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Model representation of diffusion near the triple point of argon

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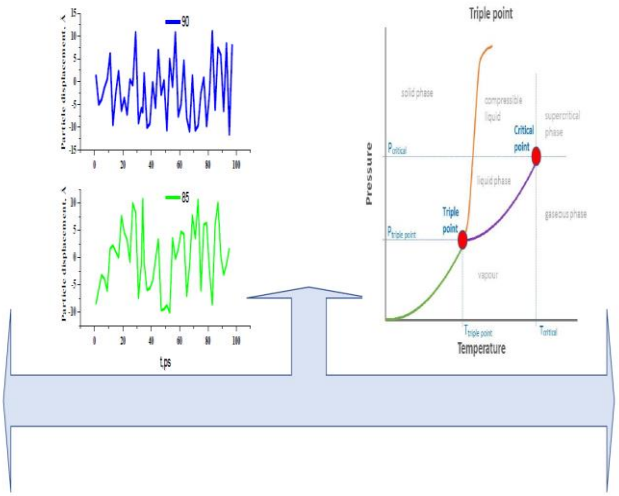
Graphical Abstract



Abstract.

We present a systematic study of the effect of temperature and pressure on the microscopic dynamics of argon near the triple point. We also provide a detailed description of the argon diffusion model and discuss the time-dependent dynamics of argon, as well the relaxation processes in the temperature and pressure range near the argon's triple point. The main goal of this work is to develop a method for determining the P-T parameters on the coexistence curve, for which there is a transition from a mixture ("solid (glass)- dense liquid")→ ("dense liquid" → "liquid") → ("liquid" -gas). We present and compare the results of a dynamic analysis of the system in various states obtained using several approaches.

Keywords
argon, triplet point, diffusion model, MD simulation

Conflicts of Interest: The author declares no conflict of interest.

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