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Molecular dynamics analysis of a equilibrium nanoscale droplet on a solid surface with periodic roughness YUMA FURUTA, Department of Mechanical Engineering, Osaka University, DONATAS SURBLYS, Institude of Phisical and Chemical Research, YASTAKA YAMAGUCHI, Department of Mechanical Engineering, Osaka University — Molecular dynamics simulations of the equilibrium wetting behavior of hemi-cylindrical argon droplets on solid surfaces with a periodic roughness were carried out. The rough solid surface is located at the bottom of the calculation cell with periodic boundary conditions in surface lateral directions and mirror boundary condition at the top boundary. Similar to on a smooth surface, the change of the cosine of the droplet contact angle was linearly correlated to the potential well depth of the inter-atomic interaction between liquid and solid on a surface with a short roughness period while the correlation was deviated on one with a long roughness period. To further investigate this feature, solid-liquid, solid-vapor interfacial free energies per unit projected area of solid surface were evaluated by using the thermodynamic integration method in independent quasi-one-dimensional simulation systems with a liquid-solid interface or vapor-solid interface on various rough solid surfaces at a constant pressure. The cosine of the apparent contact angles estimated from the density profile of the droplet systems corresponded well with ones calculated from Young's equation using the interfacial energies evaluated in the quasi-one dimensional systems.

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