Molecular Dynamics Modeling of a Ternary Semiconductor Compound in A Liquid State

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Abstract

Combination of the molecular dynamics (MD) method and the density functional theory (DFT) method was used, which takes into account the symmetries of the interaction energy of N atoms in the ternary semiconductor compound liquid state. It is shown that such a method for calculating the diffusion characteristics of a system, based on the interaction potentials of atoms taking into account the ab initio calculation of the structure and symmetry of the liquid state, competitive with other methods for calculating the characteristics of liquid multicomponent systems in quantum mechanics. The model of the three-component compound $TlInS_2$, which depends on the parameters of the NVT MD canonical ensemble, is considered. Within the framework of the MD-DFT GGA PBE model, the diffusion coefficient for the atoms of the semiconductor ternary $TlInS_2$ compound in the liquid state was calculated taking into account root-mean-square displacements at a given point in time. The FP MD-DFT GGA PBE method was used to calculate the diffusion coefficients of atoms near the melting point of $TlInS_2$: $D_{Tl} = 2.6 * 10^{-5}$ sm^2/s, $D_{In} = 2.5 * 10^{-5}$ sm^2/s u $D_S = 2.1 * 10^{-5}$ sm^2/s.

Keywords: Ab Initio Molecular Dynamics, Nvt Md Canonical Ensemble, Md-Dft Gga Pbe Calculation, Disordered Structure of Semiconductor TlinS_2, Time Displacement of Atoms, Calculation of Diffusion of Atoms in the Liquid State.

Introduction

In the method of molecular dynamics (MD), as is known, the temporal evolution of a molecular system of interacting particles is tracked by integrating their equations of motion. And the density functional theory (DFT) allows to calculate the electronic structure of molecules and condensed matter in quantum physics and quantum chemistry.

Combination of MD and DFT expands the range applications of both methods [1]. Based on first principles (FP), the FP MD-DFT technique extends molecular dynamics beyond the use of the pair potential approximation. FP MD-DFT allows to simulate large systems that include many particles with ionic, covalent and metallic bonds.

MD simulation method generates trajectories of a mate-rial point (particles) in the phase space for a system of N particles. Then, the equations of motion of these particles are integrated by appropriate algorithms. For this, different forms of force fields (FF) [1,2] are used. This enables to optimize the parameters of interatomic (intermolecular) interaction potentials of particles and to calculate long-range forces in the system. Therefore, for a specific system, from known models of force fields, it is necessary to choose fields with a set of parameters that correspond to a given problem.

The structure of ternary semiconductor compounds in a disordered state has been little studied in comparison with one- and two-component systems [3-5].

After melting, for example, silicon [3] to densify and turn into a metal with a coordination number of 6[3]. In addition, silicon becomes amorphous and amorphous Si is used in solar cells.

For liquid semiconductor binary systems, for example, $Ge_{(1-x)} Se_x$, the physicochemical properties change markedly depending on the composition of the system [5].

Based on the first principles study of the liquid Ge-Se system, it is indicated that at temperatures close to the melting point of the alloy, an intermediate order is established in the structure of liquid GeSe. Such a structure at the crystal–liquid interface is located at distances exceeding the radius of the ion in the first shell of the nearest (neighboring) molecules.

Information on the structure factors and diffusion properties of ternary semiconductor compounds in the liquid state is limited.

The purpose of this study is, within the framework of the method of molecular dynamics and first principles, modeling the interaction of particles of the semiconductor TlInS_2 ternary compound in the liquid state. As an example, simulation data of the semiconductor TlInS_2 compound is given.

In this paper, we consider the results of FP MD-DFT GGA PBE calculations for the semiconductor compound TlInS_2 near the melting temperature. The time dependences of the root-mean-square displacement of atoms and the diffusion coefficient of TlInS_2 particles in the liquid state are plotted.

Models and calculation methods

Compound TlInS_2. The TlInS_2 crystalline compound has several modifications, including a monoclinic layered structure [6-8], and can be used as a photosensitive material in nano- and microelectronics, photonics, and optics [9].

