METASTABLE STATES OF WARM DENSE HYDROGEN

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Currently, there is a sufficiently large number of works in which the influence of taking into account quantum effects of nuclei on the thermodynamic properties of systems containing hydrogen at high pressures is investigated [1, 2]. The method of path integrals together with density functional theory allows one to effectively take into account these nonlocal properties of nuclei [3].

In this work, we propose to investigate the influence of this effect on the region of existence of metastable states (atomic and molecular) of hydrogen fluid at high pressures (100â€“200 GPa) [4, 5]. The technique of calculations within the framework of the path integral molecular dynamics method using VASP and PIMD software packages has been studied. Metastable states in hydrogen fluid have been found, the existence of which is a definite indication that the observed transition is the phase transition of the first kind. This fact is especially important for phase transitions with small density jumps.

Within the framework of the VASP+PIMD method, isotherms for the temperature range 700â€“1500 K have been calculated. A method of modeling metastable states for all isotherms under study was developed and successfully applied. A phase curve and an estimate for the metastable regions are obtained. The conservation of the molecular phase along the metastable branches is evidenced by high values of the heights of the first peaks of the pair correlation function. An estimate of the heat of phase transition through the jump of the pair entropy is obtained. The pressure dependence of electrical conductivity is calculated, where metastable branches are clearly visible.

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