MM 42: Interface Controlled Properties and Nanomaterials: Nanoporous Materials and Nanolaminates

Time: Thursday 15:45–18:30 Location: SCH A 215

MM 42.1 Thu 15:45 SCH A 215

Nanoporous high entropy alloys – functional nanoscale networks — •Lukas Lührs[1], Friederike Ihle[1], and Jörg Weissmüller[1,2] — [1]Institute of Materials Physics and Technology, Hamburg University of Technology — [2]Institute of Materials Mechanics, Hybrid Materials Systems, Helmholtz-Zentrum hereon

Both, high entropy alloys as well as nanoporous metals have been the subject of considerable interest in recent years. The former topic explores alloys that are composed of multiple mayor alloying elements yielding countless opportunities for tailor-made material properties, such as outstanding mechanical performance. The latter investigates self-assembled network structures entirely composed of nanoscale elements. Owing to their large surface area to volume ratio, interfaces of nanoporous metals can be manipulated to obtain functional materials that can be used, e.g. as actuators, sensor or structural material with tunable mechanical properties.

In this work we combine both research topics to make monolithic bodies of a nanoporous high entropy alloy (np-HEA) by dealloying, a selective corrosion method, in aqueous media. Structural investigation finds a uniform, bicontinous network with feature sizes in the range of a few tens of nanometer. Moreover, samples of np-HEA exhibit a single phase microstructure with homogenous elemental distribution. Compression tests on macroscopic samples reveal considerable mechanical strength. In electrolyte, functionality is introduced by electrochemical modulation of the electrode potential which enables the generation of significant actuation strains.

MM 42.2 Thu 16:00 SCH A 215

Microstructure and mechanical behavior of hierarchical nanoporous gold-polypyrrole electrochemical actuators — •Olga Matts and Nadiia Mameka — Helmholtz-Zentrum Hereon, Geesthacht, Germany

Dealloyed nanoporous (np) metals have emerged as promising (electro-)chemical actuators that can compete with conventional actuator materials in terms of large actuation stroke, high strain energy density and low operating voltage [1]. Combining np metals with a conducting polymer polypyrrole (PPy) has been found as an effective way to enhance the actuation strain, mechanical strength and stiffness of np metals [2, 3]. Due to the synergistic effect of the two individual components at the nanoscale, such hybrid structures demonstrate enlarged actuation and tunable elastic modulus amplitudes as well as afford fast response times as compared to PPy alone [1].

In this work, we investigate an effect of structural hierarchy on actuation and elastic properties of *hierarchical* (hc) np-Au/PPy hybrids. We study the behavior in aqueous electrolyte under potential control, exploiting the ability of PPy to change its volume under reversible redox reactions. We reveal pronounced variations in the macroscopic length and Young*s modulus in response to the voltage-induced volume changes of PPy. We correlate this behavior with PPy fractions in pores and discuss the underlying mechanisms of the observations.

[1] Wittstock et al. (ed.), RCS (2012). [2] Roschning et al., Adv. Mater. Interfaces (2020). [3] Li et al., Acta Mater., 212 (2021).

MM 42.3 Thu 16:15 SCH A 215

Electrosorption-Induced Actuation in Nanoporous Silicon — •Manuel Brinker and Patrick Huber — Institut für Material- und Röntgenphysik, Technische Universität Hamburg, Denickestraße 15, 21073 Hamburg, Deutschland

Porous silicon provides a scaffold structure to study the confinement related effects of soft matter. We investigate the electro-sorption of electrolyte anions and the electrochemical behaviour of nanoporous silicon in acidic electrolytes. The silicon-electrolyte interface acts as a capacitor which allows the accumulation of electrolyte anions in a chemical double layer by an applied voltage, whose characteristics can be measured by cyclic voltammetry. The surface stresses that are caused to the monolithic porous silicon membrane by such an accumulation lead to a macroscopic strain which can be determined in-situ with a laser beam-bending setup. Comparing nanoporous silicon with a planar silicon surface yields insights on the observed electrocapillarity – in particular with respect to the importance of oxide formation and wall roughness on the single-nanopore scale.[1]

[1] Brinker, M., & Huber, P. (2021). Wafer-Scale Electroactive Nanoporous Silicon: Large and Fully Reversible Electrochemo-Mechanical Actuation in Aqueous Electrolytes. Advanced Materials, 2105923.

