MM 16: Poster Ia

Time: Monday 18:30–20:30 Location: Poster E

MM 16.1 Mon 18:30 Poster E

Investigation of excitation-induced non-thermal effects in semiconductors, metals and alloys — •Simon Kümmel and Johannes Roth — FMQ, Universität Stuttgart, Germany

Excitation-induced non-thermal melting in silicon, as well as bond-hardening in gold following strong laser irradiation with short pulse durations have been known for several years. Furthermore, several traces of excitation-induced solid-solid phase transitions have been noticed in a variety of materials.

Here, we present several approaches to identify and quantify excitationinduced effects changing the bond strength and inducing phase transitions systematically in several semiconductors, metals and alloys obtained from DFT calculations depending on the degree of excitation. These calculation are in line with previous investigations and provide new insights into the change of the bond strength and the induced phase transitions following strong laser excitation.

MM 16.2 Mon 18:30 Poster E

Ab initio study of transition paths between (meta)stable phases of Nb and Ta-substituted Nb — •Susanne Kunzmann[1,2,3], Thomas Hammerschmidt[3], Gabi Schierning[1,2,4], and Anna Grünebohm[3,5] — [1]Experimental Physics, Bielefeld University, Germany — [2]Research Center Future Energy Materials and Systems (RC FEMS), University of Duisburg-Essen, Germany — [3]Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-University Bochum, Germany — [4]Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Germany — [5]Center for Interface-Dominated High Performance Materials (ZGH), Ruhr-University Bochum, Germany

Despite being well-characterized, Niobium exhibits unexplained anomalies. To address this, we employ density functional theory to revisit the metastablephases of Nb and Nb with Ta impurities. We compare energies and groundstate volumes of selected crystal structures, explore potential transition paths to the bcc ground state and the energy landscape for tetragonal distortions. Additionally, we assess stability through phonon spectra and vibronic free energies. We discuss previously overlooked aspects: a new local energy minimum on the bcc to ω transition path, a flat energy landscape concerning uniaxial strainalong [111], and significant stabilization of the σ phase through Ta substitution.

MM 16.3 Mon 18:30 Poster E

Quantum Restored Symmetry Protected Topological Phases — •Dhruv Tiwari[1], Steffen Bollmann[1], Thomas Köhler[2], Sebastian Paeckel[3], and Elio J. König[1] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]Uppsala University, Uppsala, Sweden — [3]Ludwig Maximilian University, Munich, Germany

Symmetry Protected Topological phases are paradigmatic for the non-trivial interplay of topology, symmetry, and interactions. For a given group of symmetries, it is already known that the topological classification can be different for interacting and non-interacting systems. On the other hand, one usually resorts to a mean-field approximation to study interacting systems where the tools of non-interacting topology can be employed to study topological characteristics. This raises the natural question as to what is the role of quantum fluctuations in the topological characteristics of interacting systems. We present an example of a system that is trivial under the mean-field approximation and shows topological characteristics upon the introduction of quantum fluctuations. To this end, we present results on an array of topological Cooper pair boxes. At half-filling, we observe the restoration of topological characteristics upon the introduction of quantum fluctuations. At quarter-filling, we obtain a richer phase diagram once we take into account the contribution of quantum fluctuations.

MM 16.4 Mon 18:30 Poster E

Ab initio study of phase stability of YMn2 with different magnetic orderings — •Pavel Papež, Martin Friák, and Ilja Turek — Institute of Physics of Materials, Czech Academy of Sciences, Žižkova 22, Brno, 616 00, Czech Republic

Our work is focused on the intermetallic compound YMn2 which exhibits an anomalous thermal expansion. The origin of this phenomenon is belived to be magnetism-related but it is not completely understood yet. A puzzling aspect is e.g. a 5% volume change at the Neél temperature of 100 K. We have employed quantum-mechanical calculations to examine the thermodynamic stability of different magnetic states. Our calculations included non-collinear magnetic states which were defined employing the spin-orbit coupling. The computational cell was that of the C15 Laves phase and contained 24 atoms. The 7 different magnetic configurations were set up along the [0 0 1] direction. Our results show the most stable configuration is an antiferomagnetic (AFM) state which is followed closely by two experimentally reported configurations with the same AFM nearest neighbour configurations but pointing along different directions. Interestingly, these two magnetic configurations exhibit very similar energies. Importantly, the resulting magnetic moments on Mn atoms and lattice parameters show very good agreement with the values reported in previous experimental studies.

