

Solid-liquid phase transition of Hard core Yukawa fluid under cylindrical confinement

_____, _____, _____
(skkwak@unist.ac.kr*)

The solid-liquid phase transition of hard-core attractive Yukawa (HCY) fluid in a cylindrically hard pore of radius (R) from 3.0 to 9.0 molecular diameter was studied using molecular dynamics (MD) simulation. Modified velocity-Verlet algorithm was employed to take into account the hard collisions of particle-particle and particle-wall. This algorithm makes comparable results with previously reported data of the bulk system by González-Melchor et al. [J. Chem. Phys. 115, 3862 (2001)]. As the radius of cylindrical boundary increases, the pressure tensor component (i.e. x -axis) along the direction of cylinder was significantly decreased when the phase transition occurs. Many criteria such as structure factor, bond order parameter, and local density profile were tested to acquire the structural properties so that the solid-liquid phase transition range of the HCY fluid was accurately predicted. We also employed the free volume method to obtain the free energy of the cylindrically-confined system of the HCYukawa fluid, which has never been reported.