versity, Russia

In magnetic superlattices with interlayer exchange coupling, not only the coupling strength but also the magnetic moment of the ferromagnetic layer can be altered non-locally by modifying the electronic structure of the non-magnetic spacer layer. Specifically, changes of the electronic structure of the V spacer layers in Fe/V (001) superlattices are seen to affect the adjacent Fe layers. By reversibly loading the V layer with hydrogen, the magnetic moment of Fe increases, whereas the induced magnetic moment in V remains unchanged. The nature of this remote and non-local control of the magnetic moment is connected with a d-electron charge transfer and effective shift of the Fermi level relative to the d-bands of Fe and V, as elucidated on the basis of self-consistent electronic structure calculations [1].

We acknowledge financial support of the DFG under contract RE 2203-1/1, DFG - RFBR project 06-02-04005, INTAS-NETWORK project (03-51-4778) and from VR, the Swedish research council.

[1] A. Remhof et al, Europhys. Lett, 79 37003 (2007).

MM 41.10 Thu 18:00 Poster B

High pressure techniques for synthesis and characterization of hydrogen storage materials — •Carine Rongeat, Isabel Llamas Jansa, and Oliver Gutfleisch — IFW Dresden, Institute for Metallic Materials, P.O. Box 270116, D-01171 Dresden, Germany

High pressure reactive milling is a very effective synthesis technique for hydrogen storage materials. It was used successfully to synthesize light metal hydride by milling metal powder under high hydrogen pressure [1]. This technique can also be applied to the synthesis of novel promising complex hydrides. For example, one-step synthesis of doped-sodium alanate was performed from NaH, Al and 4

[1] Doppiu et al., J. Alloys Compd. 427 (2007) 204-208.
[2] Rongeat et al., J. Phys. Chem. B (2007) accepted.

MM 41.11 Thu 18:00 Poster B

Formation and Hydrogen Reactivity of Complex Mg-Ni-La-(Co)-H phases — •Angelika Teresiak, Annett Gebert, Valentin Bunea, Jürgen Thomas, Jürgen Eckert, and Ludwig Schultz — Leibniz Institute for Solid State and Material Research Dresden,

Currently, $Mg*Ni*RE(La)$ alloys are of great interest as new electrode materials for Ni-MH batteries. The recently discovered Mg_2NiLaH_7 hydride in the $Mg-Ni-La-H$ quaternary system shows with 2,8 wt% (109 g/l H) a much higher hydrogen content than the well-known commercial $LaNi_5H_x$- and TiV_2H_x alloys.
In the present study we investigate the formation of the complex hydride $Mg_2NiLa(Co)H_{7*x}$ by using various process routes, which aim at achieving material with nanocrystalline microstructure. The Mg_2NiLaH_7 forms completely by intensive ball milling of an inductively molten master alloy of Mg_2NiLa under hydrogen for 7.5h. Also, the gradual electrolytic charging of the master alloy using a current density of $-1mA/cm^2$ succeeded in forming the hydride. Starting from melt-spun amorphous ribbons, the crystallisation to nanocrystalline Mg_2NiLa and a subsequent hydrogenation under 0.5MPa hydrogen for 26h were performed and monitored by means of in situ high temperature XRD. Furthermore, the influence of Co additives to Mg_2NiLa on the phase formation and hydrogen absorption processes was studied.

MM 41.12 Thu 18:00 Poster B

The role of hydrogen in the development of free-machining titanium alloys — Carsten Siemers, Martin Bäker, •Hans-Rainer Sinning, and Joachim Rösler — Institut für Werkstoffe, TU Braunschweig, Langer Kamp 8, 38106 Braunschweig

Recently considerable effort has been made to improve the poor machinability of titanium and titanium alloys like Ti6Al4V. One of different possibilities is the use of hydrogen as a temporary alloying element: specimens are etched to remove surface layers, and heat treated in hydrogen atmosphere at 600-850°C to charge the Ti matrix with hydrogen (ca. 10-20 at%). Cutting operations are performed in the hydrogen-loaded state, which reduces the cutting force progressively with increasing cutting speed, up to 50% under high-speed cutting (up to 100 m/s) conditions. Finally, the hydrogen is removed from the samples by a heat treatment in vacuum, to restore the mechanical properties of the original alloy.

