MM 3: Mechanical Properties and Alloy Design I

Time: Monday 10:15–12:45 Location: SCH/A215

MM 3.1 Mon 10:15 SCH/A215

Mechanical Properties of Disordered Fe-Co Nanoparticles — •Yarden Nathan — Technion, Haifa, Israel

We synthesized Fe- 50 at.% Co nanoparticles (NPs) via solid-state dewetting of Fe-Co bilayers deposited on a sapphire substrate at the temperature of 900 *C followed by slow cooling. By employing X-ray diffraction and electron diffraction in transmission electron microscope (TEM) we demonstrated that the NPs are fully disordered α-FeCo body centered cubic (BCC) phase. We demonstrated that the size and orientations of the disordered BCC NPs can be controlled by varying their fabrication parameters. Most of the NPs were faceted single crystals with their top (110) facet oriented parallel to the substrate. The mechanical properties of the NPs were measured by employing in-situ micro compression tests in the scanning electron microscope (SEM). The near-theoretical strength of α-FeCo NPs was demonstrated. We propose that the fully disordered NPs behave similarly to the defect-free NPs of pure metals. The plasticity of these NPs is controlled by the dislocation nucleation requiring near-theoretical stress. This mechanism explains the near-theoretical strength and the distinct "smaller is stronger" size effect observed in this metastable phase.

MM 3.2 Mon 10:30 SCH/A215

Role of Structural Hierarchy on Tensile Properties of Nanoporous Metals — •Wei-Che Chang[1], Yong Li[1], Henry Ovri[1], and Shan Shi[1,2] — [1]Institute of Hydrogen Technology, Helmholtz-Zentrum Hereon, Geesthacht, Germany — [2]Research Group of Integrated Metallic Nanomaterials Systems, Hamburg University of Technology, Hamburg, Germany

Nanoporous gold (NPG) is drawing significant attention as functional, lightweight material due to its low density, high surface area, and tunable structures. Despite the inherent ductility of bulk gold, NPG often exhibits brittleness under tension [1]. Recently, hierarchical nanoporous gold (HNPG) with multiple levels of well-defined porosities has attracted significant interest for its enhanced functional performance and improved compressive properties at reduced solid fraction [2]. However, whether these mechanical enhancements under compression also extend to tension, particularly whether structural hierarchy can mitigate the intrinsic brittleness of nanoporous networks under tension, remains an important open question. In this work, we introduce an in-situ micro-tensile setup for real-time observation of deformation and fracture behaviors in a scanning electron microscope (SEM). Our results show that the hierarchical structure improves ductility by a factor of five. The mechanism of tensile deformation is further revealed by molecular dynamics simulations.

[1] N. Badwe, X. Chen, K. Sieradzki, Acta Mater. 129 (2017) 251-258
[2] S. Shi, Y. Li, B. Ngo-Dinh, J. Markmann, J. Weissmüller, Science 371 (2021) 1026-1033

MM 3.3 Mon 10:45 SCH/A215

Mechanical shielding of holes in elastic solids — •Kanka Ghosh and Andreas M. Menzel — Institut für Physik, Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg, Germany

Holes inside an elastic solid reduce its overall mechanical stiffness. We examine whether a stiff shell around the hole can act as a shield under external loading, maintaining overall mechanical properties of the solid as if the hole were absent. For this purpose, an isotropic, homogeneous, linearly elastic material, loaded uniformly under plane strain with low concentrations of holes is considered. Instead of changing the materials to conceal a hole, we suggest to adjust the thickness of the shell for given elasticity parameters. A corresponding analytical expression for the thickness of the shell is derived. We extend this idea to the atomistic level using molecular dynamics simulations of model Lennard-Jones solids. Consistency of the resulting shell thickness for mechanical shielding at the atomistic scale attests the robustness of our continuum elasticity predictions. The concept is crucial for lightweight construction without compromising elastic materials properties.

