MM 22: Microstructure and Phase Transformations

Transformations at extreme conditions

Time: Tuesday 10:15–11:15 Location: TC 010

MM 22.1 Tue 10:15 TC 010

First-principles calculations of the linear elasticity of quartz and implications for pressure induced amorphization — •Christoph Otzen[1], Silvana Botti[1], and Falko Langenhorst[2] — [1]Institut für Festkörpertheorie und Optik, Jena, Germany — [2]Institut für Geowissenschaften, Jena, Germany

Quartz is a material that is prone to amorphization at high pressures. Numerous studies have been carried out since the discovery of amorphization in the late 1980s to explore mechanisms, structural evolution, and onset of amorphization as a function of static pressure. Quartz displays however a peculiar behavior under shock metamorphism, the process under which a material reacts to dynamic pressure waves with extreme conditions. In this case, quartz develops amorphous lamellae at the nanometer scale with sharp crystalline-amorphous boundaries and most strikingly, in particular crystallographic orientations.

Here, we investigate the directional dependence of some mechanical properties of quartz in the approximation of linear elasticity and compare our results with the orientations of amorphous lamellae to gain insight into their formation mechanism. We tackle the problem by calculating second-order elastic coefficients by means of density functional theory. Our first calculations of stress-strain relations for all directions indicate indeed structural changes over pressure that are consistent with anisotropic amorphization of quartz.

MM 22.2 Tue 10:30 TC 010

Stabilization of body-centred cubic iron under Earth's core conditions — •Sergei I. Simak — Linköping University (LiU), 58183 Linköping, Sweden

The Earth's solid core is mostly composed of iron. However, the stable phase of iron under inner-core conditions remains uncertain. The two leading candidates are hexagonal close-packed (hcp) and body-centred cubic (bcc) crystal structures, but the dynamic and thermodynamic stability of bcc iron under inner-core conditions has recently been challenged. We demonstrate the stability of the bcc phase of iron under conditions consistent with the centre of the core using ab initio molecular dynamics simulations. We find that the bcc phase is stabilized at high temperatures by a novel diffusion mechanism that arises due to the dynamical instability of the phase at lower temperatures[1].

[1] A. B. Belonoshko, T. Lukinov, J. Fu, J. Zhao, S. Davis, and S. I. Simak, "Stabilization of body-centred cubic iron under inner-core conditions", Nature Geoscience 10, 312 (2017).

MM 22.3 Tue 10:45 TC 010

Hall-Petch relations of Cu-Ni alloys and their dependence on severe deformation and annealing — •Friederike Emeis, Martin Peterlechner, and Gerhard Wilde — Institute of Materials Physics, Westfälische Wilhelms-Universität Münster, D-48149

The Hall-Petch relationship is widely discussed and used as a microstructural description of different materials. In this talk the existence of different Hall-Petch relationships for the same materials, processed in different ways to achieve a variation of their grain sizes and structures is shown and connected to grain boundary characteristics. Pure Cu and Ni as well as four different compositions of Cu-Ni alloys are processed by severe plastic deformation at room temperature up to different strain levels (unsaturated and saturated severely deformed) and subsequent annealed. It is shown, that the processing and thus the characteristics of grain boundaries have in general the same effect on different materials. Furthermore, the saturated severely deformed microstructure is well described by a polycrystalline Hall-Petch relationship. It is concluded that dynamic recovery and recrystallization change the microstructure in a way that the influence of the grain boundaries on the hardness is as dominant as in a relaxed microstructure.

MM 22.4 Tue 11:00 TC 010

High-pressure torsion induced phase transformations in Cu- and Ti-based alloys — •Askar Kilmametov[1], Yulia Ivanisenko[1], Boris Straumal[1,2], Andrey Mazilkin[1,2], Mario Kriegel[3], Olga Fabrichnaya[3], David Rafaja[3], and Horst Hahn[1] — [1]Karlsruhe Institute of Technology (KIT), Institute of Nanotechnology, Karlsruhe, Germany — [2]Institute of Solid State Physics, Russian Academy of Sciences, Chernogolovka, Russia — [3]TU Bergakademie Freiberg, Institute of Materials Science, Freiberg, Germany

Severe plastic deformation not only leads to grain refinement but also accelerates mass-transfer and drives phase transformations in Cu-based alloys. Dynamic equilibrium between decomposition of (supersaturated) solid solution and dissolution of precipitates during high pressure torsion (HPT) of diluted Cu-based alloys has been studied. The precipitation of second phase particles from a solid solution and their dissolution take place simultaneously and compete with each other. The formation of high-pressure ω-phase has been studied in Ti-based alloys. A defect-rich ω-phase forms after HPT and persists in the samples also after the pressure release. The amount of retained ω-phase after HPT depends on the alloying element concentration. Based on the XRD and TEM observations, the crystallography and mechanisms of α to ω and β to ω phases transformations (which can be diffusionless as well as controlled by mass transfer) are discussed.