MM 44: Functional Materials II

Time: Friday 10:30–13:15 Location: IFW A

MM 44.1 Fri 10:30 IFW A

'The wake of Hydrogen in V, Nb and Ta at elevated temperatures: Irrreversibility and non-central forces revisited. — •Franz Reidinger — 3 Hadley Way Morristown NJ 07960 USA

At elevated temperatures U and Do of the Arrhenius equation for diffusion describe the amplitude and relaxation rate, respectively, of the stern wave wake of H. The key evidence for this hypothesis is the close correlation between the isotope dependence of U derived from measurements of the Gorsky effect 1) and the shear distortion of the orthorhombic phases of NbH(D) and TaH(D). The isotope dependence of U can be described in closed form: U=axsqrt(M)+bxsqrt(m), where M and m are the atomic weights of host metal and H isotope: a and b are 7.4 and 37 for Nb and Ta, and 0 and 55 for V, respectively, in units of meV. I explain this correlation in two steps: a) the cubic symmetry of the nearest neighbor strain field 2) of the interstitial H is the result of a dynamic superposition, possibly caused by a JT resonance 3), of two orthorhombic variants of ordered NbH0.75 and b) the successful characterization of the diffusion process as jump diffusion 4) eliminates the transition state from considerations. 1)Z Qi, J Voelkl, R Laesser and H Wenzl: J.Phys.F 13, 2053 (1983) 2)G Bauer, E Seitz, W Schmatz and H Horner: Sol. State Comm. 17, 161 (1975) 3)GC Abell: J.Phys.F 12, 1143 (1982) 4)V Lottner, A Heim and T Springer: Z.Physik B 32, 157 (1979)

MM 44.2 Fri 10:45 IFW A

Atom probe tomography analysis of deuterium distribution in V-Fe alloy film — •Ryota Gemma[1], Talaat Al-Kassab[2], Reiner Kirchheim[1], and Astrid Pundt[1] — [1]Institut für Materialphysik, Friedrich-Hund-Platz 1, D-37077, Göttingen, Germany — [2]Division of Physical Sci.& Eng., King Abdullah University of Science & Technology (KAUST), Thuwal 23955-6900, Kingdom of Saudi Arabia

In hydrogen-metal systems, investigation of hydriding properties in reduced dimension has been one of the important issues for materials development in the field of hydrogen storage and sensor applications. Atom Probe Tomography (APT) has opened up a new quantitative approach to demonstrate deuterium (D) distribution in metals. In our previous studies, it has been shown that analysis temperature in the APT analysis and oxygen-exposure of D-loaded specimen exert a major influence on D distribution. These impacts are related to diffusion behavior of D. A reliable analysis of D distribution can be achieved only in the case that the D-diffusion is suppressed. In this study, lateral and depth distribution of D in V-Fe alloy film was investigated by APT at 20 - 30 K. In the analysis of V-Fe5at% film of 10 nm-thickness deposited on a W substrate performed at 30 K, the film loaded with 0.2 Pa deuterium gas showed an average D concentration of 0.23(8) D/Metal, which was in good agreement with the expected concentration of 0.31 D/Metal. An enrichment of D near the V/W interface was observed regardless of analysis temperature, which is explained by the presence of D-trapping effect at misfit dislocations.

MM 44.3 Fri 11:00 IFW A

Blister formation on polycrystalline tungsten due to low-energy deuterium plasma loading — •Armin Manhard, Klaus Schmid, Wolfgang Jacob, Martin Balden, and Stefan Lindig — Max-Planck-Institut für Plasmaphysik, EURATOM Assoziation, Boltzmannstr. 2, 85748 Garching

When polycrystalline tungsten is loaded with deuterium due to plasma implantation with ion energies well below the sputtering threshold but with a high ion flux, the surface morphology of a well-polished specimen can change dramatically. This can be attributed to the supersaturation of the material with deuterium during plasma implantation. Depending on tungsten microstructure, ion flux and specimen temperature, various surface structures such as blisters and other protrusions appear. Their size ranges from microns to tens of microns and each one features a subsurface cavity. These cavities are typically located orders of magnitude deeper than the stopping range of the implanted ions.

