MM 26: Functional Materials V: Functional Materials

Time: Tuesday 11:45–13:00 Location: TC 010

MM 26.1 Tue 11:45 TC 010

Neutron Imaging of Metal Hydride based Hydrogen Storage Tanks — •Stefan Börries[1], Philipp Klaus Pranzas[1], Oliver Metz[1], Martin Dornheim[1], Thomas Bücherl[2], Thomas Klassen[1], and Andreas Schreyer[1] — [1]Helmholtz-Zentrum Geesthacht, Centre for Materials and Coastal Research, Max-Planck-Straße 1 D-21502 Geesthacht, Germany — [2]ZTWB Radiochemie München (RCM), Technische Universität München (TUM), Walther-Meissner-Str. 3, 85748 Garching, Germany

Hydrogen is a promising energy carrier for the future, especially for mobile applications. It can be stored safely and reversibly at high volumetric densities in hydrogen storage tanks filled with light metal hydrides. Due to the high sensitivity of neutrons towards hydrogen, Neutron Radiography (NR) is the ideal technique for in situ investigations in order to directly observe the hydrogenation behaviour of the metal hydride material inside the tank under operating conditions. Already qualitative investigations revealed interesting macroscopic structure changes for the hydorgen absorption [1,2]. In a further step, the full spectrum of available neutron energies at different imaging beamlines was used for a comprehensive quantitative study of scaled up metal hydride materials, including in operando studies as well as tomography studies. The results help for the optimization of metal hydride based hydrogen storage.

[1]*P. K. Pranzas, et al., Advanced Engineering Materials 13 (8) (2011) 730-736 [2]*Bellosta von Colbe, J.M., Int. Journal of Hydrogen Energy 37, 2012

MM 26.2 Tue 12:00 TC 010

Optimization of Tungsten-Steel Joints for Plasma Facing Components in Fusion Reactors — •Simon Heuer[1], Thomas Weber[2], Jiří Matějíček[3], Jochen Linke[2], and Christian Linsmeier[1] — [1]Forschungszentrum Jülich GmbH, Institut für Energie- und Klimaforschung - Plasmaphysik, 52425 Jülich, Germany — [2]Forschungszentrum Jülich GmbH, Institut für Energie- und Klimaforschung - Werkstoffstruktur und -eigenschaften, 52425 Jülich, Germany — [3]Institute of Plasma Physics, Academy of Sciences of the Czech Republic, 18200 Prague 8, Czech Republic

Tungsten, joint to a martensitic-ferritic EUROFER97 structure, is a promising plasma facing material composite for fusion reactors. Due to the effect of mismatch in thermo-mechanical properties direct bonding is not feasible. Current research is therefore ongoing on interlayer systems. While the adhesion was already improved by the utilization of a discrete Cu, Ti or V interlayer, that is able to relax stresses by plastic deformation, joints still do not resist the expected load cycles in a fusion reactor. Therefore, alternatives for the interface are needed. This contribution presents research on functionally graded materials (FGM). The particular microstructure of a graded interlayer allows redistributing macro stresses from a discrete interface to a greater volume while avoiding in particular Cu which tends to swell under neutron irradiation. A parameter study on the basis of finite element analysis will be presented as well as first results of several processing routes for FGM that shall be evaluated and benchmarked by mechanical as well as thermal testing.

MM 26.3 Tue 12:15 TC 010

Assembly of magnetic nano-particles close to a solid wall — •apurve saini, vassilios kapaklis, and max wolff — material physics, department of physics and astronomy, uppsala university, uppsala, sweden

Ferro-fluids are liquids with magnetic nano-particles dispersed in a solvent and show a super-paramagnetic behavior. The magnetic moment makes the particles sensitive to magnetic fields. The application of such a field can drive self-assembly and result in e.g. smectic like ordering.

We investigated the adsorption of magnetic nano-particles close to a ferrofluid-SiO2 interface as a function of external magnetic and flow fields. The particles are stabilized by surface coatings, which makes them extremely sensitive to the termination of a solid boundary and mono- or multilayers can form. The surface energy and polarity of the solid boundary is tuned by self-assembled monolayers.

In situ neutron reflectometry and grazing incidence has been utilized to obtain a detailed microscopic picture of this ordering phenomenon. Thus, the equilibrium as well as kinetics of the self-assembly is studied systematically. Both magnetic fields as well as flow facilitate pronounced layering at the interface,revealing a controlled growth of magnetically nanostructured interfaces on the time scales of hours.

MM 26.4 Tue 12:30 TC 010

Memristive behavior of $TiO_{2-\delta}$ rutile phases – an ab-initio based ground-state analysis — •Wolfgang Heckel[1], Michael Wehlau[2], Sascha B. Maisel[1], Thomas Frauenheim[2], Jan M. Knaup[2], and Stefan Müller[1] — [1]Institute of Advanced Ceramics, Hamburg University of Technology, D-21073 Hamburg — [2]Bremen Center for Computational Materials Science, University of Bremen, D-28359 Bremen

Memristive devices for various technical applications, e. g. electronic analogues to nerve cells for neuromorphic computing[1], attract growing attention. TiO_2 has been shown to serve as a memristive material.[2]

We conducted a comprehensive ab-initio based ground-state search for $TiO_{2-\delta}$ rutile phases in order to identify structural features which lead to the conductive phase of a TiO_2 memristor. A cluster expansion Hamiltonian, fitted to DFT data, enabled us to scan the entire configuration space of the oxygen vacancies. We find that O vacancies tend to form planar arrangements which relax into structures exhibiting metallic behavior. These structures are energetically less favorable, but show an even more pronounced metallic DOS than the Magnéli phases, which do not appear in our calculations due to energy barriers. Our results confirm the relation between vacancy ordering and metallic behavior in reduced oxides.

Supported by DFG, SFB 986, project A4.

[1] Jo, et al., Nano Letters **10**, 1297 (2010).
[2] Strukov, et al., Nature **453**, 80 (2008).

MM 26.5 Tue 12:45 TC 010

Bose Einstein Condensate observed in Koops-GranMat at RT — •Hans W.P. Koops — HaWilKo GmbH, Ober-Ramstadt, Germany

Giant current density is observed at room temperature in Koops-GranMat(R) with Pt- or Au-nanocrystals embedded in a fullerene matrix. The material is built with Focused Electron Beam Induced Processing. A field emission current up to 1mA was observed at 23 V (Au/C) or 70 V (Pt/C). From an emission site of 10 nm in diameter, the current density reaches in both cases > 1.5 GA/cm2. In 2009 Koops explained the apparent electron-conduction with excitonic electron states in crystal surface orbitals which obey the Bohr Eigenvalue conditions for energy states. The electrons in these excitonic surface orbitals states have a wavelength of 2 nm. The excited excitonic states having a perimeter length of 5 lambda overlap and a Bose Einstein Condensate is formed. Here electrons and holes having parallel spins form Bosons, now named Koops-pairs, they occupy one level only, and show coherent electron emission. Mapping the system on a Bose-Hubbard phase-diagram suggests super-fluidity. The estimated critical temperature for Bose-Einstein-Condensation is higher than room temperature(300K).