The monoclinic structure of TlInS_2 with the space group C2/c is formed by the growth of a single-crystal layer during the crystallization of the TlInS_2 melt (Figure 1).
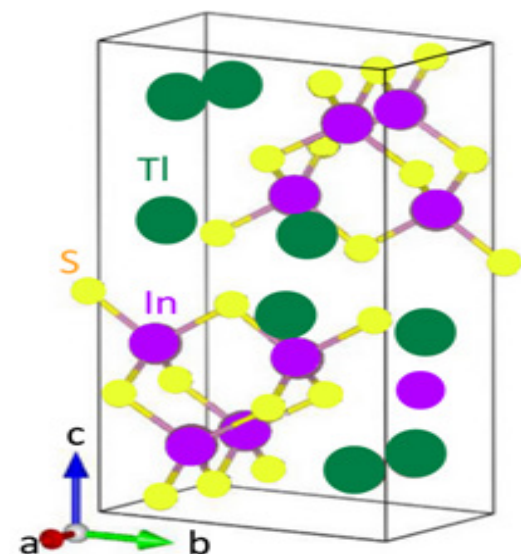

Figure 1. Primitive cell of a tlins_2 crystal with a

monoclinic structure.

As is customary in crystallography, shown in Fig. 1 elementary cell TlInS_2 of the monoclinic syngony, is built on three vectors a, b and c, having different lengths, with two straight and one indirectangles between them.

The crystal lattice parameters of TlInS_2 DFT GGA-PBE calculated by us agree with the experimental data: a = 10.942 Å, b = 10.484 Å c = 15.606 Å, α = β = 100.6°, Z = 4. [8]. The calculated lattice parameters of TlInS_2 are: a = 11.147 Å, b = 11.159 Å c = 15.378 Å, α = β = 96.883∘.

Depending on the technological mode of crystal growth, a structural rearrangement of the melt-solution occurs, which leads to the crystallization of other modifications of TlInS_2. According to DTA data, the melting temperature of TlInS_2 is ~ 1040 K [8].

Motion equation. The patterns of particle diffusion and the mechanisms of mass transfer in solid and liquid systems are known from physics and physical chemistry. In particular, various models and calculation methods for multicomponent mass transfer in ionic systems are known [10].

The behavior of an individual atom is described by the classical equations of motion [11].

$$m_i \frac{d^2 r_i(t)}{dt^2} = F_i \qquad (1)$$

where i is the number of the atom $(1 \leq i \leq n)$, n is the total number of atoms in the system, m_i is the mass of the atom, r_i is the radius vector of the atom, F_i is the resultant of the forces acting on the atom.

Interaction potential. Known interaction potentials make it possible to simulate the physicochemical and thermodynamic properties of systems with varying complexity [12–14]. The cluster potentials (for example, the empirical potential Stillinger–Weber (SW) [12]) implicitly describe two-particle interactions. In the SW functional, the parameters of pair interaction depend on the nature of the medium, where additional coefficients are taken into account. The SW potential consists of two terms responsible for attraction and repulsion.

There is also a potential describing the three-particle interaction in an implicit form, for example, the potentials Tersoff (T) [13]. In this model, it is assumed that the strength of the bond between two atoms is not constant, but depends on the local environment. The form of the potential (T), as well as SW, consists of two terms responsible for attraction and repulsion.

When atoms interact with a medium, the resultant force consists of two components:

$$F_i = -\frac{\partial U(r_{ij}...r_{ik})}{\partial r_i} + F_i^{ext} \quad (2)$$

where U is the potential energy of interacting particles, F_i^{ext} is an external force determined by interactions with the medium. The first component is the force acting on a given atom from all other atoms. The interaction between atoms is potential, and therefore the first force is written as the potential energy gradient of the system.

The total potential energy of the system is some function of the atomic coordinates, and a typical expression for force fields (FF) can be written as:

$$U(R_i) = \sum_j^{N_{bonds}} \frac{k_j^r}{2}(r-r_0)^2 + \sum_j^{N_{angles}} \frac{k_j^\theta}{2}(\theta-\theta_0)^2 + \sum_j^{N_{dihedrals}} \frac{k_j^\phi}{2}[1+\cos\{n\phi_j - \delta\}] +$$

$$\sum_j^{N_{impropers}} \frac{k_j^\omega}{2}[1+\cos(2\omega - \pi)] + \sum_{i,j=1}^{N_{LJ-pot}} 4\epsilon_{ij}\left(\frac{\sigma_{ij}^{12}}{r_{ij}^{12}} - \frac{\sigma_{ij}^6}{r_{ij}^6}\right) + \sum_{i,j=1}^{N_{coul}} \frac{q_i q_j}{r_{ij}} \quad (3)$$

where R_i are the coordinates of all atoms in the system, k_j^r and r_0 are the bond length constant and the equilibrium bond length of j, k_j^θ and θ_0 are the bond angle constant and the equilibrium bond angle of j, k_j^ϕ is the dihedral angle constant of j, k_j^ω is the irregular angle constant of ω corresponding to the deviation from flatness of angle j, $\epsilon_{(i,j)}$ is the force of dispersion interaction between atoms i and j, $\sigma_{(i,j)}$ is the contact distance between atoms i and j, q_i is the charge of atom i, r_{ij} is the distance between atoms i and j.