MM 16.5 Mon 18:30 Poster E

Investigating changes of chemical bonding upon charge density wave transition in CuTe — •Johannes Holters, Christian Stenz, and Matthias Wuttig — Institute of Physics IA, RWTH Aachen University, 52074 Aachen, Germany

Properties of solids like the electrical conductivity, band gap, phonon dispersion and dielectric function are governed by the chemical bonds between the atoms. Changes in the bonding is thus indirectly measurable by electrical and optical means. The metallic mineral CuTe exhibits a Peierls-like distortion along tellurium chains below the transition temperature of 62°C. Due to the distortion the overlap of the Cu d-orbitals and Te p-orbitals is reduced, which leads to the occurence of a quasi-1D charge density wave. This work analyses the temperature-induced structural change of polycrystalline CuTe produced by sputter deposition by electrical and optical measurements. The electrical conductivity, phonon softening and dielectric function is used to investigate changes in the chemical bonding as a consequence of the electronic rearrangement along the Te-chains.

MM 16.6 Mon 18:30 Poster E

Phase transitions and electronic properties of Fe2O3 under laser compression by ultrafast in-situ X-ray absorption spectroscopy — Juan Pintor[1], Delphine Cabaret[2], and •Marion Harmand[3] — [1]IMPMC, Sorbonne University, Paris, France. — [2]IMPMC, Sorbonne University, Paris, France. — [3]IMPMC, Sorbonne University, Paris, France.

Understanding the structural changes in hematite (α-Fe2O3) under extreme pressure and temperature is essential for gaining insights into the physical properties of planetary interiors. At ambient conditions, hematite exhibits a rhombohedral structured antiferromagnetic insulator. Its high-pressure behavior has been extensively studied, with particular focus on pressures around 50 GPa, revealing a 10% volume cell drop, a change in crystal symmetry, a Mott transition, and the collapse of iron magnetic moments (high-spin to low-spin transition). The exact nature of the phase transition in this pressure range remains controversial, with debates about whether the electronic or structural transition drives the other. This study reports ultrafast time-resolved X-ray Absorption Near Edge Spectroscopy (XANES) measurements conducted at the High Power Laser Facility of ESRF-ID24 beamline. Our data capture time-resolved transformations, revealing changes in the different XANES features within hundreds of ps, after the shock breakout from the samples. This presentation will detail a time-resolved examination of XANES changes with respect to pressure and temperature. For further understanding of the XANES features, preliminary DFT calculations will also be presented.

MM 16.7 Mon 18:30 Poster E

Spin and phase state of iron in FeS at Martian core conditions — •G. Scholz[1], C. Albers[1], H. Gretarsson[2], G. Kovalskii[3], M. Mezouar[4], W. Morgenroth[3], L. Pennacchioni[3], J. Savelkouls[1], M. Sundermann[2], N. Thiering[1], M. Wilke[3], and C. Sternemann[1] — [1]TU Dortmund, Dortmund, Germany — [2]Deutsches Elektronen-Synchrotron, Hamburg, Germany — [3]University of Potsdam, Potsdam, Germany — [4]European Synchrotron Radiation Facility, Grenoble, France

The Martian core is assumed to be comprised of molten FeNi with

up to 15 wt% S and 5 wt% O. To further understand the electronic structure of iron, we investigated the changes in phase state and spin state in FeS, a simplified core composition, which are induced by high pressure (p) and high temperature (T).

