



Monday, 13th of December, 4:30 p.m.
ICAMS Seminar room UHW 11/1102

Dr. Matous Mrovec

Fraunhofer-Institut für Werkstoffmechanik, Freiburg

Dislocation properties in alpha-iron

Mobilities of screw and edge (or mixed) dislocations in alpha-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. This extended, non-planar core is primarily responsible for most peculiarities in mechanical behavior of alpha-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 alpha-Fe using a recently constructed magnetic bond-order potential. This potential is based on the tight binding theory of chemical bond and is therefore able to describe well non-saturated 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 the discrete dislocation dynamics studies of large dislocation ensembles.