Title: Determination of Surface Premelting Point of Silver Nanoparticles by Molecular Dynamics Simulation

Abstract

A molecular dynamics (MD) simulation based on embedded atom method (EAM) was conducted to different sizes of Ag nanoparticles with diameters of 4 nm to 20 nm to find melting and surface premelting points. A comparison between our simulation and theoretical models for melting and surface premelting was reported. Obtained melting point values of NPs showed good agreement with the liquid drop model and the onset temperature of surface permeating shows good agreement with the mean field approximation model. Ag NPs with diameter smaller than 8 nm melted without passing through surface premelting stage. This finding is also in agreement with the literature.