Such H-induced reduction of the cutting force can be attributed to two effects: the stabilisation of the high-temperature bcc β phase of titanium, which is softer and more ductile than the hcp α phase, and the so-called HELP (hydrogen-enhanced local plasticity) mechanism. The latter results from the shielding of the elastic interaction between dislocations and obstacles due to hydrogen moving along with the dislocations, which eases the shear deformation in the cutting zone where the temperatures exceed 200°C. The effect becomes more pronounced at higher cutting speed, with higher local temperatures and therefore faster hydrogen diffusion in the cutting zone.

MM 41.13 Thu 18:00 Poster B

Microstructure and electrical conductivity of Cu-Ti alloys aged in hydrogen atmosphere — •Satoshi Semboshi[1,2], Ryota Gemma[2], Talaat Al-kassab[2], Astrid Pundt[2], and Reiner Kirchheim[2] — [1]Materials Science and Engineering, Osaka Prefecture University — [2]Institut für Materialphysiks, Uni. Göttingen

The influence of the aging in a hydrogen atmosphere on the electrical properties of Cu-1 and 3 at. % Ti alloys was investigated by means of electrical conductivity measurements and structural measurements using the X-ray diffraction, transmission electron microscopy and atom probe tomography. In the Cu-3 at.%Ti alloy, aging for 48 hours at 773 K in hydrogen atmosphere leads to an improvement of the electrical conductivity up to 65 % IACS (International Annealed Copper Standard), in comparison the value obtained for the alloy aged in a vacuum atmosphere. In addition, aging in hydrogen atmosphere leads to an efficient decrease of the lattice parameter of the Cu solid solution (Cuss) phase, suggesting a significant decrease of the Ti concentration in the Cuss phase. An important structural finding is the existence of not only a needle-shaped Cu$_4$Ti phase but also some cuboidal TiH$_2$ phase precipitates in the alloy aged in the hydrogen atmosphere. We, therefore, conclude that the aging in a hydrogen atmosphere strongly promotes the depletion of Ti in the Cuss phase because of the Cu$_4$Ti and TiH$_2$ precipitates formation, resulting in the significant improvement of the electrical conductivity. This work is partly supported by Inamori Foundation in Japan.

MM 41.14 Thu 18:00 Poster B

First principles analysis of Hydrogen in Manganese-rich austenitic steels — •Lars Ismer, Tilmann Hickel, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, 40237 Düsseldorf, Germany

Austenitic Mn-rich steels denote a promising new class of steels, since they combine high strength with ductility. Like other high strength steels, however, they are highly sensitive to hydrogen embrittlement (HE). Various microscopic mechanisms have been discussed as source of HE but the dominant mechanism has not been resolved so far. For a quantitative understanding a description of thermodynamic as well as kinetic aspects of the hydrogen-steel interaction is essential. We have therefore employed density functional theory to investigate the solubility and mobility of interstitial H in the austenitic phase of Fe, Mn, and Fe(x)Mn(1-x). For Fe(x)Mn(1-x) in the paramagnetic state our results show a significant increase both in the solubility and mobility of the H impurity with increasing Mn concentration. A detailed analysis shows that this effect is exclusively related to larger lattice volume induced by Mn. In addition we investigated the interaction of H with interstitial carbon. Our results show that at the high C-concentrations characteristic for the Mn steels the H solubility and mobility increase. This effect is caused by an (anisotropic) volume expansion of the lattice.

MM 41.15 Thu 18:00 Poster B

In-situ deformation study of porous nanocrystalline Pd during electrochemical charging — •Viswanath Raghavan Nadar[1], Dominik Kramer[1], and Jörg Weissmüller[1,2] — [1]Forschungszentrum Karlsruhe, Institut für Nanotechnologie, Karlsruhe, Germany — [2]Technische Physik, Universität des Saarlandes, Saarbrücken, Germany

