INVESTIGATION OF THE THERMODYNAMICS OF DECOMPOSITION OF AN ALLOY IN NANOSYSTEMS AS A RESULT OF THE FIRST-ORDER PHASE TRANSITION BY MEANS OF THE SIMULATION OF VACANCY DIFFUSION WITH THE MONTE CARLO TECHNIQUE

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S u m m a r y

A new computer model for the investigation of reactions in metal alloys with the bead-like first-order transition, including the initial stages of interdiffusion, by the Monte Carlo method is developed. The equilibrium phase diagram for a model system is obtained under the specifically matched pair potentials. The dependence of the equilibrium concentration of the solid solution at the interface with a finite-size ordered phase on its geometry is analyzed. The correlation between the size and the shape of an intermetallic particle, being at the equilibrium at a fixed temperature, is established.