
Poster Session | F. From Microstructure to Properties: Mechanisms, Microstructure, Manufacturing

[PO-F2]Poster Session 2

Symposium F

Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall

[P2-52]Intrinsic Analysis of Structural Order Parameter at Equilibrium Crystal-Melt Interfaces

○Wenliang Lu, Hongtao Liang, Yang Yang (EAST CHINA NORMAL UNIVERSITY, China)

We present atomistic simulations of precisely equilibrated crystal-melt interface under ambient pressure, for pure Ni and Fe. We demonstrate the capillary waves roughen the surface, but the intrinsic interfaces can be sharply defined. We use different types of local structural order-parameter together with a reference lattice to characterize the intrinsic interface. The statistical analysis on the structural order-parameters for the interfacial solid and interfacial liquid atoms represents universal scaling behavior, nearly independent of the order parameter type, crystal structure and interface orientations. We will discuss the potential application of such intrinsic analysis to the investigations of crystal nucleation and steady-state crystallization from melt.