

MM 7: Invited Talk: Merkert

Time: Monday 15:00–15:30

Location: SCH A 251

Invited Talk MM 7.1 Mon 15:00 SCH A 251
Molecular dynamics simulations of shock waves in alloys: Interplay of defects and phase transition — ●NINA MERKERT — TU Clausthal, Germany

The study of materials 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. These defects also influence the fracture (spallation) of the shocked iron samples.

Recently, we extended our results to high-entropy alloys (HEAs) that consist of equiatomic mixtures of five or more elements and are attracting increasing interest due to their promising material properties. We studied shock-induced spallation in HEAs and found exceptionally high spall strengths that are beneficial for high strain-rate applications.