MM 12: Computational Materials Modelling - Mechanical Properties

Time: Monday 15:45–18:15 Location: H24

MM 12.1 Mon 15:45 H24

Self-consistent scale-bridging approach to compute the elasticity of multi-phase polycrystals — •Martin Friak[1], Hajjir Titrian[1,2], Ugur Aydin[1], Dierk Raabe[1], and Joerg Neugebauer[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — [2]Universität Duisburg-Essen, Germany

A necessary prerequisite for a successful theory-guided up-scale design of materials with application-driven elastic properties is the availability of reliable homogenization techniques. We report on a new software tool that enables us to probe and analyze scale-bridging structure-property relations in the elasticity of materials. The newly developed application computes integral elastic response of randomly textured polycrystals. The application employs a Python modular library that uses single-crystalline elastic constants as input parameters and calculates macroscopic elastic moduli (bulk, shear, and Young's) and Poisson ratio of both single-phase and multi-phase aggregates. Crystallites forming the aggregate can be of cubic, tetragonal, hexagonal, orthorhombic, or trigonal symmetry. For cubic polycrystals the method matches the Hershey homogenization scheme. In case of multi-phase polycrystalline composites, the shear moduli are computed as a function of volumetric fractions of phases present in aggregates. Elastic moduli calculated using the analytical self-consistent method are computed together with their bounds as determined by Reuss, Voigt and Hashin-Shtrikman homogenization schemes. The software library can be used as a toolkit for both forward and inverse materials-design strategies.

MM 12.2 Mon 16:00 H24

Mechanical properties of fully lamellar TiAl alloys obtained from a DFT study — •Mansour Kanani, Rebecca Janisch, and Alexander Hartmaier — ICAMS, Ruhr-University Bochum, 44801 Bochum

Mechanical properties of different interfaces and bulk structures in the fully lamellar TiAl two-phase system are investigated by an ab-initio DFT (Density Functional Theory) based study with full relaxation. Interfacial energies as well as planar fault energies for γ/γ, $\alpha 2/\gamma$ interfaces and bulk structures are calculated. The tensile strength and cohesive properties for different variants are obtained from implementation of atomic scale uni-axial mechanical test. The remarkable finding is that all interfaces as well as bulk phases have comparable normal strengths. Furthermore, shear properties of the single crystals as well as interfaces are investigated on the basis of generalized stacking-fault energy surface and then the shear strength is calculated along various directions. The results show that 60-rotated and 120-rotated γ/γ interfaces display an easy shearing configuration; especially the [-1-12]γ direction shows an invariant and low shear strength for all cases. Our results are discussed and interpreted on the basis of the atomistic configurations of the investigated systems.

MM 12.3 Mon 16:15 H24

Interaction of dislocations with carbon interstitials in α-iron — •Gholamali Nematollahi, Blazej Grabowski, Johann von Pezold, Chris Race, Jörg Neugebauer, and Dierk Raabe — Max-Planck Institut für Eisenforschung, D-40237 Düsseldorf, Germany

The interaction of carbon with dislocations gives rise to the formation of Cottrell atmospheres in α-Fe. This does not only directly affect the mechanical properties of the matrix, but may also result in an indirect effect due to a dislocation-driven rearrangement of the C distribution during severe plastic deformation. Recent experimental studies of severely deformed pearlitic wires reveal a considerable refinement of the cementite layers and a substantial accumulation of C in the ferrite. It was tentatively suggested that the accumulation of C in the ferritic layers proceeds via the co-migration of C atoms with mobile dislocations gliding from the ferrite/cementite interface into the ferrite phase. In the present study, we provide molecular statics calculations addressing the proposed mechanism in detail. In particular, nudged elastic band (NEB) calculations are used to determine the effective migration barrier for an interstitial C atom in the vicinity of an edge and screw dislocation in α-Fe, using a semi-empirical EAM potential. Carbon diffusion barriers of 0.2 eV are found in the core of the dislocation suggesting that carbon is more mobile than in bulk iron (barrier: 0.9 eV). The Portevin-le Chatelier effect that suggests the mobile solute atoms can diffuse with the moving dislocation at high temperature and moderate strain rate. These conditions are satisfied about C in the dislocation core already at room temperature.

