Poster Session | C. Crystal Plasticity: From Electrons to Dislocation Microstructure

[PO-C1]Poster Session 1

Symposium C

Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall

[P1-15]Investigation of dislocation core structure in Aluminum by using a generalized Peierls-Nabarro model

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We investigate the dislocation core structure in Aluminum (Al) by using generalized Peierls-Nabarro (PN) model.
Same as classical PN model, a generalized PN model expresses the total energy of dislocation core as a sum of local misfit energy and non-local elastic energy.
To integrate micromechanics in classical PN model, the generalized PN model can flexibly and efficiently evaluate the non-local elastic energy [1].
Especially, in isotropic case, the generalized PN model can evaluate the non-local elastic energy with high accuracy [1,2].
In this work, we calculate the generalized stacking fault energy surface by density functional theory (DFT) calculation and empirical atomic potential and evaluate dislocation core structure in Al.
Then we discuss the accuracy of generalized PN model by comparing to result of empirical atomic potential.
We also demonstrate that the generalized PN model is a useful tool to investigate the mesoscopic dislocation behavior.

[1] H.Wei,Y.Xiang and P.Ming: Commun. Comput. Phys. 4 (2008) 275-293
[2] V.V.Bulatov and W.Cai: Computer simulations of dislocations (Oxford,2006)