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Phase behavior of hard rods between two walls: Phase change of particles without occurring phase transition

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Abstract

In this study, we investigated the phase behavior of rods with square ($D \times D$) and circular (diameter D) cross sections between two hard walls using the Parsons-Lee theory and applying the Zwanzig approximation. Our focus is to find wall-to-wall separations (H) and the size of particles in which the phase of the system changes without occurring a phase transition. It was determined that if the distance between the plates is smaller than the length of the particles, for any particle whose length (L) to diameter ratio is greater than 1, the second order phase transition occurs, and most of the particles are placed in a certain direction parallel to the plates, which this type of phase transition takes place at lower densities with increasing particle's aspect ratio. We also came to the conclusion that if the distance between the plates is greater than $2D$ and $1D < L < 2D$, despite the phase change of the system with increasing particle density, no phase transition will occur. In addition, it was found that the cylindrical shaped particles show some unexpected behaviors, which could be due to the inappropriate performance of the applied theory or their real physical behavior, which requires more detailed studies to resolve the ambiguity.

Keywords: liquid crystal, phase transition, rods, confined, nematic

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