MM 21: Functional Materials II

Time: Monday 17:15–18:45 Location: IFW D

MM 21.1 Mon 17:15 IFW D

Hydrogen induced defects in the palladium/rutile titanium dioxide model system — •Marian David Bongers[1], Mohsen Sotoudeh[2], Vladimir Roddatis[1], Jakub Čížek[3], Carsten Nowak[1], Martin Wenderoth[4], Peter Blöchl[2], and Astrid Pundt[1] — [1]Institut für Materialphysik, Univ. Göttingen — [2]Institute for Theoretical Physics, Clausthal Univ. of Technology — [3]Department of Low-temperature Physics, Charles Univ. in Prague, Czech Republic — [4]IV. Physikalischen Institut, Univ. Göttingen

The palladium (Pd)/titanium dioxide (TiO_2) system is used in a range of applications where in particular the interaction with hydrogen (H) is of interest. We use in-situ transmission electron microscopy (ETEM) and electron energy loss spectroscopy (EELS) on cross-sectional Pd/TiO_2 lamella focusing on the interface. The EELS studies show a small change of the Ti L edge signal in the 3 nm close vicinity of the interface, for hydrogen gas pressures of about 10^{-1} mbar. These small changes can be attributed to a shift in the density of states (DoS) by about 1 eV, by the presence of hydrogen. This is supported by projector augmented wave (PAW) code simulations using the local hybrid density functional PBE0r [1]. We suggest interstitial hydrogen to be the dominant hydrogen induced defect in bulk, while it is the oxygen-vacancy filled with hydrogen nearby the interface. These defects determine the corresponding Fermi level position in bulk and at the interface. This work is supported by the Deutsche Forschungsgemeinschaft via SFB1073, project C06 and C03 as well via the Heisenberg grant PU131/9-2. [1] M. Sotoudeh, M. Bongers, et al., submitted

MM 21.2 Mon 17:30 IFW D

Magnetocaloric properties of melt-spun NiCoMnAl Heusler ribbons — •Bruno Weise[1], Niclas Teichert[2], Andreas Becker[2], Lars Helmich[2], Maria Krautz[1], Andreas Hütten[2], and Anja Waske[1,3] — [1]IFW Dresden, Institute for Complex Materials, Dresden, Germany — [2]CSMD, Department of Physics, Bielefeld University, Bielefeld, Germany — [3]Institute of Materials Science, TU Dresden, Dresden, Germany

Within the group of magnetocaloric Heusler alloys NiCoMnAl is a promising alloy system for magnetic refrigeration. It is rare-earth free, non-toxic and none of the constituent elements is short on stock. In thin films of NiCoMnAl, an entropy change of up to $\Delta S = 17.5\ J/kgK$ for a magnetic field change of $\Delta\mu_0 H = 5\ T$ was observed [1], hence thin films can be used as a model system to test new materials. This subsequent study applies these results to bulk materials.

Samples of the nominal composition $Ni_{40}Co_{10}Mn_{30}Al_{20}$ have been produced by melt spinning to achieve near net shaped thin plates for the use in a refrigeration bed. The ribbons were annealed for up to 50 h and the structure was checked with XRD. With electron microscopy the microstructure of the ribbons was studied. An optimal heat treatment time for highest entropy change was found and the adiabatic temperature change for this annealing time was determined.

[1] N. Teichert et al., Phys. Rev. B 91, 184405 (2015).

MM 21.3 Mon 17:45 IFW D

In-situ dehydrogention and positron annihilation spectroscopy of Mg2Fe thin films — •Thu Trang Trinh[1,2], Marciej Oskar Liedke[2], Andreas Wagner[2], Rene Heller[2], Herman Schreuders[3], Bernard Dam[3], Kohta Asano[4], and Kay Potzger[2] — [1]Technische Universität Dresden, 01062 Dresden, Germany — [2]Helmholz-Zentrum Dresden Rossendorf, 01328 Dresden, Germany — [3]Delft University of Technology, 2629HZ Delft, Netherlands — [4]AIST, Tsukuba 8565, Japan

Mg2Fe hydride belongs to the most promising candidates for application as light weight storage material in a future hydrogen economy. Recently, it has been shown that due to chemochromism, Mg2Fe is also a low-cost and rare-earth-free candidate for switchable mirrors upon hydrogen loading. However, the interaction between defects and hydrogen on the atomic scale remains not completely understood, despite the fact that the behaviour of hydrogen in metals is strongly affected by the presence of defects. Due to the positive binding energy between hydrogen and vacancy, the hydrogen atoms get trapped at existing defects which thus play an important role for the hydride formation.

