STUDY OF THE PHASE DIAGRAM OF ZIRCONIUM BY MOLECULAR DYNAMICS METHOD

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Zirconium is an important structural material, however, its phase diagram has not been fully studied. The method of molecular dynamics allows to calculate phase transition curves by different methods. The purpose of this work is to compare the results of such methods as two-phase and single-phase modeling, calculation of thermodynamic potentials by the vibration density of states for the BCC-HCP and BCC-melt transitions. The calculations are carried out for two potentials: EAM-potential #2 [1] and ADP-potential [2]. The two-phase simulation method is based on the observation of the phase boundary motion in a two-phase system. The single-phase simulation method is based on extrapolation of the transition temperature between the phases at different heating or cooling rates in a single cristal. The calculation of thermodynamic potentials by vibration density of states received from the calculations of the velocity autocorrelation function. All simulations were carried out in LAMMPS.

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