Molecular modeling [14-18]. The calculation of the evolution of atomic systems containing ≥ 106 atoms is possible using the MD method. For this, the equation of motion of atoms is solved, including interaction potentials depending on the coordinates of atoms. The solution requires an adequate choice of difference schemes for calculating the MD equations and interaction potentials of atoms.

The MD equations for atoms are written in the form of Hamilton's ordinary differential equations. The Hamilton equation is solved at a fixed point in time in a canonical transformation in phase space. Here time is a conversion parameter.

Canonical equations are solved numerically using difference schemes, in which the differential operator is replaced by explicit and/or implicit difference schemes [19–26]. In the numerical scheme, the difference operator must include the properties of the canonical transformation. Computer programs allow you to control the limitation on the integration step. In our problem, explicit schemas were preferred.

Consider the motion of N point particles of mass m, including the coordinate (x_i) and momentum (p_i) of the i-th particle. The Hamiltonian of this system has the form

$$H = K(p_i) + U(x_i) \quad (4)$$

where K is the kinetic energy of particles, V is the potential energy of particle interaction;

$$K = \sum_{i=1}^{3N} \frac{p_i^2}{2m}, \quad U = U(x_i), i = 1, ..., 3N.$$

The equations that include the coordinate (x_1) and momentum (p_1) of the i-th particle, as well as the force (F_1) acting on the particle for the Hamiltonian (4), have the form [11].

$$\frac{dx_i}{dt} = \frac{p_i}{m_i}, \quad \frac{dp_i}{dt} = F_i, \quad F_i = -\frac{dU(x_i)}{dx_i} \quad (5)$$

For a non-closed system of N particles, the potential of the interaction of particles with the environment $U_i^{ext}(x_i)$ is added to the right side of the Hamiltonian (4), and for the momentum, the contribution

$$F_i^! = -\partial U_i^{ext}/\partial x_i.$$

The Lammps software package was used to calculate molecular dynamics. In the framework of a two- and three-dimensional problem with periodic boundary conditions, physical quantities were calculated for the semiconductor TlInS_2 with a monoclinic structure near the melting temperature [27].

The integration step was taken as 2 femtoseconds (timestep = 0.002). The number of atoms of the simulated compound TlInS_2 in the single-phase state was 8000 atoms, and for two-phase states it was 16000 atoms. The calculations were carried out according to the Verlet scheme, which consists of four stages of the algorithm implementation [14, 28].

DFT GGA calculation [6,7,29-35]. DFT GGA (generalized gradient approximation) calculation of the system in the liquid state has been carried out. Along with the structural data, the form of the exchange-correlation energy functional was also taken into account. In a functional, for example, GGA+U, the total energy is expressed as (4) [32].

$$E^{GGA+U} = E^{GGA} + \frac{U-J}{2} \sum_\sigma \left[\left(\sum_{n} n_{m,n}^\sigma \right) - \left(\sum_{m,m'} n_{m,m'}^\sigma n_{m',m}^\sigma \right) \right] \quad (6)$$

where U is the Coulomb parameter, J is the exchange parameter, (U–J) is the effective interaction parameter, n is the occupation matrix of 3d-orbitals with indices, m is the index of the d-orbital (quantum number of the angular momentum), σ is the index referring to the spin.

Discussion Of Results

New information about the structure of the liquid-crystal interface and the parameters of kinetic processes occurring at the interface are important for crystallization control. There are high requirements for obtaining materials with a given composition. Slight changes in the structure and concentration of the components of the system can affect the properties of the material. In technological operations for the production of semiconductor devices, processes are used that include the phenomena of interfacial mass transfer. Plausible models, using MD calculation methods, make it possible to describe the totality of such processes.