In order to explore this topic, we conducted *in situ* (resonant) X-ray emission spectroscopy at beamline P01, PETRA III (DESY) using a von Hamos spectrometer. We used diamond anvil cells in combination with a double-sided Yb:YAG-laser heating setup to achieve pressure and temperature conditions up to 64 GPa and 3000 K, respectively. The phase state of FeS was evaluated at beamline ID27, ESRF with X-ray diffraction combined with double-sided *in situ* laser heating up to 43 GPa and 3000 K.

In both experiments, our focus was set on the temperature induced phase transition from FeS-III to -IV and -V and the potential spin state change at p/T-conditions of the FeS-IV and -V phase transition boundary.

MM 16.8 Mon 18:30 Poster E

Characterization and improvement of the hydrogen embrittlement properties of AM316L — •Kai Lagemann, Stefan Wagner, and Astrid Pundt — Karlsruher Institute for Technology (KIT), Institute for Applied Materials Materials Science and Engineering (IAM WK), Karlsruhe

In this project, powder bed-based laser melting (PBF-LBM) is used to investigate additively manufactured 316L steel, which is planned to be used as a structural material in hydrogen technology in the future. It is investigated how the microstructure changes through the application of a remelting (RM) strategy and whether printing defects can be minimised as a result.

The RM parameter study identifies optimal manufacturing parameters. It is shown that the RM strategy melts remanent powder particles and reduces the melt pool distance. However, the microstructure of the steel can only be influenced to a limited extent.

The fracture behaviour of the printed steel shows a complex interplay of porosity, crystallographic grain orientation and hydrogen concentration. The combination of these effects influences the active failure mechanism during fracture. The elongation at fracture and the necking behaviour change, while the modulus of elasticity and tensile strength are minimally affected. For hydrogen-loaded RM specimens, a strain rate dependence of the failure mechanisms was demonstrated.

MM 16.9 Mon 18:30 Poster E

LPBF processed crack-free high-strength Al alloy — •Irena Paulin, Nejc Velikajne, Črtomir Donik, and Matjaž Godec — Institute of Metals and Technology, Lepi pot 11, Ljubljana, Slovenia

The ambitious goal of our research involves the development of a new high-strength Al alloy suitable for the AM process, which will facilitate the production of crack-free components combined with improved mechanical and corrosion properties. To achieve this goal, we prepared samples from commercially available AA7075 aluminium powder on a laboratory LBPF device. We changed various process parameters and optimized the production of simple samples in the form of 10x10x10 mm3 cubes, where we achieved the highest densities. Cracks were visible in all samples, regardless of the variety of process parameters used.

To avoid cracks, we process the samples at different temperatures of the preheated baseplate, where it turned out that higher temperatures do not have a favourable effect on the production of material without cracks. Surprisingly, lower preheating temperatures ensured better remelting in the material and thus less porosity in the material. In order to try to produce a material without cracks, in the next steps we started mixing AA7075 and AlSi12 powder, adding Si to the base material and thus reducing the difference in solidification temperature. Microstructural characterization showed that we successfully made a material without cracks.

MM 16.10 Mon 18:30 Poster E

PBF-LB of Soft Magnetic Fe-Based Metallic Glasses — •Felix Römer[1], Florian Spieckermann[1], Parthiban Ramasamy[2], and Jürgen Eckert[1,2] — [1]Montanuniversität Leoben, Leoben, Austria — [2]Erich Schmid Institute of Materials Science, Leoben, Austria

Reducing the energy losses is a key requirement in the development of soft magnetic materials.

In recent years, interest has focused on nanocrystalline soft magnetic alloys, whose magnetic properties benefit from their chemical and structural variations at the nanoscale. Unfortunately, the nanocrystalline Fe- BMG's suffers from extreme embrittlement. Thus, they must be annealed in the final core geometry and handled very carefully.

