MM 22: Mechanical Properties and Alloy Design: Porous and Nanostructured Materials

Time: Tuesday 14:15–15:45 Location: SCH A 118

MM 22.1 Tue 14:15 SCH A 118

tailoring mechanical properties of lightweight 1D Nanostructures — Samuel Baltazar[1,2], Javier Rojas[1,2], •Felipe Valencia[2,3], Sebastian Allende[1,2], Rafael Gonzalez[2,4], Eduardo Bringa[5], and Pierre Cocco-Magnard[2] — [1]Physics Department, Universidad de Santiago de Chile, Chile — [2]Center for the development of Nanoscience and Nanotechnology, Universidad de Santiago de Chile, Chile — [3]Engineering Faculty, Universidad Catolica del Maule, Chile — [4]Centro de Nanotecnología Aplicada, Universidad Mayor, Chile — [5]CONICET & Facultad de Ingeniería, Universidad de Mendoza, Argentina

1D Nanostructures such as nanowires (NW) and nanotubes (NT) have gained a lot of attention due to their mechanical and electronic properties. The deformation of NT and NW has been previously studied, finding different fracture mechanisms. Tension and compression deformations show elastic regimes until a sudden stress drop due to the fast generation of dislocations. Synthesis of polycrystalline NW allows the reinforcement of the material's response. We report the mechanical properties are studied for mono and bimetallic systems by means of molecular dynamics simulations. Interatomic potentials were used to model Ni, Fe, and bimetallic NTs and NWs with dimensions similar to the experimental setup. Ni NT shows an asymmetry in the stress response under tension and compression, mediated by twins and stacking-faults dislocations, with no significant degradation of mechanical properties up to 60% mass reduction than NW, opening the generation of new lightweight and resistant materials.

MM 22.2 Tue 14:30 SCH A 118

Comparing structural response of filled and porous 3D Titanium network structures by application of nanotomography and graph theory — •Stefan A. Berger[1], Markus Ziehmer[1], and Jürgen Markmann[1,2] — [1]Helmholtz Zentrum Hereon — [2]Technische Unoversität Hamburg

Recently, refinements of the classical Gibson-Ashby relation have been invoked to extend its applicability to the description of the mechanical properties of bicontinuous, nanoporous metals. In particular, the network connectivity has been identified as a crucial parameter that needs to be taken under consideration. So far, global parameters like connectivity or genus (density) have been employed, However, these do not uniquely identify the underlying microstructure. This can be achieved by making use of graph theoretical aspects, as demonstrated in Ziehmer et al[1]. In this work, we have investigated the changes in the network structures of porous Titanium and Ti-Mg composites, fabricated by Liquid Metal Dealloying, during compression tests in a x-ray nanotomograph. The reconstructed sample volumes were simplified by skeletonization, the resulting skeletons transferred into a weighted graph representation, and further decomposed into the constituent rings that built the network. This approach allowed for a statistical description of the behavior of the ring elements under load. One major result is that the essential part of deformation is carried by larger rings. [1] M. Ziehmer, E. T. Lilleodden, Acta Materialia 199 (2020).

MM 22.3 Tue 14:45 SCH A 118

Hierarchical-structural effects on mechanical behavior of nanoporous gold in electrochemical environment — •Hansol Jeon[1], Shan Shi[3,1], and Jürgen Markmann[1,2] — [1]Institute of Materials Mechanics, Helmholtz-Zentrum Hereon, 21502 Geesthacht, Germany — [2]Institute of Materials Physics and Technology, Hamburg University of Technology, 21073 Hamburg, Germany — [3]Research Group of Integrated Metallic Nanomaterials Systems, Hamburg University of Technol-ogy, 21073 Hamburg, Germany

Recently, hierarchical nanoporous gold (HNPG) has been emerged with having multiple-level structures. HNPG is more active because of higher surface area than nanoporous gold (NPG) since Au ligaments are supposed to be converted into another porous structure with smaller ligaments and pores. Regarding mechanical behavior, especially with the same solid fraction for both, it has been not directly compared yet whether HNPG would have better me-chanical properties. Here, we investigated the mechanical properties of NPG and HNPG with the same solid fraction by conducting compressive tests at the micro-scale. The NPG and HNPG were prepared from the same precursor alloy Ag85Au15 by dealloying. The pillars were milled by a focused ion beam (FIB), and compressive tests were performed by a nanoindenter with a flat-punch tip. We discussed the difference of dislocation activities and connectivity for NPG and HNPG. Finally, by conducting additional compressive tests in an electrochemical environment, we explored the role of surface state on the mechanical behavior of NPG and HNPG by impos-ing electrode potential.