This presentation focuses on the formation of blisters on rolled and subsequently polished and stress-relieved tungsten. The abundance and size distribution of the blisters is discussed depending on the specimen temperature. The influence of the initial surface morphology such as, e.g., surface roughness is also addressed. The influence of the tungsten microstructure is examined by investigating recrystallized and subsequently implanted tungsten specimens. In this context, the formation of different types of protrusions which appear on the surface of recrystallized tungsten for very high ion fluxes is also discussed.

MM 44.4 Fri 11:15 IFW A

Combined impact of microstructure and mechanical stress on PdHc thin films electrical resistivity — •Stefan Wagner and Astrid Pundt — Institut für Materialphysik, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Physical properties of metal thin films strongly depend on their microstructure and stress state. [1] Palladium hydrogen (PdHc) thin films are used as a model system to determine the impact of microstructure and mechanical stress release on the electrical resistivity of thin film metals and alloys that undergo structural phase transitions. The results are compared with bulk resistivity models. Nanocrystalline, multi-oriented and epitaxial films in the thickness range from 5 nm to 2 μm are investigated, yielding initial terminal resistivities of 152 - 200 Ωnm. The hydrogen-related resistivity changes of epitaxial films are shown to approach the predicted α-phase bulk increment $\Delta\rho/\Delta cH = 451\ \Omega$nm, while hydrogen trapping in nanocrystalline films strongly reduces the resistivity response. In the two phase field the resistivity is shown to be modified by the sterical distribution and geometry of the hydride precipitates, yielding different proportions of serial and parallel conduction. Film delamination from the substrate strongly reduces the resistivity increment due to the Gorsky effect. [2,3]

[1] Wagner S, Pundt A: APL 2008;92:051914. [2] Wagner S, Pundt A: Acta Mat 2010;58:1387. [3] Wagner S, Pundt A: Acta Mat, accepted.

MM 44.5 Fri 11:30 IFW A

Positron lifetime measurements for monitoring vacancies and vacancy clusters in hydride forming free standing Mg films. — •Luca Ravelli[1], Werner Egger[1], Günther Dollinger[1], Roberto Brusa[2], and Riccardo Checchetto[2] — [1]Institut für Angewandte Physik und Messtechnik, Universität der Bundeswehr München, Neubiberg, Deutschland — [2]Dipartimento di Fisica, Università degli Studi di Trento, Trento, Italy

Pd-capped free-standing Mg-based film samples (thickness 10 micrometers) were produced by r.f. magnetron sputtering[1]. The presence of vacancies and the formation of vacancy clusters were studied in the as-prepared sample and in samples submitted to 1, 2, 4 and 8 H2 absorption and desorption cycles by positron annihilation lifetime spectroscopy. For this task a monoenergetic pulsed positron beam of variable energy is necessary to control the implantation depth of the positrons and to depth-profile the defect structure in the Mg films. The measurements were performed with the Pulsed Low Energy Positron System (PLEPS)[2] at the high intensity positron source NEPOMUC (NEutron-induced POsitron source MUniCh) of the research reactor FRM II. Disappearence of vacancies due to their clustering was observed after the second H2 sorption cycle.

[1] N. Bazzanella et al., Appl. Phys. Lett. 85 (2004) 5212-5214.

[2] P. Sperr et al., Appl. Surf. Science 255 (2008) 35-38.