The possibility of additive manufacturing of metallic glasses has drawn a lot of attention. This technique provides high heating and cooling rates, making it suitable for producing metallic glass parts with dimensions much bigger than their critical casting diameter. Besides the high heating and cooling rates, the layer-by-layer construction of the part results in a complex heat treatment of the preceding layers. Understanding the behavior of metallic glasses under these high rates and complex treatment is the key to printing dense, crack-free parts with suitable magnetic properties.

In the current study we show the effects of double scanning and random line strategy as well as preheating of the building platform on the microstructure, crack formation and thermal properties of KUAMET6B2 Fe72.6Si11.3B10.9Cr2.2C3.0 (at%).

MM 16.11 Mon 18:30 Poster E

Investigation of the Anisotropic Conductivity in Printed Nanosilver — •Lennart Schwan[1,2], Michael Feige[1], Laila Bondzio[2], Hütten Andreas[2], and Sonja Schöning[1] — [1]Bielefeld Institute for Applied Materials Research (BIfAM), Hochschule Bielefeld - University of Applied Sciences and Arts — [2]Thin Films & Physics of Nanostructures, Bielefeld University

3D printing is an emerging technology with a wide range of applications. The modern multi-material jetting process, such as that used in the Nano Dimension Dragonfly Pro LDM, makes it possible to print dielectric and conductive materials in a single process. In addition to printing flat structures such as printed circuit boards, three-dimensional structures such as antennas, coils or cooling elements can also be realized.

A special characteristic of the printed conductive material is the anisotropy of the electrical conductivity. Our investigation is dedicated to the origin of the anisotropy.

Investigations in the SEM show a direction-dependent crack structure. In order to investigate the influence of the cracks, we generate geometries from SEM images of the surface and simulate the current flow and the influence/impact on the effective conductivity using FEM. A further explanation results directly from the printing process, in which the surfaces are created from alternating offset printing lines. In order to investigate the influence of the resulting boundary layers on the anisotropic conductivity, we create additional boundary layers by manipulating the printing process.

MM 16.12 Mon 18:30 Poster E

Usability and Performance Analysis of 3D-Ink-Jet-Printed Load Cells with Resistive and Capacitive Strain Gauges — •Michael Feige, Lennart Schwan, and Sonja Schöning — Institute for Applied Materials Research (BIfAM), Hochschule Bielefeld - University of Applied Sciences and Arts, Bielefeld, Germany

Strain gauges can be used in a variety of different measurements e.g., to measure forces in manufacturing systems, to continuously monitor displacement of building structures. Furthermore, are they used in simple bathroom scales, kitchen scales and precision instruments with accuracies up to thousands of a gram. We utilize a 3D-Ink-Jet-Printer to manufacture flexible plastic devices with integrated strain gauges consisting of traces for resistive measurements or electrode arrays for capacitive measurements made of sintered silver ink. This additive manufacturing process provides a big advantage in scalability and flexibility over conventional methods and can avoid the necessity of bonding the strain gauges to a substrate adhesively. Printing measuring devices with dimensions of several millimeters up to several centimeters, an adaption to fulfill different geometric constraints e.g., due to housing or mounting, and fine tuning by thinning or thickening materials in particular areas is possible without great effort. Even more or less complex formations of multiple strain gauges combined in one device are feasible. We print different designs and examine them with regard to their sensitivity, hysteresis, non-reversible effects of stress and temperature stability.