MM 22.4 Tue 15:00 SCH A 118

Mechanical properties and oxidation performance of nanostructured self-passivating WCrY material — •Jie Chen[1], Andrey Litnovsky[1], Jesus Gonzalez-Julian[1,2], Jan Willem Coenen[1], and Christian Linsmeier[1] — [1]Forschungszentrum Jülich GmbH, Institut für Energie- und Klimaforschung - Plasmaphysik, 52425 Jülich, Germany — [2]Institute of Mineral Engineering, RWTH Aachen University, 52074 Aachen, Germany

Self-passivating W-11.4wt%-0.6wt%Y alloy have been considered as a promising plasma-facing material in fusion power plants. In the present work, bulk material are fabricated via holding at 1300C for 2 minutes in field-assisted sintering. As a result, an average matrix's grain size of 98.9nm and 6.7% surface area of Cr-rich phase was obtained. Cr-rich phase is formed on the surface of particles during sintering and over 70 at% of Cr is detected by EDX. A hardness HV0.5 of 1287.6 is obtained as a result of small grains while a fraction of Cr-rich phase in the microstructure softens material to some extent. Three point bending tests at temperature up to 1000C are performed to measure fracture toughness and ductile brittle transition temperature. This is done combining with fractography study to investigate the effect of grain size as well as Cr-rich phase on the thermo-mechanical properties. Reduction in grain size down to the order of sub-micrometer range is proven to improve material's anti-oxidation performance in previous study. Oxidation test was performed at 1000C to investigate performance of the microstructure developed. Details of the work are presented in this contribution.

MM 22.5 Tue 15:15 SCH A 118

Study of the oxidation mechanism of Cr_2AlC MAX phase through nanoscale analysis of alumina scale formation — •Anicha Reuban[1,2], Jesus Gonzalez-Julian[1,2], Ivan Povstugar[1], Andrey Litnovsky[1], and Christian Linsmeier[1] — [1]Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — [2]Institute of Mineral Engineering, RWTH Aachen University, 52074 Aachen, Germany

In a Concentrated Solar Power (CSP) plant, the receiver must withstand temperatures >800 °C, be resistant to oxidation by air and/or corrosion by molten salts and maintain its properties over time. MAX phases, which are ternary carbides and nitrides with a unique combination of ceramic and metallic properties, are candidate materials for the receiver. In this work, the oxidation mechanism of the alumina-forming MAX phase Chromium Aluminium Carbide (Cr_2AlC) is studied. The samples are oxidized in a thermogravimetric analyzer (TGA) at 1000 °C and 1200 °C in humid air. The oxide scale is characterized using XRD, FIB-SEM, EDX and STEM. The alpha alumina layer formed consists of needle-like grains on top, with larger grains at the bottom, below which is a layer of chromium carbide. The elemental distribution across grain boundaries and interfaces of various regions of the oxide scale, carbide and bulk material are being analyzed with Atom Probe Tomography (APT), since these are possible pathways for the diffusion of aluminium and oxygen ions to form the oxide layer. The effect of dissolved chromium in the oxide scale and the segregation of impurities such as iron and silicon to interfaces is examined.

MM 22.6 Tue 15:30 SCH A 118

Phase stability of iron and its alloys from first principles dynamical simulations and thermodynamic integration — •Davide Gambino and Björn Alling — Linköping University, Linköping, Sweden

In recent years, thermodynamic integration (TI) based on first principles simulations has been shown to accurately reproduce phase diagrams and is now able to guide the design of functional materials and alloys. For what concerns iron and steels, this methodology is complicated by the presence of magnetic degrees of freedom (DOF) and

their interplay with electronic and vibrational DOFs. Here I will show how the phase stability of iron and its alloys can be obtained from first principles employing atomistic spin dynamics - ab initio molecular dynamics (ASD-AIMD) simulations and TI accounting for all DOFs [1].

The free energy difference between bcc and fcc Fe was calculated close to the melting point in the magnetically disordered state, carrying out TI over stress-strain variables along the Bain path, and then propagating it to low temperatures with TI over temperature employing the ASD-AIMD energies. The method captures the $\alpha \rightarrow \gamma \rightarrow \delta$ transitions, with the latter transition temperature reproduced within 50 K from experiments, and the calculated Gibbs free energy difference being within 5 meV/atom from the CALPHAD estimate over the whole temperature range. The method is then applied to $Fe_{1-x}Mn_x$ alloys for concentrations of $x = 0.05, 0.10$ and for temperatures T $\geq$ 1400 K and results are compared with the experimental phase diagram.

[1] Gambino et al., arXiv:2210.14718 [cond-mat.mtrl-sci]