MM 44: Materials Design II

Time: Wednesday 16:15–17:15 Location: H5

MM 44.1 Wed 16:15 H5

Design strategy for biodegradable Fe-based alloys for medical applications — •Michael Schinhammer, Anja C. Hänzi, Jörg F. Löffler, and Peter J. Uggowitzer — Laboratory of Metal Physics and Technology, Department of Materials, ETH Zürich, Switzerland

Iron is a promising metallic element for bioabsorbable medical implants. The aim of this article is to describe a design strategy for the development of new biodegradable Fe-based alloys for temporary implant applications, in terms of both an enhanced degradation rate compared to pure iron, and suitable strength and ductility. The design strategy is based on electrochemical, microstructural and toxicological considerations. The influence of alloying elements on the electrochemical modification of the Fe matrix and the controlled formation of noble intermetallic phases is deployed. Manganese and palladium have been shown to be suitable alloying additions for this design strategy: Mn lowers the standard electrode potential, while Pd forms noble (Fe,Mn)Pd intermetallics acting as cathodic sites. We discuss the efficiency and the potential of the design approach, and evaluate the resulting characteristics of the new alloys. The newly developed Fe-Mn-Pd alloys reveal an increased degradation rate compared to pure iron. Additionally, the mechanical performance is shown to be adjustable not only by the choice of alloying elements but also by heat treatment procedures; high strength values >1400 MPa at ductility levels >10% can be achieved. Thus, the new alloys offer an attractive combination of electrochemical and mechanical characteristics considered suitable for biodegradable medical applications.

MM 44.2 Wed 16:30 H5

Superconductivity in $FeSe_{1-x}$: a simple system with ambiguities — •Amir-Abbas Haghighirad, Mariano de Souza, Ulrich Tutsch, Sebastian Köhler, Daniel Hofmann, Michael Lang, and Wolf Assmus — Physikalisches Institut, Goethe-Universität, Max-von-Laue Str. 1, D-60438 Frankfurt (M), Germany

Recently, superconductivity has been reported at ~ 8.5 K in FeSe with the α-PbO-type structure [1]. One of the interesting aspects of superconductivity in FeSe is the enormous effect of T_c [2,3] when pressure is applied. The latter indicates an extraordinarily high sensitivity of the superconducting state to structural deformations [4,5]. However, the accurate structure and the terminology for describing the FeSe phase that exhibits superconductivity is still not well understood. Several groups, as well as ours, have undertaken the effort to refine the synthesis steps to produce better quality single-crystalline samples of FeSe, which is crucial for resolving the physical properties, such as "anomalous" resistivity, the role of the structural phase transition as well as the role of magnetism in enabling superconductivity. We have improved our methods of synthesis using ambient- and high-pressure techniques. The effect of stoichiometry on the phase purity of FeSe and its superconducting properties were investigated. We will provide an overview of the progress seen so far. [1] F.C. Hsu *et al.*, Proc. Natl. Acad. Sci. U.S.A. **105**, 14262 (08); [2] K.W. Yeh *et al.*, Europhys. Lett. **84**, 37002 (08); [3] S. Medvedev *et al.*, Nat. Mat. **8**, 576 (09); [4] S. Margadonna *et al.*, Chem. Commun. **43**, 50607 (08); [5] T.M. McQueen *et al.*, Phys. Rev. Lett. **103**, 057002 (09).

MM 44.3 Wed 16:45 H5

Mesoporous metal catalysts formed by ultrasound — •Jana Schäferhans, Nicolas Pazos Perez, and Daria Andreeva — Physikalische Chemie II, Universität Bayreuth, Deutschland

We study the ultrasound-driven formation of mesoporous metal sponges. The collapse of acoustic cavitations leads to very high temperatures and pressures on very short scales. Therefore, structures may be formed and quenched far from equilibrium. Mechanism of metal modification by ultrasound is complex and involves a variety of aspects. We propose that modification of metal particles and formation of mesoporous inner structures can be achieved due to thermal etching of metals by ultrasound stimulated high speed jets of liquid. Simultaneously, oxidation of metal surfaces by free radicals produced in water during cavitation stabilizes developed metal structures. Duration and intensity of the ultrasonication treatment is able to control the structure and morphology of metal sponges. We expect that this approach to the formation of nanoscale composite sponges is universal and opens perspective for a whole new class of catalytic materials that can be prepared in a one-step process. The developed method makes it possible to control the sponge morphology and can be used for formation of modern types of catalysts. For example, the sonication technique allows to combine the fabrication of mesoporous support and distribution of metal (Cu, Pd, Au, Pt etc.) nanoparticles in its pores into a single step.

MM 44.4 Wed 17:00 H5

Large grain systems based on experimental EBSD-data and influence of elastic forces — •Michael Selzer, Marcus Jainta, Mathias Reichardt, Andreas Unser, and Britta Nestler — Institute for Materials and Processes, Karlsruhe, Germany

Phase-field simulations are applied to investigate the evolution of large polycrystalline grain structures from the melt or using EBSD data from experiments as initial condition. We study the dependence of grain boundary anisotropy on the evolution of the grain size distributions and the effect of misorientation distributions on the growth laws in 2D and 3D. Additionally it is possible to predict the failure and strength properties of the investigated metallic alloys. To achieve this it is necessary to take in account the influence of elastic forces. When applying a sufficient amount of stress, the grain structure breaks and forms a crack. In numerical simulations, we investigate crack propagation in polycrystalline metallic alloys for mode I and III. The shape of such cracks depends on the applied loads and on the grain distribution of the observed material. Suitable simulations require many grains in a relatively large domain. For this goal, we present a parallel, optimized multi phase field model featuring efficient modeling of large three dimensional phase systems coupled with a model for elastic stresses. We show results for 2D and 3D crack developments along grain boundaries and in polycrystalline systems based on experimental EBSD data.