MM 12.4 Mon 16:30 H24

Atomistic modelling of α-Fe and Fe-C by analytic bond-order potentials including magnetism — •Sebastian Schreiber, Thomas Hammerschmidt, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum

The mechanical properties of steels are to a large degree determined by plastic deformations on the microstructural level. Understanding the involved processes at such length-scales calls for atomistic simulations of the movement of line defects. This may help to explain, e.g., the influence of temperature and carbon content on dislocation glide in α-Fe and to make direct contact to recent atom-probe experiments. However, simulating the interaction of dislocations and other defects with atomic resolution requires computationally efficient methods that are able to treat million-atom simulation cells. To this end, we develop analytic Bond-Order potentials (BOP) that are footed on recently parametrised tight-binding (TB) models of Fe and Fe-C. The analytic BOP provide an approximate solution to the TB problem and include the treatment of magnetism within the Stoner model. Here, we demonstrate the transferability of taking the Fe and Fe-C TB parameters to the analytic BOP formalism and discuss first results of large scale BOP simulations that will lead us to the calculation of the Peierls stress for dislocation movement. Moreover, we will present benchmarks of the computational performance of the analytic BOP with respect to system size and parallelisation.

MM 12.5 Mon 16:45 H24

First-principles calculations of the key atomistic parameters related to hydrogen embrittlement in FeMn — •Aurab Chakrabarty, Johann von Pezold, Robert Spatschek, Tilmann Hickel, and Joerg Neugebauer — Max-Planck Institute for Iron Research, Duesseldorf, Germany

Hydrogen embrittlement in high-manganese steels has been in the centre of attention for automotive applications. It is difficult to perceive the role of hydrogen of these steels solely from experiments. However, key atomistic parameters such as H-H interaction, elastic constants, solution energies and stacking fault energies can be systematically determined from first-principles calculations. They can be used to create a fully ab-initio based continuum scale simulation and validate commonly assumed assumptions of H-segregation on stacking faults, cracktips and cleavages and eventually to understand phenomena such as HELP (hydrogen enhanced local plasticity).

In this work we apply density functional theory to investigate the role of hydrogen in FeMn. Starting with the crystal and magnetic structure for H-interstitials, we calculated the hydrogen solution energy in a hydride phase and H-H interactions in Fe and Mn in order to investigate the possibility of hydrogen congregation. The energetic preferences of the interstitial sites for a hydrogen atom in Fe-Mn alloy based on the number of Fe/Mn neighbours, have been determined. These parameters, including their chemical and elastic contributions were analyzed in order to understand the nature of the defect and implications for alloys those are less sensitive to H-embrittlement.

MM 12.6 Mon 17:00 H24

Shear instabilities in perfect bcc crystals during simulated tensile tests — •Miroslav Černý[1,2], Petr Šesták[1,2], Jaroslav Pokluda[2], and Mojmír Šob[1,3] — [1]Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Republic — [2]Faculty of Mechanical Engineering, Brno University of Technology, Brno, Czech Republic — [3]Faculty of Science, Masaryk University, Brno, Czech Republic

This work demonstrates a simple but efficient way how to determine the existence of shear instabilities in ideal bcc crystals under uniaxial loading. The theoretical tensile strengths are derived from calculated values of the theoretical shear strength and their dependence on the superimposed normal stress. The presented procedure enables us to avoid complicated and time-consuming analyses of elastic stability of crystals. Results of first-principles simulations of coupled shear and tensile deformations for two most frequent slip systems ($\{110\}\langle 111\rangle$

and {112}⟨111⟩) in six ideal cubic crystals are used to evaluate the uniaxial tensile strengths in three low-index crystallographic directions (⟨100⟩, ⟨110⟩, and ⟨111⟩) by assuming a shear instability in the weakest shear system. While instabilities occurring under ⟨100⟩ tension are mostly related to the shear in {112} plane, those occurring during loading in the other two directions are associated with {110} planes. The results are consistent with those predicted by available elastic analyses. The weakest tendency to fail by shear is predicted for uniaxial tension along ⟨100⟩. This is consistent with occurrence of {100} cleavage planes in bcc metals.