The above can be specified. For example, by studying the process at the phase boundary, a semiconductor crystal is a condensed phase, one can estimate the magnitude of potential barriers at the boundary, establish the mechanism of transport phenomena and the structure of the transition layer. The structure and properties of the melt-crystal boundary layer determine the kinetics of interfacial mass transfer. The study of processes in the boundary layer in a model system is difficult. Whereas, the method of molecular dynamics and / or the Monte Carlo method, allow modeling the thermodynamic and structural properties of substances in various states of aggregation [19-25]. Such data are important in the absence of experimental results. The FP MD-DFT GGA PBE method for studying processes occurring in heterophase systems makes it possible to evaluate the quantitative characteristics of processes in both gas and condensed phases.

In the FP MD-DFT GGA PBE calculations of the transport parameters of atoms and/or chemical particles in a disordered system, it was assumed that the particles propagate only by diffusion. In such a system, the root-mean-square displacement of particles characterizes the deviations of the position of the particle from the reference position over time during random motion.

Then the trajectories of the root-mean-square displacement (MSD) of particles of type α in a disordered system can be calculated by the equation (7)

$$\text{MSD} = \langle \Delta r_\alpha^2(t) \rangle \equiv \langle |\eta_\alpha(t) - \eta_\alpha(0)|^2 \rangle = \frac{1}{N_\alpha} \langle \sum_{i=1}^{N_\alpha} |r_{i\alpha}(t) - \eta_\alpha(0)|^2 \rangle \quad (7)$$

where N_α is the total number of chemical particles of type α, $r_{i\alpha}(t)$ is the coordinate of the i-th particle of type α.

Consider a disordered system at the atomic level, where atoms or particles of type α migrate by successive jumps between neighboring sites in a three-dimensional isotropic lattice.

Assume that in an isotropic lattice the distance between the nearest neighboring sites is equal to rα and the atom a makes n random jumps during the time t. Then the root-mean-square displacement of a particle of type α is $\langle r_\alpha^2(t) \rangle = n a^2$
Hence the well-known relation for the diffusion coefficient of a spherical particle

In view of the above, in the diffusion regime for the self-diffusion coefficient we obtain:

$$D_\alpha = \lim_{t \to \infty} \frac{\langle \Delta r_\alpha^2(t) \rangle}{6t} = \frac{1}{6N_\alpha t} \langle \sum_{i=1}^{N_\alpha} |r_{i\alpha}(t) - \eta_\alpha(0)|^2 \rangle \quad (8)$$

Thus, equation (8) refers to random jumps of atoms with a spherical shape. It enables to calculate the statistical average number of diffusing atoms depending on time. With such diffusion of atoms, successive jumps of the atoms of the system do not depend on each other.

Correlations between successive jumps of atoms in a system depend on the diffusion mechanism. This is taken into account by introducing the correlation coefficient ($f \leq 1$) into the right side of equation (8).

In view of the above, the FP MD-DFT GGA PBE method was used to calculate the diffusion coefficients of TlInS2 atoms in the liquid state along an extended trajectory. This was achieved by using a relatively long relaxation time, which takes into account the diffusion of atoms in an equilibrium system.

In other words, it was assumed that the TlInS$_2$ system is in a liquid state and has an isotropic lattice. In such a lattice, a particular type of atom migrates by jumping from one lattice site to the nearest neighboring site.
Note that the exact configuration of the chemical structural components and individual atoms in TlInS$_2$ in the liquid state is not known. This makes it difficult to assess the degree of accuracy in calculating the atomic diffusion coefficient obtained for small samples and hundredths of ps.

Assume that in the disordered TlInS$_2$ system, the structural components of InS4, as in the TlInS$_2$ crystal lattice, co-exist with homopolar bonds and uncoordinated atoms.

Then the new atomic positions and several equivalent positions that structurally make up InS4 of the TlInS$_2$ compound in the liquid state will be comparable with the coordinates of a crystal with the space group C2/c.

Near the melting point of TlInS2 (1045 K) i.e., when the temperature is close to the transition of the liquid into the solid phase, the TlInS2 microparticles will begin to move more and more orderly. In FP MD-DFT GGA PBE calculations, we used disordered TlInS2 system consisting of 120 atoms: N = 120 (30 Tl, 30 In, and 60 S atoms). FP-MD simulation is performed in the NVT canonical ensemble while keeping constant measure [14, P. 136].

