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Molecular dynamics study of phase transition in substrate-supported nanoparticles of bcc metals YASUSHI SHIBUTA, TOSHIO SUZUKI, The University of Tokyo — The phase transition between liquid and solid phases of substrate-supported nanoparticles of bcc metals with size ranging from 2000 to 31200 atoms was investigated using a molecular dynamics simulation. The effect of the interaction energy between the nanoparticle and the substrate on the contact angle, melting point and nucleation temperature was focused on. Unidirectional solidification and inward melting after surface melting were observed in the substrate-supported nanoparticles during cooling and heating, respectively. The depression of the melting point from the bulk melting point was proportional to the inverse of the effective radius of the substrate-supported nanoparticles [1]. The gradient of proportionality increased with decreasing contact angle and deviated from that of freestanding nanoparticles [2]. On the other hand, the undercooling temperature for solidification decreased with decreasing contact angle, which agrees with the theory of heterogeneous nucleation. [1] Y. Shibuta, T. Suzuki, Phys. Chem. Chem. Phys., 2010, DOI:10.1039/b919869e. [2] Y. Shibuta, T. Suzuki, J. Chem. Phys. 129 (2008) 144102.

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