MM 44.6 Fri 11:45 IFW A

Nuclear Magnetic Resonance study of $LiMnPO_4$ with different Li concentrations — •Christian Schmidt, Hans-Joachim Grafe, Nadja Wizent, Lothar Dunsch, and Bernd Büchner — Leibniz-Institut für Festkörper- und Werkstoffforschung, Dresden, Germany

$LiMnPO_4$ is a promising material for building the cathode of Li-ion batteries due to its high stability and large cation mobility. Yet, the mobility of the Li-ions in this material is not well understood. Here, we present ^{7}Li and ^{31}P Nuclear Magnetic Resonance (NMR) measurements on Li_xMnPO_4 single crystals for different doping levels (x=0.6, x=0.8, and x=1). NMR is a powerful tool to investigate the microscopic ionic jump processes rather than the macroscopic material transport. The nuclear spin lattice relaxation rate, $1/T_1$, and the linewidth, σ, of the resonance lines show characteristic temperature dependencies related to the ionic jump processes that set in at a certain energy or temperature, respectively. The advantage of the use of single crystals is that the linewidth is not broadened by a distribution of linewidths as in a powder sample, but can show a fine structure that could be related to different sites in the crystal. Furthermore, single crystals allow for an orientation dependent investigation of the Li-ion mobility, where certain crystal orientations are preferred by the Li-cations.

MM 44.7 Fri 12:00 IFW A

$SrTi_{1-x}Nb_xO_{3-\delta}$ glass-ceramics as oxidic thermoelectric materials

— •Julian Lingner[1,2], Martin Letz[1], and Gerhard Jakob[2] — [1]Schott AG, Hattenbergstraße 10 Mainz — [2]Johannes Gutenberg-Universität Mainz

Thermoelectrics are materials that convert waste heat into electrical power. The quality of a thermoelectric substance is characterized by the dimensionless figure of merit $ZT = \frac{S^2\sigma}{\kappa}T$. One essential advantage of glass-ceramics is their low thermal conductivity κ together with the high temperature stability of up to 700°C. The crystal phase $SrTiO_3$ is a wide bandgap semiconductor, doping with niobium and with oxygen vacancies shifts the Fermi level into the donor band resulting in a insulator-metal transition. Furthermore, nanoscale structure offers a possibility to improve the performance and allows to adjust the material to the required application. Nano crystalline conducting crystal grains effectively reduce the dimensionality of the conducting material, which allows to modify the density of states and therefore the Seebeck coefficient S and the electrical conductivity σ, thus increasing the thermoelectric figure of merit. Using a short range infrared heat treatment, a controlled crystallization in the glass samples can be induced so that nanoscale $SrTiO_3$ crystals are formed in the glass-ceramic. We show results of thermoelectric properties of first glass-ceramic systems containing doped $SrTiO_3$.

MM 44.8 Fri 12:15 IFW A

Hybrid electrode for electrochemical capacitors consisting of a MnO_2 infiltrated carbon aerogel

— •C. Weber[1], V. Lorrmann[1], G. Reichenauer[1], V. Dyakonov[1,2], and J. Pflaum[1,2] — [1]Bavarian Center for Applied Energy Research e.V. (ZAE Bayern), D-97074 Würzburg — [2]Julius-Maximilians-University of Würzburg, Institute of Physics, Experimental Physics VI, D-97074 Würzburg

Electrochemical capacitors (EC) bridge the gap between conventional capacitors with high power but low energy density and batteries with high specific energy density but rather low power density. There are two types of EC: Double-layer capacitors, based on the electrostatical storage of charges in the Helmholtz-layer between the electrolyte and the electrode of large surface area, the latter typically consisting of activated carbon. In pseudocapacitance capacitors charging is of faradaic nature, e.g. by redox processes in oxides of transition metals. We have prepared EC hybrid electrodes by infiltrating a carbon aerogel with manganese oxide (MnO_2).

Variations in structure of the carbon aerogel backbone and the amount of deposited MnO_2 were characterized electrochemically and structurally. Due to the MnO_2 deposition, the gravimetric capacitance was augmented by a factor 2, whereas the volumetric capacitance was increased by a factor 5, compared to the capacitance of the bare carbon aerogel, respectively. Remarkably, these findings are independent of the concentration of MnO_2 in the precursor.