MM 42.4 Thu 16:30 SCH A 215

Structural analysis of hierarchical nanoporous gold — •Lukas Riedel[1], Jürgen Markmann[1,2], Jörg Weissmüller[2,1], and Shan Shi[3,1] — [1]Institute of Materials Mechanics, Helmholtz-Zentrum Hereon, Geesthacht, Germany — [2]Institute of Materials Physics and Technology, Hamburg University of Technology, Hamburg, Germany — [3]Research Group of Integrated Metallic Nanomaterials Systems, Hamburg University of Technology, Hamburg, Germany

Hierarchical nanoporous metals offer the possibility to produce mechanically stable materials with a reduced solid fraction [1], which therefore qualify for lightweight application. Here, hierarchical nanoporous gold is produced from Ag90Au10, following a three-step procedure which consists of first dealloying, coarsening and second dealloying. The ligament size on the upper and the lower hierarchy level can be tuned independently. In addition to scanning electron microscopy (SEM), small- and ultra-small-angle X-ray scattering (SAXS/USAXS) are applied for structural analysis and show consistent results. Descriptive parameters including length scale, specific surface area and pore volume fraction are obtained. From a comparison of the length scale parameters, ligament diameter and mean ligament distance, a conversion factor is yielded. Ultra-small-angle X-ray scattering was found to be suitable for the analysis of structures with a ligament size range of several hundreds of nanometers.

[1] S. Shi, Y. Li, B.-N. Ngo-Dinh, J. Markmann and J. Weissmüller, Scaling behavior of stiffness and strength of hierarchical network nanomaterials, Science 371 (6533), 2021.

MM 42.5 Thu 16:45 SCH A 215

Self-detachment of nanoporous thin films — •Gideon Henkelmann[1], Diana Waldow[1], Maowen Liu[1,2], Lukas Lührs[1], Yong Li[1,2], and Jörg Weissmüller[1,2] — [1]Institute of Materials Physics and Technology, Hamburg University of Technology, Hamburg, Germany — [2]Institute of Materials Research, Materials Mechanics, Helmholtz-Zentrum Geesthacht, Geesthacht, Germany

Experiment shows thin films of dealloyed nanoporous gold (NPG) spontaneously detaching from massive gold base layers. NPG can also densify near its external surface. This is naturally reproduced by kinetic Monte Carlo (KMC) simulations of dealloying and coarsening and so appears generic for nanoscale network materials evolving by surface diffusion. This talk focuses on how the KMC simulation manages to predict intricate physical phenomena with few and simple assumptions to the kinetics. This contrasts with contemporary popular efforts to fit a multitude of independent energy barriers to quantum mechanical calculations. Simplified kinetics significantly speed up computation, provide clearer understanding of the underlying processes, while still reproducing relevant phenomena. The KMC simulation model is further motivated by thermodynamic principles.

15 min. break

MM 42.6 Thu 17:15 SCH A 215

Wetting and Drying Dynamics in Hierarchically Porous Silicon: An In-Situ X-Ray Microscopy Study — •Stella Gries[1,2,3], Laura Gallardo Domínguez[1,2,3], Mark Busch[1,2,3], Mariia Liseanskaia[1,2,3], Juan Sánchez Calzado[1,2,3], Mathis Boderius[1,2,3], Silja Flenner[4], Imke Greving[4], and Patrick Huber[1,2,3] — [1]Institute for Materials and X-Ray Physics, Hamburg University of Technology, Hamburg, Germany — [2]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — [3]Center for Hybrid Nanostructures CHyN, University of Hamburg, Hamburg, Germany — [4]Institute of Materials Physics, Helmholtz Zentrum Hereon, Geesthacht, Germany

Hierarchical porosities consist of small, often nano-scaled pores as well as large, macroscopic pores to simultaneously achieve large inner surfaces in combination with optimized mass transport. The investigation of capillary dynamics within optically opaque hierarchically porous

membranes necessitates sophisticated microscopy techniques. First hints to unveil the dynamics are obtained from lab-scale experiments, e.g. mass-uptake as a function of time or the mechanical response depending upon wetting and drying in dilatometry. However, these techniques do not spatially resolve on the rising liquid front, which is achieved with transmission X-ray microscopy (TXM). The samples are scanned in radiography (2D) and tomography (3D) to resolve both the static structure and the capillary dynamics. These findings can help to tailor hierarchical porous materials for their designated application and to tune the dynamics depending on the needs.