We present a comparative and systematic study on the defects in Mg2Fe and their interaction with hydrogen by means of positron annihilation spectroscopy (PAS). We present first results of the temperature dependence of the open volume defects during annealing of Mg2FeH6 thin films, which was performed by an unique high vacuum system for defect manipulation and analysis (AIDA) at the positron beamline at the Helmholtz-Zentrum Dresden-Rossendorf.

MM 21.4 Mon 18:00 IFW D

Compliant on-skin compass for artificial magnetoception — •Gilbert Santiago Cañon Bermúdez, Jürgen Fassbender, and Denys Makarov — Helmholtz-Zentrum-Dresden-Rossendorf e.V., Dresden, Germany

Flexible electronics has inspired novel concepts like electronic skins[1] and more recently, magnetosensitive skins[2], i. e., artificial skins which allow humans to perceive magnetic fields. This ability to detect and respond to magnetic fields, commonly referred to as magnetoception, has sparked several legends since the old sailing times. Back then, it was believed that compass rose tattoos would allow sailors to always find the way home. Here, we present a flexible electronics platform to turn this ancient belief into a functional on-skin compass system. The highly compliant compass is prepared on 6-micron-thick polymeric foils and relies on the anisotropic magnetoresistance (AMR) effect in magnetic thin film sensors. Its response is tailored to be linear and possess maximum sensitivity around the earth's magnetic field by using a barber pole scheme, which forces the current in the sensor to flow 45 degrees skewed with respect to the easy axis of the AMR stripes. We envision that this on-skin compass could support research efforts on biomagnetic orientation and novel magnetic interactive devices. In the latter case, the applications span a plethora of tasks from virtual or augmented reality systems to touchless security systems and magnetic tags.

[1] D. H. Kim et al., Science 333, 838 (2011).
[2] M. Melzer et al., Nature Commun. 6, 6080 (2015).

MM 21.5 Mon 18:15 IFW D

Photoemission Spectrscopy of Type-II Weyl Semimetal Candidate MoTe2 — •Andrew Patton Weber[1,2], Nan Xu[1,2], Stefan Muff[1,2], Mauro Fanciulli[1,2], Arnaud Magrez[1], Phillipe Bugnon[1], Helmuth Berger[1], BQ Lv[3], Bin Bin Fu[2,3], Christian Matt[2], Joel Mesot[1,2,4], Hong Ding[3], Ming Shi[2], and Jan Hugo Dil[1,2] — [1]Institute of Physics, École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland — [2]Swiss Light Source, Paul Scherrer Institute, Villigen-PSI, Switzerland — [3]Beijing National Laboratory for Condensed Matter Physics and Institute of Physics, Chinese Academy of Sciences, Beijing, China — [4]Laboratory for Solid State Physics, ETH Zurich, Zurich, Switzerland

Topological matter can often be identified by signatures presented by the surface electron-structure. Type-II Weyl semimetal candidates, in which surface Fermi arcs can overlap with the projection of bulk Fermi pockets, have proven to be more difficult to characterize by these means, leading to controversies. The present work clarifies the situation for the case of the octahedral polytype of MoTe2 through temperature-dependent spin- and angle-resolved spectroscopy experiments. It is found that the appearance of large spin-polarized Fermi arcs (extending over more than 12% of a reciprocal lattice vector and exhibiting nearly full spin-polarization), occurs as a consequence of the transition from the inversion-symmetric 1T' structure to the inversion-symmetry-breaking Td structure. Moreover, helical spin-textures are found to be absent near the large Fermi arcs. These results indicate a topological origin for Fermi arc-like states.

MM 21.6 Mon 18:30 IFW D

Identifying detrimental effects for multi-band superconductivity - Application to Sr_2RuO_4 — •Aline Ramires[1] and Manfred Sigrist[2] — [1]Institute for Theoretical Studies, ETH Zurich, 8092 Zurich, Switzerland — [2]Institute for Theoretical Physics, ETH Zurich, 8093 Zurich, Switzerland

We propose a general scheme to probe the compatibility of arbitrary pairing states with a given normal state Hamiltonian by the introduction of a concept called *superconducting fitness*. This quantity gives a direct measure of the suppression of the superconducting critical temperature in the presence of key symmetry-breaking fields. A merit of the superconducting fitness is that it can be used as a tool to identify

nontrivial mechanisms to suppress superconductivity under various external influences, in particular, magnetic fields or distortions, even in complex multiorbital systems. In the light of this concept we analyze the multiband superconductor Sr_2RuO_4 and propose a new mechanism for the suppression of superconductivity in multiorbital systems, which we call interorbital effect, as a possible explanation for the unusual limiting feature observed in the upper critical field of this material.