

MM 20: HV Mrovec

Time: Wednesday 10:15–10:45

Location: IFW A

Invited Talk

MM 20.1 Wed 10:15 IFW A

Atomic-scale modeling of dislocations in iron — ●MATOUS MROVEC — Fraunhofer IWM, Freiburg, Germany — IZBS, Karlsruhe Institute of Technology, Karlsruhe, Germany

Mobilities of screw and edge (or mixed) dislocations in α -iron, like in other bcc metals, are markedly different at low temperatures. While the mobility of edge dislocations remains large and independent of temperature, the mobility of screw dislocations decreases strongly with decreasing temperature. The reason of this distinct behavior has been traced to a non-planar core structure of the $1/2\langle 111 \rangle$ screw dislocation. The non-planar core is primarily responsible for most peculiarities in mechanical behavior of α -iron and other bcc metals such as

the strong temperature dependence of the flow and yield stresses, the brittle-to-ductile transition, and the non-Schmid behavior.

We performed extensive atomistic simulations of dislocation properties in α -Fe using a recently constructed magnetic bond-order potential. This potential is based on the tight binding theory of chemical bonds and is therefore able to capture non-saturated covalent directional bonds originating from the d-electrons as well as magnetic interactions. It is also computationally efficient so that it enables to simulate complex dislocation configurations under arbitrary stress conditions. We will discuss the behavior of dislocations at the atomic scale and show how the atomistic studies enable to formulate mobility laws that can be implemented in mesoscopic discrete dislocation dynamics studies of large dislocation ensembles.