The length of porous nanocrystalline palladium in a nearly neutral aqueous NaF (0.7 M) electrolyte was measured using a commercial dilatometer as a function of the applied electrode potential and of the charge. As expected, the sample expands during formation of the palladium hydride phases. However, the length is not just a simple function of the faradaic charge, but shows a remarkable fine structure which we discuss using a comparison with other nanoporous samples, e.g. gold and platinum. Even without hydrogen ad- or absorption, the length of nanometals varies as a function of charge due to the variation of surface stress with charge density, which causes large variations of the bulk pressure of nanomaterials due to their large ratio of the number of surface atoms relative to the number of bulk atoms. The surface stress behaviour of palladium observed at potentials positive of the hydrogen adsorption is qualitatively similar to that of porous

platinum, although there is a quantitative difference if one relates the expansion to the charge density, e.g. by calculating the surface stress-charge coefficient. The highly reproducible cyclic strain caused by hydrogen absorption and -desorption in Pd is larger than the surface stress effects by more than an order of magnitude.

MM 41.16 Thu 18:00 Poster B

Absolutbestimmung der Wasserstoffkonzentration innerhalb der plastischen Zone der Aluminiumlegierung AA6013 — •Christian Lenk, Thorsten Loewenhoff, Matz Haaks und Karl Maier — Helmholtz Institut für Strahlen- und Kernphysik, Universität Bonn, Nussallee 14-16, D-53115 Bonn, Germany

In ersten ortsaufgelösten Messungen an einer wechselverformten CT-Probe aus der Legierung AA6013 konnte bereits eine erhöhte Wasserstoffkonzentration in der plastischen Zone vor der Rissspitze nachgewiesen werden. Findet die Wechselverformung in einer korrosiven Umgebung statt, so dass Wasserstoff in die Probe diffundieren kann, führt dies zu einer erhöhten Rissausbreitungsgeschwindigkeit und einem verzögerten Ausheilverhalten von Fehlstellen in der plastischen Zone. Der Nachweis erfolgt dadurch, dass im UHV Späne mit einer Dicke von wenigen μm aus einer Probe herausgesägt und in situ ausgeheizt werden. Der folgende Anstieg des Partialdrucks wird mit einem Massenspektrometer aufgenommen. Es wird eine Methode vorgestellt, mit der es möglich ist, die absolute Wasserstoffkonzentration im Span aus der plastischen Zone zu bestimmen.

MM 41.17 Thu 18:00 Poster B

Hydrogen in ZnO - a challenge to experiments and theory — •Gerhard Brauer[1] and Jan Kuriplach[2] — [1]Forschungszentrum Dresden-Rossendorf e.V., Dresden, Germany — [2]Charles University, Prague, Czech Republic

Positron lifetime spectroscopy, nuclear reaction analysis and X-ray diffraction have been combined to investigate various, nominally undoped, ZnO single crystals. Hydrogen is detected in all crystals in a bound state (0.3 - 0.8 at.-%), and in some cases also in an unbound state (0.7 * 1.9 at.-%), which can be removed by annealing. A single positron lifetime of 180-182 ps and 165-167 ps is measured for all hydrothermally and melt grown crystals, respectively. These lifetimes are attributed to zinc vacancy-hydrogen complexes, as deduced from ab initio studies of various vacancy-hydrogen defect configurations in ZnO and related positron calculations. In addition, various defect studies of hydrothermally grown (0001) oriented ZnO crystals electrochemically doped with hydrogen are presented. It is demonstrated that a very high amount of hydrogen (up to ˜30 at.-%) can be introduced into the crystals by electrochemical doping. It is found that more than half of this amount is chemically bound, i.e. incorporated into the ZnO crystal lattice.

MM 41.18 Thu 18:00 Poster B

Hydrogen in V-8at%Fe single-layered films and Fe/V multi-layered films — •Ryota Gemma, Talaat Al-Kassab, Reiner Kirchheim, and Astrid Pundt — Institut fuer Materialphysik, Friedrich-Hund-Platz 1, D-37077, Goettingen, Germany

The influence of out-of-plane lattice parameter a_0 of V layer on the plateau slope of electromotive force (EMF) curves of V-8at%Fe films and Fe/V multi-layered films was investigated by applying in-situ XRD and in-situ stress measurements equipped with electrochemical hydrogen loading set up. For the films with small a_0, the plateau slope and hydrogen-induced stress were found to be larger than those with larger a_0. This trend can be qualitatively understood if we consider that hydrogen atoms predominantly occupy O_z sites in vanadium hydride phase, unlikely for the materials with isotropic site occupation as Pd. The deuterium distribution in the same kind of (110) films was also investigated by atom probe tomographic analysis (APT). The depth profile of the Fe/V films showed D atoms concentrated in V layers, as expected from the fact that V has bigger enthalpy for hydrogenation than that of Fe. However, the D concentration was not homogeneous in a V layer and far below the expected value from EMF curve. A similar phenomenon was found also for V-8at%Fe single-layered film. The results will be discussed in terms of difference in the microstructure and initial stress of the films.