MM 16.13 Mon 18:30 Poster E

Electrochemical study of Hydrogen Embrittlement in Al-Si coated stainless steels — •Neil Reon Mathias[1], Alisa Svirina[2], Sebastian Pentz[1], and Ferdinand Haider[1] — [1]Chair for Experimental Physics I, University of Augsburg, Universitätsstraße 1, 86159 Augsburg (Germany) — [2]Institute de Mécanique et Ingéniere, Université de Bordeaux (France)

There is a compelling business case for optimizing stainless steels for

usage in hydrogen storage tanks. One method of reducing the penetration of hydrogen and accordingly the embrittlement of stainless steels is by coating it using the hot-dip process, which forms a layer of Al-Si on the surface to mitigate the embrittlement process. This study performs electrochemically controlled hydrogen permeation on different coated and uncoated stainless steels using a Devanathan-Stachurski cell to understand the nature of protection offered by these coatings. A set of commercial-grade austenitic, ferritic, duplex, and hot-dipped stainless steels are investigated for changes in their microstructure and fracture behaviour at room temperature. Evolution of trapped hydrogen is measured through thermal desorption spectroscopy to validate the electrochemical measurements. The hot-dip coating seems to reduce the hydrogen permeation considerably, thereby resulting in less hydrogen embrittlement compared to uncoated stainless steels. Microstructural changes indicate that the uncoated stainless steels show greater degree of intergranular fracture compared to the coated stainless steels. Tensile test results demonstrate the increased elongation of coated stainless steels in comparison to their uncoated counterparts.

MM 16.14 Mon 18:30 Poster E

Effect of Ilmenite reduction pathway on TiFe hydrogen storage properties obtained by Sieverts apparatus measurement — •Matthieu Ramond[1,2], Alexander Haack[1,2], Gabby Hunter-Smith[3], Mohammad Zarar[3], Karl Shaffer[4], Karl Dahm[5], Chris Bumby[3], Paul Jerabek[2], Thomas Klassen[2,6], Nigel Lucas[1,7], and Claudio Pistidda[2] — [1]University of Otago, Department of Chemistry, Dunedin, New Zealand — [2]Helmholtz-Zentrum Hereon, Institute of Hydrogen Technology, Geesthacht, Germany — [3]Victoria University of Wellington, Paihau-Robinson Research Institute, Wellington, New Zealand — [4]Victoria University of Wellington, Ferrier Research Institute, Wellington, New-Zealand — [5]Callaghan innovation, Lower Hutt, New Zealand — [6]Helmut Schmidt University, Faculty of Mechanical Engineering, Institute of Materials Science, Hamburg, Germany — [7]MacDiarmid Institute for Advanced Materials and Nanotechnology, Wellington, New Zealand

New Zealand has large quantities of naturally occurring ilmenite (TiFeO3) ore. Samples of this easily available oxide were thermally reduced to a titanium-iron alloy under a variety of experimental conditions, e.g., temperatures, durations, and grind sizes at Victoria University of Wellington. After thermal activation under dynamic vacuum, hydrogen adsorption and desorption cycles were measured. The hydrogen uptake properties of the alloys can be determined using a specially-built Sieverts apparatus. The gravimetric storage and kinetics of the samples were evaluated by numerical fitting, enabling these properties to be linked to the reduction process.

MM 16.15 Mon 18:30 Poster E

Experimental and computational study of the effects of metal-based additives on the dehydrogenation process of the 2NaBH4 + MgH2 system — •Yuanyuan Shang[1], Archa Santhosh[1], Ou Jin[2], Fahim Karimi[1], Thi Thu Le[1], Dorothée Vinga Szabó[2], Stefan Wagner[2], Christian Kübel[2], Paul Jerabek[1], Astrid Pundt[2], and Claudio Pistidda[1] — [1]Department of Materials Design, Institute of Hydrogen Technology, Helmholtz-Zentrum hereon GmbH, 21502, Geesthacht, Germany — [2]Institute for Applied Materials, Karlsruhe Institute of Technology, 76131, Karlsruhe, Germany

We report a systematic investigation of the effect that selected metal-based additives have on the dehydrogenation properties of the reactive hydride composite (RHC) model system 2NaBH4+MgH2. Compared to the pristine system, the material doped with 3TiCl3*AlCl3 exhibits superior dehydrogenation kinetics. The addition of 3TiCl3*AlCl3 alters the controlling mechanism of the second dehydrogenation step making it change from a two-dimensional interface-controlled process to a two-dimensional nucleation and growth controlled process. Nanostructured metal-based phases, such as TiB2/AlB2 particles, appear to act as heterogeneous nucleation sites for MgB2. For this reason, the properties of the TiB2/MgB2 interface were investigated by first-principles calculations utilizing density functional theory (DFT).

