

Prediction of Equation of States for Hard-Sphere Crystals via Free Volume Approach

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The free volume is a volume available to a hard-sphere to move around surrounding hard-spheres at fixed positions. Using this statistical property, we predicted equations of state of FCC and HCP hard-sphere crystals with a help of molecular dynamics simulation, which is only used for providing system configurations at several points of time. A usual manner for the density reduction, where particles and volumes are correspondingly increased, was not followed. Instead it is done by the gradual omission of particle while keeping the volume constant. Thru this approach, it was possible to trace the equation of state including a specific density where the Maxwell equal area is constructed. The free volume method is not sensitive enough to obtain differences in equations of states of FCC and HCP crystals over high density region, yet it was clearly observed that their fluid-solid phase transitions were distinguishable.