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Effects of carbon interstitials on the Peierls stress in Fe using atomistic-continuum coupling

Karthik Chockalingam[1,*], Rebecca Janish[2] and Alexander Hartmaier[3]

[1] ICAMS Ruhr-Universität, Universitätsstr. 150, Germany 44801,
karthikeyan.chockalingam@rub, http://www.icams.de

[2] ICAMS Ruhr-Universität, Universitätsstr. 150, Germany 44801,
rebecca.janisch@rub, http://www.icams.de

[3] ICAMS Ruhr-Universität, Universitätsstr. 150, Germany 44801,
alexander.hartmaier@rub, http://www.icams.de

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Carbon as a ubiquitous alloying element in steel and an interstitial atom in the iron lattice, segregates to dislocation cores to form so-called Cottrell clouds. This is energetically favorable due to the low solubility of C in the iron matrix and the release of strain energy at the dislocation core. Carbon clouds are pinning dislocations, resulting in an increase in yield strength. To better understand the influence of carbon on the critical stress to move a dislocation in the crystal lattice, i.e. the Peierls stress, its effect on edge and screw dislocations was investigated. We found that the relative increase in Peierls stress is higher for edge dislocations than for screw dislocations.

For this analysis we implemented an atomistic-continuum framework in which the dislocation core is modeled atomistically, and the material away from the dislocation core is described in a continuum-elasticity finite-element approach using anisotropic elasticity. Thus, the atomistic domain is restricted to a small region around the core, resulting in a significant reduction of the number of atoms required to model a dislocation. Initially we use an embedded atom method (EAM) type potential for the interatomic interactions, but the coupled framework is not limited to a particular choice of interaction and can also be used in combination with ab-initio methods.

REFERENCES

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