

Abstract Submitted
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Molecular dynamics study of the phase transition in the bcc metal nanoparticles YASUSHI SHIBUTA, TOSHIO SUZUKI, The University of Tokyo
— The phase transition between liquid and solid phases in bcc metal nanoparticles was investigated using a molecular dynamics simulation. The nucleation from an undercooled liquid droplet was observed during cooling in all nanoparticles considered. A nucleus was generated near one side of the particle and solidification spread toward the other side during nucleation process. On the other hand, the surface melting and subsequent inward melting of the solid core of the nanoparticles were observed during heating. The depression of the melting point was proportional to the inverse of the particle radius due to the Gibbs–Thomson effect [1]. However, the depression of the nucleation temperature during cooling was not monotonic with respect to the particle radius since the nucleation from an undercooled liquid depends on the event probability of an embryo or a nucleus.

[1] Y. Shibuta, T. Suzuki, J. Chem. Phys. 129 (2008) 144102.

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