Molecular dynamics simulations of edge dislocations interacting with grain boundaries

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Aim of the project

Plasticity in iron is governed by the motion of dislocations. Grain boundaries in the material, whether between similar or between dissimilar phases, act as a barrier for dislocation motion.

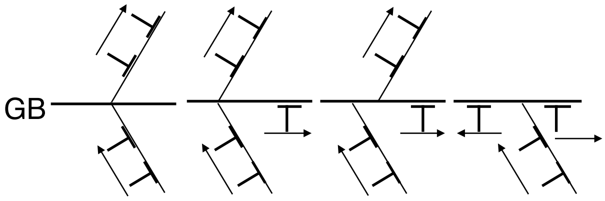

Figure 1: Possible dislocation behaviour at grain boundary

Aim: to quantify the effect of dislocation impingement at a grain boundary such that this can be translated in cohesive laws, which in turn can be used in dislocation dynamics simulations.

Approach

Molecular dynamics simulations of edge dislocations interacting with a grain boundary between a bcc and a fcc phase.

New EAM-potential

- bcc phase described with EAM Fe-potential[1] for proper description of edge dislocations in α-iron
- fcc phase described with EAM Ni-potential[2] for proper description of edge dislocations in fcc material
- two potentials combined with interaction described by EAM Fe-Ni-potential[3]

Demands on system

- dislocation line parallel to grain boundary
- periodicity in dislocation line direction
- dislocation glide direction not parallel to grain boundary
- both grains have to fit into the system with minimum stress given their orientations and lattice constants

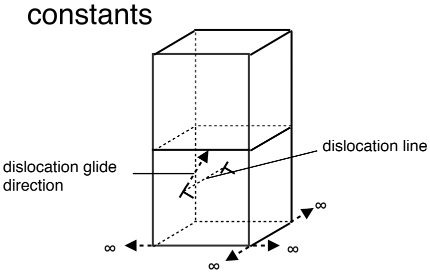

Figure 2: System set-up

Grain boundaries

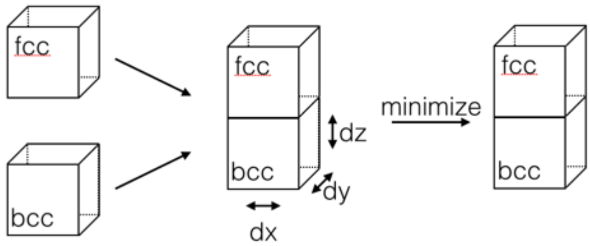

Figure 3: Creating a system with a grain boundary of given orientation relation between a bcc and a fcc grain

Slip systems in iron

{110}<111> slip system in bcc, active at low temperature
{111}<110> slip system in fcc
➔irrational interface, non-close packed planes at interface

Stresses

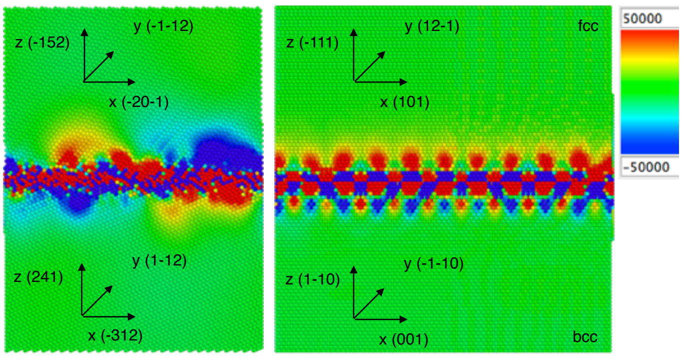

Figure 4: Stress distribution at grain boundary between fcc and bcc grain for irrational interface (left) and Nishiyama-Wassermann interface (right) (σ_{xx} in bar/Å^3)

The irrational interface is seen to have a less regular stress distribution. Knowledge of stresses turns out to be very important for an efficient and correct simulation of dislocation behaviour. Due to these stresses and the stress field of a dislocation, large systems are needed. Work on these issues is currently ongoing.

References

1. L. Malerba *et al.*, Journal of Nuclear Materials (2010) 406 7–18.
2. A.F. Voter and S.P. Chen, MRS Symp. Proc. (1987) 82, 175
3. G. Bonny *et al.*, MSMSE (2009) 17, 025010

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