Prediction of phase transition of FCC and HCP hard-sphere crystals via Free Volume Approach

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Free volume is a volume available to a particle center to move around without the alteration of the other particle positions. Using this statistical geometric-property, we predicted equations of state of FCC and HCP hard-sphere crystals with a help of molecular dynamics simulation. It is only used for providing system configurations to calculate free volumes of each particle at different points of time trajectory. A usual manner for the volume expansion and contraction, where particles and volumes are correspondingly varied, was not followed. Instead the step-by-step omission of a particle while keeping the volume constant was done in this approach. By doing so, it was possible to trace the equation of state including a specific density where the Maxwell equal area is satisfied. 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 at the vicinity of the absolute instability.