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

[PO-F2]Poster Session 2

Symposium F

2018年10月31日(水) 17:45 ～ 20:00 Poster Hall

[P2-51]Molecular-Dynamic Simulation of Rapid Solidification of Dipolar Molecular Crystal from Its Melt

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We present results of molecular dynamics (MD) simulations of crystal growth from the melt. The work focuses on a face-centered-cubic molecular crystal consist with molecules modeled by an extended point dipole model. We will present results of non-equilibrium MD growth simulations as a function of temperature and molecular dipole moment. An analysis of the interfacial position as the function of simulation time was employed to extract the steady-state, and the data of the kinetic coefficients vs. molecular dipole moments and their anisotropies were calculated and will be presented. Values of the kinetic coefficient for the (100), (110) interfaces are compared quantitatively to the prediction of Mikheev-Chernov (MC) theory. Our study suggest that incorporating a second relaxation time due to the dipolar fluctuation beside the relaxation time of density waves, is necessary for extending MC theory to be applicable for molecular crystals.