MM 42.7 Thu 17:30 SCH A 215

Scaling between elasticity and topological genus of nanoporous metals — •Seoyun Sohn[1,2], Claudia Richert[1], Shan Shi[3,1], Jürgen Markmann[1,2], Norbert Huber[1,2], and Jörg Weissmüller[2,1] — [1]Institute of Materials Mechanics, Helmholtz-Zentrum Hereon, Geesthacht, Germany — [2]Institute of Materials Physics and Technology, Hamburg University of Technology, Hamburg, Germany — [3]Research Group of Integrated Metallic Nanomaterials Systems, Hamburg University of Technology, Hamburg, Germany

Nanoporous gold (NPG) made by dealloying has emerged as a model material for random networks and specifically for studies of their mechanics. The mechanical behavior of such open-cell foam structures has been expressed by classical Gibson-Ashby relations. They highlight the solid volume fraction as the most obvious descriptor of strength and stiffness. Yet, recent research acknowledges that Young's modulus, Y, of NPG may significantly depend on additional microstructural descriptors, specifically on the scaled topological genus, g, as a measure of the network's connectivity. It represents the number of connections within a representative volume element of the microstructure. Here, we explore the nature of the dependency of Y on g, and we condense the observations into a scaling law that explicitly involves the scaled genus. Our study inspects and assesses the implications of the existing database, from experiment and simulation, and it adds simulation data for random networks with various scaled genera. The results suggest a common scaling that is broadly comparable to experimental observations.

MM 42.8 Thu 17:45 SCH A 215

An Improved Kernel-Based NMR Cryoporometry Characterization of Mesoporous Solids — •Henry R. N. B. Enninful and Rustem Valiullin — Faculty of Physics and Earth Sciences, Felix Bloch Institute for Solid State Physics, Leipzig University, Linnéstraße 5, 04103, Leipzig, Germany.

NMR cryoporometry is a pore space characterization technique for industrial and natural materials such as catalysts, gas storage materials, cartilage, bones, rocks and many more. While gaining wide use, the fundamental phenomena underlying solid-liquid phase transitions in geometrically disordered porous materials is still not fully understood. This may lead to inaccurate pore size distributions from the NMR cryoporometry technique.

In this work, we have developed a new approach to NMR cryoporometry. Herein, it takes account of cooperativity effects in pores, the existence of a variable non-frozen layer (NFL) thickness between the frozen core and pore wall and the effect of curvature on thermal fluctuations in pores which hitherto are missing in the current approach. In the first place, we compile a family of transition curves characterizing the phase state in pores with different pore sizes, so called kernels. Thereafter, we apply a general framework for predicting phase equilibria in collection of pores. We demonstrate the new approach by first applying it to ordered porous materials such as MCM-41 and SBA-15. Further more, the technique is used to characterize a highly disordered random porous material where we reproduce all states seen in the material. A more accurate pore size distribution (PSD) is, thus, obtained.

MM 42.9 Thu 18:00 SCH A 215

Interface-related defect annihilation in high entropy amorphous/crystalline nanolaminates under ion irradiation — •qi xu[1], daniel sopu[1], xudong yuan[1], and jürgen eckert[1,2] — [1]Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Jahnstraße 12, Leoben A-8700, Austria — [2]Department of Materials Science, Chair of Materials Physics, Montanuniversität Leoben, Jahnstraße 12, Leoben A-8700, Austria

The main challenge of designing nuclear materials that possess a high irradiation resistance is accumulation of point defects-induced structural damage. The interfaces and grain boundaries play a critical role on the defect generation and annihilation in nanostructured materials. In this work, the irradiation-induced microstructure evolution as well as defect production and recovery in metallic glass (MG) / high entropy alloy (HEA) nanolaminates were investigated by molecular dynamics (MD) simulations. The displacement cascades were simulated for the energies of primary knock-on atoms (PKA) at 5, 10 keV and 15 keV. It was found that, there are more displaced atoms in the thermal spike phase for MG/HEA laminate compared with free-standing MG and HEA. In addition, the interface acts as defect sink and accelerates the recombination and annihilation of interstitial in HEA plate, which leads to more residual vacancies in crystalline plate. Moreover, the residual vacancies diffusion induces the generation of dislocation loops in the HEA plate. Furthermore, the interface acts as a transfer medium that accelerates the crystallization of MG plate during irradiation.

MM 42.10 Thu 18:15 SCH A 215

Anode engineering via ultrathin alumina membrane for next-generation stable sodium metal batteries — •Jiajia Qiu, Changfan Xu, Huaping Zhao, and Yong Lei — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Sodium metal batteries are recognized as one of the most promising candidates for next-generation batteries, owing to their high theoretical specific capacity and energy density. However, a major bottleneck is the mossy or dendritic growth of Na in the repetitive stripping/plating process with an unstable solid electrolyte interphase (SEI), which limits the Coulombic efficiency and even leads to short circuit risks. In this work, ultrathin alumina membrane (UTAM) is first validated as a functional layer to effectively protect the Na anode for Na-metal batteries. By protecting Na metal with UTAM, the mossy or dendritic growth of Na has been suppressed, resulting in uniform electrodeposition. This highly ordered alumina oxide nanostructure improved electrochemical performance significantly and has the potential to be applied to other metal anodes. The novel design of UTAM protected metal Na anode may bring in new opportunities for next-generation high performance Na metal batteries.