Prediction of Surface Melting Behavior of Cu metal of Lennard-Jones Potential

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We investigate surface melting of copper (100), (110), and (111) using molecular dynamics (MD) simulation, where Lennard-Jones potential is used to describe the interatomic interaction. By constant-temperature MD the structural information of bulk and surfaces of copper were investigated at temperatures from 800K and 1400K. Internal energy, density of atoms, diffusion coefficient, and radial distribution function were calculated for detailed analyses. The surface models of (100), (110), and (111) were melted at about 1313K, 1310K, and 1350K, respectively, which were lower than the melting point of bulk copper. Diffusion coefficients in normal direction to each surface plane were smaller than that in parallel, and this finding indicates enhanced tendency for disordering and eventual initiation of melting in the lateral direction.