INVESTIGATION OF PROPERTIES AND PHASE STATE OF HELIUM BY THE METHODS OF MOLECULAR DYNAMICS AND THERMODYNAMICS

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Abstract: The applicability of interatomic pair Lennard–Jones (LD) potential to helium ^{4}He was studied by the molecular-dynamic modeling technique by analizing its structure, phase state, and thermal properties. The parameters of the paired interatomic potential of the LD were determined and verified against available experimental data. It is shown that the found potential parameters reliably reproduce the properties of ^{4}He in a wide range of pressure and temperature, including domains of solid, liquid, and gaseous helium. The properties of ^{4}He along isotherms are calculated for temperatures ranging from 20 to 3000 K. The structures and phase state of ^{4}He are analyzed at high pressure. The melting line of ^{4}He is estimated. It is found that there is a stable crystal body-centered cubic phase for ^{4}He at a temperature of 300 K and a pressure of 16 GPa.

Keywords: molecular-dynamic simulation; phase diagram; intermolecular interaction potential; melting line; helium

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