MM 7: Materials for the Storage and Conversion of Energy

Hydrogen related Surface Effects

Time: Monday 15:45–17:00 Location: H22

MM 7.1 Mon 15:45 H22

Effect of stress induced nanohydride formation on dislocation nucleation and pinning in FeCr alloys — •Ali Tehranchi[1], Jing Rao[2], Lekshmi Sreekala[2], Jazmin Duarte[2], Gerhard Dehm[2], Jörg Neugebauer[2], and Tilmann Hickel[1] — [1]BAM Federal Institute for Materials Research and Testing, ali.tehranchi@bam.de, Germany — [2]Max Planck Institute for Sustainable Materials

The detrimental effects of hydrogen (H) on the mechanical properties of metals are universally acknowledged. However, the mechanisms behind these effects remain unclear. In situ nano-indentation experiments are powerful tools for probing the effect of H on the hardness and plasticity of metals. In this work, ab initio calculations and stress dependent phase diagrams in chemical potential space are used to clarify the effect of nanohydrides on the pop-in load of in situ nanoindentation of FeCr alloys. It is shown that the anisotropic stress field of the indenter with a radius of 170 nm facilitates the formation of nanohydrides with significantly lower elastic constants and containing high eigen shear strain. The shear stress associated with these inhomogeneous inclusions is responsible for the experimentally observed reduction in critical shear for dislocation nucleation and the pop-in loads in these indentation experiments. On the other hand, for indenters with a larger radius, the pop-in load is increased due to the pinning of the pre-existing dislocations by the same nanohydrides which are not capable to form underneath the indenter because of the lower magnitude of its induced stress field. The formation of nanohydrides under loading has significant implications for H-embrittlement and H-storage.

MM 7.2 Mon 16:00 H22

Spherical nanoindentation during electro chemical nanoindentation — •Verena Maier-Kiener, Stefan Zeiler, and Anna Jelinek — Montanuniversität Leoben, Leoben, Österreich

Nanoindentation enables efficient characterization of material flow behavior, offering reliable results with minimal effort. While established for hardness and Young*s modulus, its potential for deriving localized flow curves remains underexplored due to challenges in correlating spherical indentation and uniaxial data. A calibration procedure addressing tip imperfections allows strain-rate-controlled experiments and accurate constraint factor evaluation. Using an innovative in-situ electrochemical charging method, side-charging cell, it is shown that electrochemical charging increases hardness and flow stress while reducing the constraint factor, providing valuable insights into deformation behavior.

MM 7.3 Mon 16:15 H22

Hydrogen-based reduction of iron oxide surfaces studied by ab-initio calculations — •Ahmed Abdelkawy, Mira Todorova, and Jörg Neugebauer — Max Planck Institute for Sustainable Materials, Max-Planck-Str.1, 40470 Düsseldorf

The production of pure iron from the iron oxide ores is a very energy-intensive process. Additionally, the dependency on carbon and carbon monoxide as reducing agents results in CO2 as an intrinsic byproduct of the reaction. Consequently, the steel industry is responsible for more than 6% of the global CO2 emissions. Using Hydrogen (H) as a reducing agent would result in water being released instead. Two important aspects in this context are (i) the relative thermodynamics stability of iron oxide facets under different conditions, as this will determine their abundance and (ii) the interaction of H with the oxide surfaces, as these will catalyse the reaction. This work, which is an initial step toward understanding the complex process of the H-based reduction of iron oxides, focuses on Hematite (Fe2O3). Using density functional theory (DFT) calculations we explore the surface stability of different facets under relevant thermodynamic conditions. Additionally, we use transition state theory to describe different H reaction paths and their activation barriers. Keeping in mind the impact the description of the electronic structure may have on the considered quantities, the calculations were performed using both GGA-PBE and GGA-PBE+U. While our results indicate that both methods result in the same preferential reaction path, the electron localization from the (+U) term results in a significant reduction in the activation barrier.

MM 7.4 Mon 16:30 H22

Atomic Cluster Expansion potential for hydrogen-based direct reduction of iron oxides — •Baptiste Bienvenu[1], Mira Todorova[1], Jörg Neugebauer[1], Matous Mrovec[2], Yury Lysogorskiy[2], Ralf Drautz[2], and Dierk Raabe[1] — [1]Max Planck Insitute for Sustainable Materials, Max-Planck-Straße 1, 40237 Düsseldorf, Germany — [2]Interdisciplinary Centre for Advanced Materials Simulation, Ruhr Universität Bochum, 44780 Bochum, Germany

Modeling atomistic mechanisms underlying hydrogen-based direct reduction of iron oxides poses many great challenges, due to the combined structural and electronic complexities of the bulk materials, but also due to the involved chemical reactions. To allow for atomic scale modeling of such processes over the relevant length and time scales, an accurate yet affordable interatomic potential is needed.

Following our previous work, which focused on the development of an Atomic Cluster Expansion (ACE) potential for iron and its oxides, we present in this work the extension of the model to include hydrogen. Based on an extensive DFT-computed database encompassing both iron and its oxides in a wide range of atomic environments involving hydrogen, we fit the extended ACE potential, also including magnetic degrees of freedom. To demonstrate the capabilities of the ACE potential, we focus on its ability to capture some basic mechanisms involved in the hydrogen-based reduction of iron oxides in various environments, including iron oxides-hydrogen (reactions at surfaces, bulk defects), iron oxides-water (surface oxidation), iron-water (surface reactions) and iron-hydrogen (trapping, interactions with defects).

MM 7.5 Mon 16:45 H22

Investigating phase diagram and phonons in superconducting Lanthanum Hydride through an accurate treatment of anharmonicity and nuclear quantum effects — •Abhishek Raghav[1], Kousuke Nakano[2], and Michele Casula[1] — [1]Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie (IMPMC), Sorbonne Université, Paris, France — [2]Center for Basic Research on Materials, National Institute for Materials Science (NIMS), Tsukuba, Japan

Hydrogen rich materials with clathrate structures are an important class of superconducting materials. Lanthanum hydride (LaH_{10}) is one such material, demonstrated to show superconductivity at 250 K and 170 GPa. Phase diagram, phonon spectrum and electron-phonon coupling are important ingredients used to predict superconductivity, being of BCS type. However, computing these accurately for hydrogen clathrate materials requires including anharmonicity due to nuclear quantum effects (NQE). In this work, we use the path integral molecular dynamics (PIMD) and the stochastic self-consistent harmonic approximation (SSCHA) to study NQE and finite temperature on the phase stability and phonons. In order to speed up PIMD and SSCHA calculations, we employ a machine learning potential generated using MACE. This allows us to explore the theoretical LaH_{10} phase diagram over an unprecedentedly wide range of temperatures and pressures. We found that, when quantum effects are included, hydrogen cage symmetrization occurs at lower pressures than in classical simulations, placing the maximum of T_c measured in experiments close to the quantum transition region.