MM 15 Hydrogen in Metals II

Time: Tuesday 11:45–12:45 Room: IFW D

MM 15.1 Tue 11:45 IFW D

Surface morphology changes and time dependency of hydride formation in thin epitaxial Nb-films — •Kai Nörthemann, Reiner Kirchheim, and Astrid Pundt — Institut für Materialphysik, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

The growth and arrangement of precipitates in thin epitaxial films is presented in this contribution, using the model system Niobium-Hydrogen.

With the surface sensitive scanning tunneling microscopy (STM) it is possible to distinguish between matrix and precipitates because of the different lattice parameter of niobium and niobium hydride. The STM measurements of thin epitaxial niobium films are taken during hydrogen loading, therefore the time dependency of the hydride formation and the orientation of the hydride can be examined. Two different types of hydride precipitates were found. Their appearance will be discussed. Their expansion is fitted to a Johnson-Mehl-Avrami kinetic. The stability of the α-phase and the hydride in the two phase field will be discussed.

This work is financially supported by the DFG via SFB 602.

MM 15.2 Tue 12:00 IFW D

Catalytic effect of oxides for decomposition of magnesium hydride explained by the gateway model. — •Andreas Borgschulte and Rüdiger Bormann — GKSS-Research Center, Geesthacht GmbH, WTP, building 59, Max-Planck-Straße 1, 21502 Geesthacht

The kinetics of the reversible reaction of hydrogen gas with magnesium forming MgH_2 is enhanced significantly by the addition of transition metals oxide catalysts and by using nanostructured powders. Hydrogen absorption and desorption properties of such systems were studied by high pressure differential scanning calorimetry (DSC) under hydrogen atmosphere, from which the heat of hydride formation and decomposition of magnesium hydride is revealed. We find an additional, slightly destabilized phase, which is formed within the first desorption. Its amount depends on the degree of nanostructuring and the used additive. The phase is attributed to destabilized magnesium hydride near grain boundaries. It is the intermediate step before the more stable, stoichiometric MgH_2-phase is formed. Thus the phase acts as a gateway for de-hydrogenation of MgH_2. The results correspond to neutron diffraction measurements, in which a $MgH_{x<<2}$ was found [1].

[1] H. Gijs Schimmel, Jacques Huot, Laurent C. Chapon, Frans D. Tichelaar, and Fokko M. Mulder, J. Am. Chem. Soc. **127**, 14348 (2005).

MM 15.3 Tue 12:15 IFW D

Optical characterisation of MBE grown neodymiumhydride films — •S. Weber, H. Schröter, and J. Schoenes — Institut für Physik der Kondensierten Materie, Mendelssohnstr. 3, D-38106 Braunschweig

Many rare earth metals have attracted attention because of their metal-insulator transition during hydrogen loading. Neodymium takes a special place among these as in addition to the opening of a large gap a transition to a ferromagnetic state has been reported.

Thin films of Nd have been grown onto CaF_2 and Si-substrates using the MBE technique. In order to prevent corrosion in ambient air and to allow hydrogenation of the samples a protective layer of palladium is mandatory. A Nb-bufferlayer is used to prevent interdiffusion between the Pd-layer and the Nd-film which strongly deteriorates the quality of the samples. Temperature dependend measurements on hydrogenated samples have been performed using a FT-IR-spectrometer in the energy range of 5meV to 1eV. The spectra show 5 phonon modes which can be assigned unambiguously to hydrogen vibrations by comparison with deuterium loaded samples. The transmission spectra of the samples which are multiple layer systems can be simulated using a thin film model. Subsequently, the optical properties of NdH_x can be determined. The modelling parameters indicate an expansion of the films by a factor of about 2 during hydrogenation which was confirmed by AFM measurements. Furthermore, the optical band gap was measured by UV/Vis-spectrometry.

MM 15.4 Tue 12:30 IFW D

Raman spectroscopy study of strong correlation effects in $YH_{3-\delta}$ — •A.-M Racu and J. Schoenes — Institut für Physik der Kondensierten Materie - TU Braunschweig Mendelssohnstrasse 3, 38106 Braunschweig

Temperature dependent Raman measurements on insulating $YH_{3-\delta}$ thin films have been performed from 4 K to 450 K. The most striking effect is the broadening by a factor of almost 6 between 4 and 300 K of a particular mode, which is assigned to a breathing vibration of the yttrium atoms. For higher temperatures, the line-width of this mode saturates, which is rather unusual for a phonon.

We developed a model which discusses the line broadening in terms of a coupling between this breathing mode and the electron excited from an octahedral H-vacancy into the 4d conduction band of Y. The data strongly support the correlated electron theory proposed by Ng *et al.* [1] for the metal-insulator transition in YH_x.

[1] K. K. Ng, F. C. Zhang, V. I. Anisimov, T. M. Rice, Phys. Rev. B **59**, 5398 (1999).