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Reference: K. Ghosh and A. M. Menzel, Mechanically concealed holes, arXiv:2511.00135

MM 3.4 Mon 11:00 SCH/A215

Synthesis and mechanical properties of multi-scale hierarchical Ni and Cu foams — •Ulrike Dette[1,2] and Shan Shi[1,3] — [1]Research Group of Integrated Metallic Nanomaterials Systems, Hamburg University of Technology, 21073 Hamburg, Germany — [2]Institute of Materials Physics and Technology, Hamburg University of Technology, 21073 Hamburg, Germany — [3]Institute of Hydrogen Technology, Helmholtz-Zentrum Hereon, 21502 Geesthacht, Germany

As functionalized materials gain importance and component miniaturisation advances, there is an increasing demand for optimized structured materials. This talk presents a novel and straightforward alloying-dealloying approach to fabricate metals such as Ni and Cu with two- and three-level hierarchical network structures. Due to the significant difference in vapour pressures between the target metals, vapor phase alloying (VPA) of a metal foam with Zn resulted in Zn-based intermetallic alloy foams. This is then followed by vapor phase dealloying (VPD) which removes Zn and creates a finer porosity, resulting in a second level. A subsequent VPA-VPD cycle produces a third hierarchical level. Compression tests on these hierarchical foams with varying solid fractions were performed to determine Young's modulus and strength. The experimental results align well with the predictions of our new scaling law.

15 min. break

MM 3.5 Mon 11:30 SCH/A215

Formation and properties of crystalline and amorphous high-entropy ZrTiTaMoWNi thin films using magnetron sputtering of a segmented target — •Anna Kornyushchenko[1,2], Vyacheslav Perekrestov[2], Marilena Tomut[1,3], Harald Rösner[1], Martin Peterlechner[4], and Gerhard Wilde[1,5] — [1]Institute of Materials Physics, University of Muenster, Muenster, Germany — [2]Laboratory of Vacuum Nanotechnologies, Sumy State University, Sumy, Ukraine — [3]GSI Helmholtz Center for Heavy Ion Research, 64291 Darmstadt, Germany — [4]Karlsruhe Institute of Technology, Laboratory for Electron Microscopy, 76131 Karlsruhe, Germany — [5]Herbert Gleiter International Institute, Liaoning Academy of Materials, Shenyang, China

Using direct current magnetron sputtering of a segmented target under conditions of thermodynamical equilibrium, single-phase bcc or amorphous ZrTiTaMoWNi high entropy alloy layers have been formed. The crystalline layers have been obtained in the form of nano-patterns, with crystal growth occurring preferentially on the basis of (310) crystallographic plane, which aligns parallel to the substrate surface. The amorphous layers have smooth surface, featureless morphology and demonstrate structural stability. TEM studies have shown that their crystallization into a single bcc phase occurs at the annealing temperature of 800 C. The microhardness of the amorph and the crystalline films has measured to be 10 GPa and 4.6 GPa, correspondingly. Resistance to impact of swift heavy Au ions irradiation with energies 4.8 MeV/u have been compared for amorph and crystalline layers.

MM 3.6 Mon 11:45 SCH/A215

Microstructural and Chemical Analysis on MoSiTi samples with PDC coating for High Temperature Application — •Ingrit Nurak[1], Daniela Camacho[2], Lukas Korell[3], Giorgia Guardi[1], Heike Störmer[1], Svetlana Korneychuk[1], Yolita M. Eggeler[1], Astrid Pundt[1], and Samuel A. Kredel[2] — [1]Karlsruher Institut für Technologie, Karlsruhe, Germany — [2]Technische Universität Darmstadt, Darmstadt, Germany — [3]Dechema Forschungszentrum, Frankfurt, Germany

MoSiTi material is of high interest for high temperature applications, such as Mo-20Si-52.8Ti [Schliephake et. al., 2019]. In this presentation, we investigate the combination of this material with a Cr-bond coat and a Si(Hf, Ta)BCN(O)-polymer derived ceramic (PDC) upper layer. The structural and chemical evolution of the layered material, depending on the specific synthetic routes used and additional thermal treatments will be addressed by using different scanning and transmission electron microscopy (SEM, TEM) techniques. TEM will be applied to the (i) polymer-derived ceramic nanocomposites coating, to the development of (ii) ultra-high temperature silicides and to the (iii) Cr bond coat layer. Heat treatments will be addressed at 1200°C and

1400°C both in air and in argon atmosphere. The experimental outcomes demonstrate that the Materialsystem exhibits the capacity to withstand temperatures of 1200°C for an hour without delamination. Notwithstanding the application of heat treatment at 1400°C, there is no oxygen penetration into the MoSiTi substrate occurred. Moreover, the PDC coating was found to remain partially amorphous.

