-x}Ti_6O_{13}$ ($x = 0...2$)** — •Kai Volgmann and Paul Heitjans — Leibniz Universität Hannover, Inst. f. Phys. Chemie u. Elektrochemie, Callinstraße 3 - 3a, D-30167 Hannover

Titanate systems attract much attention as anode material for secondary Li ion batteries due to advantages compared to graphite. $TiO_2$ is a prominent example within the system $Li_2O$ - $TiO_2$. In the present work, $Li_xNa_{2-x}Ti_6O_{13}$ (space group $C2/m$) has been chosen as a model system because of its channel-like crystal structure. The alkali atoms are solely located inside the channels. The samples with different Li/Na ratios were characterized by powder x-ray diffraction and inductively coupled plasma optical emission spectroscopy (ICP-OES). Impedance spectroscopy measurements were performed over a wide temperature range (200-1000 K). Thin films of graphite or Pt were used as electrodes. The frequency dependent conductivity data yielded activation energies $E_A$ which partly depend on the Li/Na ratio. Whereas $E_A$ values calculated from the DC plateau are essentially independent of $x$, the AC contribution has a maximum $E_A$ value for $x = 0.33$. Cole-Cole plots of the complex impedance show a depressed semicircle. Thus no separation of bulk and grain boundary contributions is visible. Plotting the complex modulus vs. frequency shows different relaxation modes corresponding to different bulk processes. Comparison of the various representations gives information on the diffusivity of the alkali ions on macroscopic and microscopic scales.

MM 27.5 Tue 12:45 IFW B

**Short Range Silicon Migration in Amorphous Silicon Observed by Neutron Reflectometry** — •Florian Strauss[1], Harald Schmidt[1], Jochen Stahn[2], and Thomas Geue[2] — [1]TU Clausthal, AG Mikrokinetik, Institut für Metallurgie, Deutschland — [2]Paul Scherrer Institut, Villigen, Schweiz

Amorphous silicon (a-Si) is a simple model system of covalent amorphous semiconductors, widely used in solar cells and flat screen displays and a promising electrode material in Li-ion batteries. Yet, there exist no experimental data on self-diffusion in the amorphous state. The expected low diffusivities and intrinsic metastability of a-Si require measurement by time-of-flight neutron reflectometry (NR), a method capable of determining diffusion lengths of 1 nm and below [1,2]. $^{29}Si/^{28}Si$ isotope multilayers are prepared by ion beam sputtering and thermally treated in Ar atmosphere at temperatures below the crystallisation temperature in order to induce interdiffusion. The samples are isotope modulated but amorphous and chemically homogenous as shown by TEM and XRD. Previous measurements have pointed to an onset of movement above 350 °C and short range atomic diffusion processes on the length scale of 1.5 - 2 nm. New data from NR and SIMS are discussed, focussing on time dependent diffusion processes and long range motion at temperatures between 400 °C and 600 °C. The influence of impurities on diffusion and structure is also part of the on-going investigation.

[1] H. Schmidt et al.; Acta Mater. 56 (2008), 464
[2] E. Hüger et al., Appl. Phys. Lett. 93 (2008), 162104