Iinfluence of external factors (high temperatures, pressures) on soft matter systems

N.A.Atamas^{*}, D.A. Gavryushenko

National Taras Shevchenko University of Kyiv, Physics Department, 2 Glushkov Ave., Kyiv 03124, Ukraine Keywords: high pressure, high temperature, thermodynamic properties, MD simualtion.

*e-mail: atamasphys@mail.univ.kiev.ua

A consequence of the influence of external factors (high temperatures, pressures) on physical systems is the appearance in these systems of new components that differ from the components of the unperturbed system as the interaction energy, and the physical characteristics of the particles. Therefore, the formalism of the distribution functions is convenient from the point of view of the interpretation of both the structural changes that have occurred in the system and from the point of view of computing the change in the basic macroscopic characteristics of the system. Present work is dedicated to the investigation of temperature influence on those thermodynamic properties of liquid Ar, which are defined by the shift of chemical potential of the regarded system and its components under the influence of temperature. It was shown, that temperature of coexisting phases in stationary state leads to the shift of the parameters of phase transitions of the first order. Also the presented research

studied the effect of temperature on the structural and dynamic properties of liquid Ar at high temperature and pressure by using the MD. A model relating the structural and dynamical properties of the Ar systems introduced. These data suggest that changes in temperature in a given interval leads to a change in the dynamic properties of liquid Ar. Analysis of the temperature and the time dependence of diffusion allowed to build a model representation describing the mechanisms of diffusion of the Ar systems and calculate their characteristic times. Qualitative analysis of the characteristic of the molecules of Ar, made from the the diffusion coefficient indicates the existence of various mechanisms of diffusion in Ar. To confirm the theoretical predictions, a qualitative comparison of the model with the existing experimental data on temperature influence on the physics properties of liquid Ar is performed.