MM 41.19 Thu 18:00 Poster B

Wechselverformungsmaschine für spezielle Anforderungen — •Thorsten Loewenhoff, Christian Lenk, Matz Haaks und Karl Maier — Helmholtz Institut für Strahlen- und Kernphysik, Universität Bonn, Nussallee 14-16, D-53115 Bonn, Germany

Zur Untersuchung dünnwandiger Al-Legierungen für den Flugzeugbau wurde eine Wechselverformungsmaschine konstruiert, um den speziellen Anforderung an die Probendimensionen zu genügen. Der Aufbau erlaubt mittels einer Piezokeramik Wechselverformungen im Bereich von einigen 10 μm Amplitude mit Frequenzen von 0,1 Hz bis 50 Hz. Die entwickelte Steuerungssoftware stellt verschiedene Signalformen (Sinus, Dreieck, Rechteck) zur Verfügung und nimmt Daten (Kraft auf die Probe, Verformungsamplitude) zur späteren Analyse auf. Im Gegensatz zu hydraulischen Verformungsmaschinen lässt die Piezokeramik Rechtecksignale mit guter Flankensteilheit zu. Dies ermöglicht Untersuchungen der Eindiffusion von Wasserstoff an Rissspitzen in Al-Legierungen.

MM 42: Phase Transitions III

Time: Thursday 14:00–15:30 Location: H 0107

MM 42.1 Thu 14:00 H 0107

Stress Induced Martensite in Epitaxial Ni-Mn-Ga Films — •Michael Thomas[1,2], Jörg Buschbeck[1], Oleg Heczko[1], Ludwig Schultz[1,2], and Sebastian Fähler[1,2] — [1]IFW Dresden, P.O. Box: 270116, 01171 Dresden, Germany — [2]Institute for Solid State Physics, Department of Physics, Dresden University of Technology, 01062 Dresden, Germany

Martensitic epitaxial Ni-Mn-Ga films with a thickness of about 500 nm were deposited at different temperatures on MgO(001) substrates. Some films are in an orthorhombic martensite state at room temperature though their compositions suggest far lower martensitic transformation temperatures. The martensite transformation is stress induced which was confirmed by X-ray stress analysis. The film structure can be explained as having an austenite layer at the interface between film and substrate. A hierarchical twinned martensite phase is grown on this austenite layer separated by a (101)-habit plane. The distribution of the twin boundaries is controlled by the stress state arising from the substrate constraint. Additionally non-modulated Ni-Mn-Ga films with a tetragonal phase and a coexisting cubic austenite phase were grown. Peeling this films off the substrate leads to the vanishing of the residual austenite phase. The strongly acting stress during the peeling may induce a fully tetragonal non-modulated martensite phase.

MM 42.2 Thu 14:15 H 0107

Microstructure and mechanical properties of sputter deposited NiMnGa magnetic shape memory alloy thin films — •Guido J. Mahnke and S. G. Mayr — 1. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

While bulk magnetic shape memory alloys (MSMA) are well established - and even commerically available, miniaturization as thin functional films still remains an open issue. The relation of microstructure and mechanical properties is one of the key ingredients to understand the martensitic transformation behaviour as well as twin boundary movement in MSMA thin films. To achieve this, highly textured and epitaxial NiMnGa MSMA thin films were preprared on different substrates at variable temperature by ion beam sputtering from a multicomponent target, and charcterized with respect to phase, microstructure and growth stresses. While growth usully occurred in the austenitic phase, a twinned martensitic state usually could be obtained during cooling down, accompanied by changes in the stress state. The relation of mechanical properties and microstructure is discussed.

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MM 42.3 Thu 14:30 H 0107

Growth of epitaxial and highly textured FePd shape memory alloy thin films — •Lisa Kühnemund, Tobias Edler, and S.G.