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

[P1-18]Machine learning interatomic potentials for molecular dynamics simulations of dislocations

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The mechanical response of crystalline materials is largely controlled by the mobility of dislocations. It is possible to study the mobility of individual dislocations using molecular dynamics simulations, e.g. [1], but the validity of these studies depends on the quality of the interatomic potentials employed. In the present contribution we employ machine learning techniques for the construction of interatomic potentials using ab-initio data as input, validate the interatomic potential accuracy against experimental and ab-initio observables and apply to the study of dislocations.

[1] E. Oren, E. Yahel, G. Makov, Dislocation kinematics: a molecular dynamics study in Cu, Model. Simul. Mater. Sci. Eng. 25 (2017) 25002.

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