INTERATOMIC INTERACTION OF LEAD AND TIN CHALCOGENIDE CRYSTALS WITH THE STRUCTURE OF NaCl

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S u m m a r y

To study the structural and energetical parameters of a crystal and its defect subsystem by molecular-dynamics simulations, it is necessary to define the interaction potentials and interacting structural particles. Three simple models of potential-particle are considered to investigate lead and tin chalcogenide crystals with the structure of NaCl. The parameter K is proposed to determine the model. This parameter is calculated using the experimental data on the nearest-neighbor distance R_0, lattice energy U_0 and bulk modulus B.