
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

[P1-11]Dislocation transmission behaviors of bi-crystal BCC Tantalum with high and low angle symmetric tilt grain boundaries: Multiscale simulation study

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In this research, we conducted multiscale (molecular dynamics and dislocation dynamics) simulations to study dislocation transmission behaviors of bi-crystal BCC Tantalum (Ta) with high and low angle symmetric tilt grain boundaries. To investigate dislocation transmission behaviors, we introduced a dislocation loop to describe the Frank-Read source, one of the dislocation multiplications in molecular dynamics simulation. We put dislocation loop on the slip plane where maximum resolved shear stress occurs. In molecular dynamics simulation, we observed interactions between dislocation and grain boundary such as dislocation transmission and absorption. Furthermore, we performed dislocation dynamics simulation to observed similar dislocation transmission behaviors. Finally, we analyzed mechanical property changes (e.g. stress-strain response) as dislocation interacts with grain boundary.

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