

Abstract Submitted  
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**A Molecular Dynamics Study of the Melting and Nucleation of Iron Nanoparticles** YASUSHI SHIBUTA, TOSHIO SUZUKI, Department of Materials Engineering, The University of Tokyo — The melting and nucleation of iron nanoparticles were investigated by molecular dynamics simulation using a Finnis-Sinclair potential. The nanoparticle of the bcc single-crystal was uniformly melted from the surface at a melting point during heating, whereas a nucleus was generated near one side of an undercooled liquid droplet and the solidification spread toward another side at a lower temperature during cooling. The melting point and nucleation temperature decreased with particle radius. Moreover, the solid-liquid interfacial energy was estimated to be  $0.101 \text{ J/m}^2$  using a Gibbs-Thomson equation, which is of the same order as the experimental value based on Turnbull-Fisher's classical nucleation theory.

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