Poster Session | E. Deformation and Fracture Mechanism of Materials

[PO-E1]Poster Session 1

Symposium E

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

[P1-21]Large-scale molecular dynamics simulations: coupling with dislocation dynamics

○Pavel A. Pokatashkin, Denis K. Ilnitsky, Alexei V. Yanilkin (Dukhov Research Institute of Automatics (VNIIA), Russia)

Various dislocation-related mechanisms: phonon drag, forest-harderning, thermal activated processes (climb, cross-slip) contribute to material properties e.g. strength. Until recently, studying of deformation via molecular dynamics (MD) considered simulations of only extremely high strain-rates. However contribution of various mechanisms might change significantly while proceeding to lower strain rates. Therefore the accuracy of dislocation dynamics (DD) models used for large strain rate range is an open question due to extrapolation.

Recent advances in computational powers increased both spatial and temporal scales available for atomistic modeling. Therefore it is possible to make coulping between MD and DD for strain rates ~10^7 s^{-1} and higher. We consider such materials as: iron, molybdenum, and uranium.