In the NVT ensemble, instead of the total energy, only the kinetic energy of the molecules (temperature) is fixed. The change in kinetic energy is modeled by rescaling the velocities of the atoms of the molecular system at each step:

$$\lambda = \sqrt{1 + \frac{\Delta t}{\tau_1}\left(\frac{T_0}{T\left(t - \frac{\Delta t}{2}\right)} - 1\right)} \quad (9)$$

where λ is the rate recalculation factor, τ_1 is the time constant of the order of 1 ps
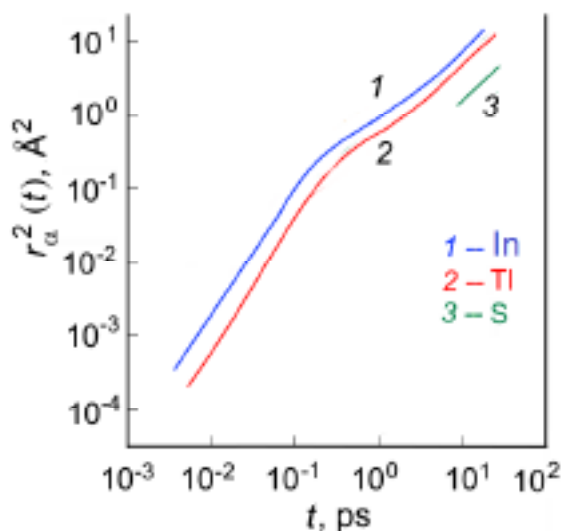
Figure 2: Theoretical Time Dependence of The Root-Mean-Square Displacement of Atoms (or particles α) of the tlins_2 Compound in the Liquid State At t = 1045 k. The Straight Line after the Slope Corresponds to the Diffusion Regime.

The results of calculations of the root-mean-square displacement of atoms (or particles α) of the semiconductor TlInS2 compound in the liquid state are shown in Figure 2.

Time dependence of the diffusion coefficient of atoms in the liquid TlInS_2 compound according to calculations by the FP MD-DFT GGA PBE method is shown in Figure 3.
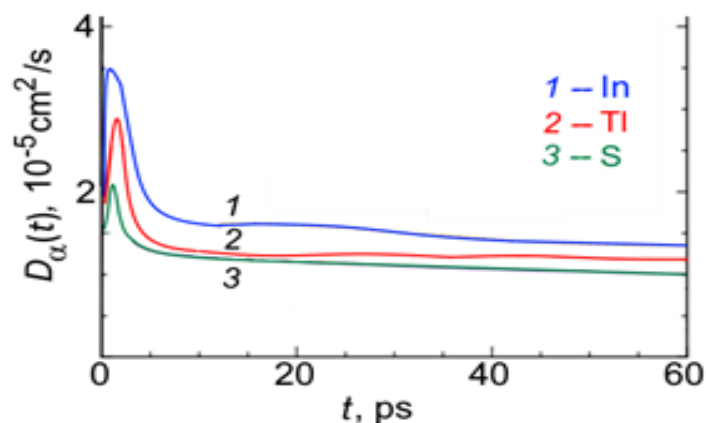
Figure 3: Diffusion coefficients of atoms (or particles α) of the TlInS_2 compound at T = 1045 K calculated by the FP MD-DFT GGA PBE method, taking into account root-mean-square displacements at time t.

The plateau values in fig. 3 are achieved after 4 ps and give the diffusion coefficients of ternary compound TlInS$_2$ atoms in the liquid state on the order of ~ 10^5 cm2/s, which is typical for semiconductors at high temperatures.

Conclusion

Method FP MD-DFT GGA PBE calculated diffusion coefficients atoms, near the melting point of ternary compound TlInS$_2$, for atoms are:

$$D_{Tl}=2.6 *10^{-5} \text{ sm}^2\text{/s}, \ D_{In}=2.5 *10^{-5} \text{ sm}^2\text{/s и } Ds=2.1*10^{-5} \text{ sm}^2\text{/s}.$$

The calculation of the diffusion of atoms of the TlInS2 compound at T = 1045 K FP MD-DFT GGA PBE method provides an adequate description of the properties of the near and medium range. The sensitivity of the calculation of the diffusion of atoms of a disordered system to the GGA PBE functional is moderate.

Conflicts of Interest

The author declares no conflicts of interest regarding of this publication paper.

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