MM 16.16 Mon 18:30 Poster E

Electrochemical loading of magnesium-palladium thin films in KOH — •Giorgia Guardi[1], Angelina Sarapulova[1], Sonia Dsoke[1], Stefan Wagner[1], Luca Pasquini[2], and Astrid Pundt[1] — [1]Institute for Applied Materials (IAM), Karlsruhe Institute of Technology (KIT), Germany — [2]Department of Physics and Astronomy, University of Bologna, Italy

The magnesium-hydrogen system is of interest for hydrogen storage applications due to the high hydrogen density (7.6 wt.%) achievable in magnesium hydride (MgH_2). There are however drawbacks, such as the slow diffusion of hydrogen in MgH2. This drawback can be overcome by using nanostructured materials such as thin films, where the hydrogen diffusion coefficient increases due to the high concentration of grain boundaries. This leads to faster hydride formation.

Hydrogen charging of magnesium by means of electrochemistry is challenging due to its high corrosion tendency. In this work we show how the electrochemical hydrogen loading of Mg-Pd thin films can be optimised in KOH. It is revealed how the loading potential influences the hydride formation mechanism, and how its optimal value can be found by performing cyclic voltammetry and hydrogenography experiments.

MM 16.17 Mon 18:30 Poster E

Measurement of Tritium Content with a novel Detector System — •Joris Müller, Christoph Kirchlechner, and Xufei Fang — IAM, KIT, Karlsruhe, Germany

Hydrogen Embrittlement (HE) and the involved mechanisms are still being heatedly debated today. It yet remains a challenge to quantify the embrittlement due to the difficulty in precisely detecting hydrogen via most existing methods, while ones with high precision (e.g., Atom Probe Tomography) are limited to very local areas under special conditions (e.g., deuterium charging). Here, we present a concept of using a high-resolution, spatially-resolving direct electron detector, akin to a radiation camera, by taking advantage of using the radioactive hydrogen isotope tritium. After exposing samples to tritium, the β-decay can then be detected to enable a positionally accurate depiction of its position in the crystal lattice. One proposed concept makes use of a parallel-hole collimator for direction-wise filtering in order to achieve a parallel projection image in combination with a stacked microchannel plate (MCP) array for amplification, followed by a phosphorescent screen and high-resolution camera functioning as an electron to photon and finally signal converter. A setup like this will, in an ideal case, enable in situ real-time tracking of tritium during micromechanical tests, allow quantification of the mechanical properties with the presence of hydrogen in the materials' defects (e.g., grain boundaries), and help to gain a better understanding of the hydrogen embrittlement mechanisms in metals.

MM 16.18 Mon 18:30 Poster E

Microstructural Influencing Factors on Susceptibility of High Strength Steels against Hydrogen Embrittlement — Ingrit Sisilia Rosari Nurak[1] and •Michael Brilz[2] — [1]KIT, Karlsruhe (Gebäude 30.25, Raum 217) — [2]MPA IfW Darmstadt

This thesis aims to conduct a materials science-based analysis of the relationship between microstructural, chemical, and fracture mechanical factors and the susceptibility to hydrogen embrittlement. For this purpose, metallographic and fracture mechanical examinations are done via VVT tests. To analyze the correlation between microstructural and fracture mechanical parameters, three materials with different microstructures are loaded with a constant HCl concentration and then strained, while for the investigation of the correlation between chemical and fracture mechanical parameters, identical samples are loaded with different HCl concentrations and then strained. An important microstructural influencing factor for quenched and tempered steels is the grain size of former austenite grains.