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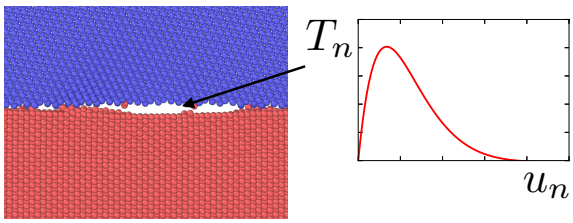
Research topics: iron/precipitate interfaces, steel, molecular dynamics, interface decohesion, cohesive laws, dislocations, dislocation loops

Nano-scale failure in steel

Research activities:

Interface decohesion

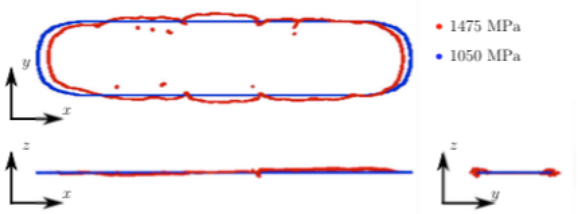
Cohesive laws have been derived to describe the relation between tractions and separations at interfaces between the soft iron matrix of steel and hard precipitates. With the aid of molecular dynamics simulations, the influence of dislocations and various loading modes is taken into account in describing both the crack nucleation and crack growth behaviour at various iron/precipitate interfaces. The resulting cohesive laws can be implemented in material models at the next, larger, length scale such as discrete dislocation plasticity.



Interface decohesion at iron/precipitate interface and shape of cohesive law relating tractions T_n to separations u_n at interface.

Dislocation shear loops

The equilibrium size and shape of dislocation shear loops in iron is determined with molecular dynamics simulations, as well as the growth behaviour. Since dislocation shear loops consist of both edge and screw dislocation parts, both kinds of dislocations should be properly described in the molecular dynamics simulations. From the current available interaction potentials for iron which are capable of describing the large systems needed to contain a dislocation loop, no potential is known to describe both edge and screw dislocations correctly. By combining the description of single edge and screw dislocations as well as dislocation shear loops by various potentials selected on either their proper description of just edge or just screw dislocations, or an acceptable description of edge and screw dislocations, the equilibrium sizes, shapes and shear stresses of dislocation loops are found.



Example of two expanding dislocation shear loops under different applied shear stress levels σ_{xz}, starting from different initial sizes.

Teaching activities:
Guest lecture in Ghent University on molecular dynamics simulations

Key publications 2018:

- A. Elzas, T.P.C. Klaver, B.J. Thijsse, Cohesive laws for shearing of iron/precipitate interfaces, Computational Materials Science, 152, 2018, 417-429
- A. Elzas, B.J. Thijsse, Cohesive laws describing the interface behaviour of iron/precipitate interfaces under mixed loading conditions, Mechanics of Materials, 129, 2019, 265-278
- A, Elzas, Nano-scale failure in steel, interface decohesion at iron/precipitate interfaces, PhD thesis