MONTE CARLO STUDY OF THERMODYNAMIC AND STRUCTURAL PROPERTIES OF A LENNARD-JONES FLUID AT DIFFERENT TEMPERATURES

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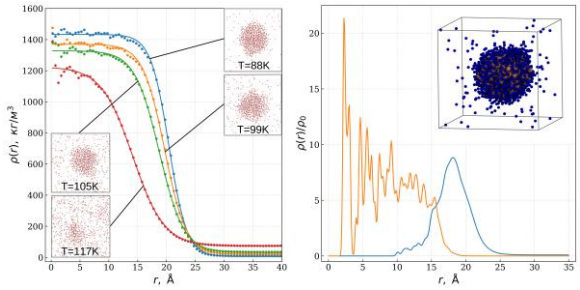
We present the results of computer simulation of one-component and two-component Lennard-Jones fluids in the canonical statistical ensemble using the Monte Carlo method [1-2]. The purpose of the study is to analyze the influence of temperature, size and composition of the considered systems on their structural and thermodynamic properties. A one-component system consisting of argon molecules has been simulated in the temperature range from 80 to 120 K. The formation of droplets surrounded by the vapor phase has been observed during the simulations (see Figure). The dependence of the density profile on the temperature at a fixed concentration of argon in the simulation cell has been studied. The obtained results are consistent with the data presented by other authors [3]. Our calculations show that the density of the vapor phase increases and the density of the liquid phase decreases with the increase of temperature. A two-component system consisting of argon and neon molecules has been also studied. Analysis of structural properties of the system has revealed the formation of a liquid film consisting of neon molecules on a solid core consisting of argon molecules at the temperatures below 60 K (see Figure). The influence of argon and neon concentrations, as well as temperature, on the density profiles, energy and heat capacity of the considered systems has been studied.



Density profiles and snapshots of one-component (argon) and two-component (argon and neon) Lennard-Jones fluids

1. Metropolis N. et al. // J. Chem. Phys. 1953. V. 21. No. 6. P. 1087–1092.
2. Allen M.P., Tildesley D.J. // Computer Simulation of Liquids. 2 ed. Oxford University Press, 2017.
3. Maruyama S. et. al. // Proc. Int. Heat Transfer Conf. 10. 1994. P. 409–414.