MM 3.7 Mon 12:00 SCH/A215

Understanding Alloying Effects on Grain Boundary Adhesion in Nickel Alloys by Atomistic Simulation — •Aljoscha F. Baumann[1], Reyhaneh Ghassemizadeh[1], and Daniel F. Urban[1,2] — [1]Fraunhofer IWM, Freiburg, Germany — [2]Freiburger Materialforschungszentrum, Freiburg, Germany

When increasing the in-service performance of engineering metallic materials, interfaces such as phase or grain boundaries (GB) may act as the weakest links. For the nickel-base superalloy Alloy 718 intergranular cracking can be a relevant damage mechanism as a result of high-temperature fatigue in an oxygen-rich environment. The reliable prediction of adhesion and mechanical stability at grain boundary interfaces from atomistic calculations remains a challenge due to the high-dimensional parameter space of chemical compositions and GB structures. Recently developed machine learning interatomic potentials (MLIPs) such as GRACE offer a promising solution to explore this parameter space by combining high accuracy with computational efficiency. Here we use a MLIP to perform cleavage simulations on grain boundaries in fcc Ni with Cr and Fe as alloying elements at varying concentrations and statistical distributions. This approach provides a pathway for atomistic simulations towards a more comprehensive modelling of alloys and their interface mechanical properties, thereby providing insights into intergranular failure mechanisms. Our results can be used to parametrize traction separation laws used in finite element modelling, allowing for microstructure-sensitive modelling of fatigue crack formation and growth.

MM 3.8 Mon 12:15 SCH/A215

Phase stability and surface segregation in multinary noble-metal alloys: an atomistic study with universal models — •Quentin Bizot, Matous Mrovec, and Ralf Drautz — Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-University Bochum, 44780 Bochum, Germany

Multinary alloys are complex solid solutions composed of several elements. They rarely behave like ideal solid solutions due to differences in phase stability, atomic size, and crystalline preferences. In bulk, short-range order can therefore be significant, leading to the formation of specific phases or distortions across the lattice. In addition to the effects in the volume, surface segregation affects the order and composition of the few first layers at the surface. A detailed understanding of these effects at the atomic scale is essential to predict and control the distribution and ordering of surface atoms, as well as their influence on material properties.

In this work, we investigate complex solid solutions based on noble metals with atomistic simulations demonstrating the formation of stable phases in the bulk as well as the segregation of specific elements at the surface. For this purpose, we used tailored GRACE model capable of describing interactions for 25 transition metals as well as universal GRACE models trained on diverse datasets.

MM 3.9 Mon 12:30 SCH/A215

First-principles study of aluminum alloy - polymer interfaces: From surface structures to adsorbate interactions — •Zhengqing Wei[1], Inna Plyushchay[2], Nebahat Bulut[1], Florian Lehmann[4], Philip Grimm[5,6], Maik Gude[4], Julia Hufenbach[5,6], and Sibylle Gemming[1,3] — [1]Inst. Physics, TU Chemnitz, Germany — [2]Natl. Taras Shevchenko University of Kyiv, Ukraine — [3]MAIN Center, TU Chemnitz, Germany — [4]ILK, TU Dresden, Germany — [5]IFW Dresden, Germany — [6]Inst. Materials Science, TU-BA Freiberg, Germany

Aluminum alloy surfaces face strict demands regarding extreme environmental conditions. The joining of aluminum alloy materials with engineering plastics enhances the overall resilience of composite. This study employs density functional theory (DFT) to model aluminum alloy surfaces while including electronic structure considerations. The surface stability was investigated as functions of alloying composition particularly on surfaces doped with Mg, Zr, and Si. The study includes the alloy's diffusion tendency, which shows that differential electron density variations occur simply at the outermost surface layer in contact with vacuum. Surface vacancy and migration barriers, and when the surface is bonded to the polymers, the interactions between atomic species of polymer side chains and aluminum alloy surfaces as well as surface vacancy sites were also analyzed. The modeled adsorbates on aluminum alloy surfaces provides modified local potential parameters for classical modeling of large-scale aluminum alloy–polymer surface and interfacial regions.