Phase Transition of Lennard-Jones Fluid in the Confined System

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The molecules in the confined systems play the important role in the lubrication, adhesion and fabrication of nanomaterials. It is important for new physics that relate to finite-size and reduced dimensionality effects. The experimental study of actual molecular films were performed. [1] This study shows that the thermal properties of the molecules in the confined system is significantly different from its properties in the bulk system. The freezing point and melting point depends on the width of the parallel slit pore in those confined system. We study the phase transition of Lennard-Jones particles in the confined system. We performed the Monte Carlo simulation. To realize the sampling in the wide energy space or wide volume space, we employed the multicanonical approach. The conventional Monte Carlo method samples the conformations or coordinates at the constant temperature and the constant pressure. The multibaric-isothermal (MUBA) ensemble and the isobaric-multithermal (MUTH) ensemble was proposed. [2] The MUBA ensemble is aiming for the flat probability distribution in volume space. The MUTH ensemble is aiming for the flat probability distribution in energy space.

References

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[2] Okumura, H.; Okamoto, Y. *Phys. Rev. E* **2004**, *70*, 026702.