MM 48: Invited talk Gunkelmann

Time: Thursday 9:30–10:00 Location: BAR 205

Invited Talk MM 48.1 Thu 9:30 BAR 205

Molecular dynamics simulations of pressure induced phase transformations in iron and iron-carbon: Interplay of defects and phase transition — •Nina Gunkelmann[1], Hoang-Thien Luu[1], Ramon J. Ravelo[2], Timothy C. Germann[3], Eduardo M. Bringa[4], and Herbert M. Urbassek[5] — [1]TU Clausthal, Germany — [2]University of Texas, El Paso, USA — [3]Los Alamos National Laboratory, USA — [4]University of Mendoza, Argentina — [5]TU Kaiserslautern, Germany

The study of iron under high-pressure conditions is essential not only for industrial activities but also for geological and astronomical applications. We consider iron and iron-carbon alloys showing a pressure induced phase transformation from the bcc to the hexagonal close-packed phase at around 13 GPa depending on the carbon content. We study compression waves in polycrystalline Fe and Fe-C using interatomic potentials that faithfully incorporate this phase transition at the desired equilibrium pressure. Our simulations show that the phase transformation is preceded by plastic activity, leading to the so-called 3-wave structure: An elastic compression wave is followed by a plastic wave, which then leads to a phase-transformation front. We investigate the interplay of defects in bcc with the transformation process. The role of twins, dislocations, and Cottrell atmospheres has a strong influence on the crystalline iron structure during the phase transformation. Our results show that the presence of Cottrell atmospheres surrounding an edge dislocation in bcc iron retards the development of the hcp phase.