



INTERDISCIPLINARY CENTRE FOR
ADVANCED MATERIALS SIMULATION

ICAMS Seminar

Dr. Roman Gröger

Academy of Sciences of the Czech Republic
Institute of Physics of Materials
Brno, Czech Republic

Monday, April 23, 4:30 p.m. ICAMS Seminar room

Atomic-level foundations of the plastic deformation of bcc metals

Plastic deformation of body-centered cubic (bcc) metals is governed by the glide of screw dislocation whose non-planar cores give rise to high lattice friction (Peierls) stresses. We have recently shown that these atomic-level details percolate through all length scales and thus determine the macroscopic behavior of these materials. If this coarse-graining is to be performed systematically, one has to find the shape of the Peierls barrier that represents the variation of the energy of the dislocation when it moves in the crystal. However, atomistic simulations provide only the maximum slope of this barrier and so its shape remains unknown.

We will demonstrate that the straightforward application of the Nudged Elastic Band method leads to clustering of the dislocation positions and thus overestimation of the Peierls stress. To solve this problem, we introduce a modification of this approach in which the NEB method is applied only to a limited number of degrees of freedom around the dislocation, while the rest are obtained by molecular statics relaxation. This guarantees uniform distribution of dislocation positions along the path and thus provides the Peierls barrier that is in agreement with a direct application of stress.

For more information contact STKS secretary: Hildegard.Wawrzik@rub.de

ICAMS/ Uni-Hochhaus-West/ Stiepelers Str. 129/ 44801 Bochum