MM 12.7 Mon 17:15 H24

Modeling of pressure-induced phase transformation in Si using a two phases strategy — Sebastien Groh, •Michael Budnitsky, and Meinhard Kuna — TU Bergakademie Freiberg, Freiberg, Germany

We have carried out constant pressure molecular dynamics simulation with a Tersoff interatomic potential to study the pressure-induced phase transformation in Si using a two-phases model. The simulations successfully reproduced the diamond-cubic to β-Sn structural transformation under hydrostatic pressure. The pressure level at which the transformation occurred is in agreement with both experimental data and thermodynamics considerations. Moreover, the mechanism of phase transformation by inhomogeneous shear deformation was revealed by the calculations. Furthermore, as the β-Sn cannot transform back to diamond-cubic structure, it was observed in the simulation that the two-phases model transformed to a diamond- cubic and an amorphous Si for pressure lower than the transition pressure. Although such a transformation from β-Sn to amorphous Si was already observed by simulation of nanoindentation of Si using MD, it is the first that time this transformation is reported under hydrostatic loading conditions using molecular dynamics simulations.

MM 12.8 Mon 17:30 H24

Extended Modules Material Assembly — •Matthew S Dyer, Christopher Collins, Darren Hodgeman, Philip Chater, Antoine Demont, Simon Romani, Ruth Sayers, Michael F Thomas, John B Claridge, George R Darling, and Matthew J Rosseinsky — University of Liverpool, Liverpool, UK

Computational approaches have a growing influence on the search for new materials. However, potential functional materials with complex structures still pose the problem of an excessive number of permutations needing consideration and screening. Here we present the Extended Modules Material Assembly (EMMA) method to address this issue. EMMA constructs a set of structures based on layered building blocks, combined using predefined rules.

In the present study, we investigate layered perovskite oxides within the Y-Ba-Ca-Fe-Cu-O phase diagram. A new material was identified, synthesised, and its structure determined using a combination of the EMMA method and experimental diffraction methods. This complex structure has 6 elements in 20 distinct sites, and a longest lattice constant of 61 Å. We have shown experimentally that the new material is a functional cathode for solid oxide fuel cells.

Many functional materials, even those with complicated structures, can be described as a periodic combination of constituent layers. The EMMA method is particularly well suited to these materials, where brute force approaches cannot be used and chemical knowledge needs to be used to guide structural searches. It is a pragmatic, practical method aiding the discovery of new functional materials.

MM 12.9 Mon 17:45 H24

Massively parallel detection of contacts for packing problems using NVIDIA CUDA — •Jakob Nixdorf and Eckard Specht — Otto-von-Guericke-University Magdeburg, Department of Experimental Physics/Material Physics

High density packings of particles are often used as models of the structure of liquid, glassy and crystalline states of matter, granular media, heterogeneous materials and even biological systems.

In this work the packing of millions of unequal spheres is studied. The crucial and by far most time-consuming part of such computer simulations is the detection of contacts and overlaps between the spheres and the container. A massively parallel approach has been implemented using the CUDA toolkit for programming NVIDIA Tesla graphics cards. Problems and results of this implementation are discussed and compared with a serial implementation as well as the efforts of other groups.

MM 12.10 Mon 18:00 H24

Direction Dependent Field Evaporation of Pure Materials in Atom Probe Tomography — •Torben Boll and Talaat Al-Kassab — King Abdullah University of Science and Technology, Division of Physical Sciences and Engineering, Thuwal, 23955-6900, Saudi Arabia

In the field of atom probe tomography (APT) the process of field evaporation governs the progress of an analysis. The field evaporation field (FEF) is known to exhibit different strengths for different crystallographic directions for pure metals. However this is not considered in currently used APT-models. This paper will present a method to calculate small differences in the FEF for crystallographic directions from experimental APT data of Al, W and Si. Furthermore we will discuss how this can be used to adjust parameters for geometry based APT-simulations.

To obtain this information we developed an upgraded version of the AtomVicinity algorithm, which is mostly identical to what is also called *spatial distribution maps*.

The results were acquired with two different commercial atom probes, the Laser assisted Wide Angle Atom Probe (LA-WATAP) and the Local Electrode Atom Probe (LEAP 4000). Additionally, this approach allows a comparison of the spatial resolution of these two devices.