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MM 44.9 Fri 12:30 IFW A

Stability of polymer-ceramics interfaces in hybrid materials: The role of coupling agents and surfactants

— •Wolfgang Heckel, Kristina Brandt, Tobias C. Kerscher, Sascha B. Maisel, Gerold A. Schneider, and Stefan Müller — Technische Universität Hamburg-Harburg, Institut für Keramische Hochleistungswerkstoffe, Denickestr. 15, D-21073 Hamburg

The mechanical properties of hierarchically structured materials like ceramics-polymer systems heavily depend on the composition of the interface materials and the choice of an optional adhesive. As an example we have investigated the Titaniumdioxide-PMMA system by application of different experimental techniques. In order to control the properties of the system, we use density functional theory to analyze the stability of this interface and compare different surfactants, adhesives and coupling agents. Indeed, a detailed knowledge of the local electronic and energetic behaviour at the polymer-agent-ceramics interface is crucial. The resulting energetics and electronic properties depend on both the agent-ceramics and the agent-polymer bond stength.

MM 44.10 Fri 12:45 IFW A

Magnetoelectric FeCoBSi/PVDF bilayers

— •Kerstin Meurisch, Robert Jahns, Eric Woltermann, Thomas Strunskus, Vladimir Zaporojtchenko, and Franz Faupel — Tecnical Faculty of the University of Kiel, Germany

In Magnetoelectric composites magnetostrictive and piezoelectric materials are combined in a way that changes in the dimension of the magnetostrictive material by an external magnetic field will lead to a measurable polarization change of the piezomaterial. It was already demonstrated that laminates fabricated by gluing of a FeCoBSi foil to a PVDF (polyvinylidene fluoride) foil provide a fairly high magnetoelectric response [1], but downsizing and integration into devices is rather complicated. To avoid these problems and to achieve a better mechanical coupling at the metal-polymer interface we deposited the FeCoBSi directly onto a piezoelectric PVDF foil by DC magnetron sputtering. An in situ applied magnetic bias field was used to improve the magnetic field direction sensitivity. The influence of the substrate preparation, sensor design and sputter parameters on the magnetoelectric output signal will be discussed.[1] Zhai, J.; Dong, S.; Xing, Z.; Li, J. & Viehland, D;. Giant magnetoelectric effect in Metglas/polyvinylidene-fluoride laminates; Appl. Phys. Lett.; 2006, 89, 083507

MM 44.11 Fri 13:00 IFW A

Novel method to produce catalysts for oxygen reduction re- action by dual plasma process

— •Christian Walter[1], Volker Bruser[1], Antje Quade[1], Klaus-Dieter Weltmann[1], Kurt Kummer[2], and Denis Vyalikh[2] — [1]INP Greifswald e.V. Felix-Hausdorff-Str. 2 17489 Greifswald — [2]TU Dresden Inst. für Festkörperphysik Helmholtzstraße 10 01069 Dresden

Polymer electrolyte membrane fuel cells (PEMFCs) have been recognised as a potential future power source for zero emission vehicles [1]. Today, Pt is the only efficient catalyst for the oxygen reduction reaction (ORR) in PEMFCs. But for reasons of availability and cost efficiency there is a great desire to replace Pt with inexpensive and abundant catalysts (Non-noble-metal catalysts (NNMCs)). Metal (Co/Fe)/N/C composites have emerged as the most promising alternatives within the NNMcs. Those composites are either prepared by pyrolisation of Co- or Fe-N_4-macrocycles at high temperatures in an inert atmosphere or by introducing the metal and the nitrogen precursors separately onto carbon support and subsequent pyrolisation [2]. But it has also been shown that metal-polymer-composites can be produced by a dual PECVD/PVD process [3]. In this contribution, such a dual process is used with pyrrole as the polymer and cobalt as metal to obtain catalytically active composites. Advantages and shortfalls of this technology are discussed.

[1] R. Bashyam and P. Zelenay; *Nature*, **2006**, 443,63-66
[2] F. Jaouen et al.; *ACS Appl. Mater. Interfaces*, **2009**, 1 (8), 1623
[3] C.Walter et al.; *Plasma Process. Polym.*; **2009**, 6, 803-812