INTRODUCTION

Methods of computer molecular dynamics are the most powerful calculation methods of analyzing the structure and predicting the physicochemical properties of materials [1, 2]. In order to calculate the classical trajectories of individual atoms, the characteristics of dynamic interaction of particles in molecular systems, methods of molecular dynamics enable one to provide the high space–time resolution and obtain the information on the processes taking place at atomic–molecular level for several nanoseconds. The predecessors of the methods of computer molecular design include the methods of quantum and mathematical chemistry, which recently united to the methods of quantum molecular dynamics. In conventional molecular dynamics models, equations of statistical mechanics are used to calculate the trajectory of motion of individual atoms, ions, and fragments of polymer chains. Primary national studies on molecular dynamics were performed at the Institute of Applied Mathematics of USSR Academy of Sciences and Institute of Physical Chemistry of the USSR Academy of Sciences. Results of works by these authors on the development of methods of molecular dynamics were widely used in various institutes of the USSR Academy of Sciences, in particular, the Institute of Physical Chemistry of USSR Academy of Sciences, where the problem of integrating multidimensional systems of Newton and Langevin equations was solved under the supervision of A. G. Grivtsov [1, 2].

The contemporary development of computer facilities enables one to simulate the dynamics of molecular systems composed of the large number of particles (from dozens to hundreds thousands) with the assumption of the large set of parameters and various conditions imitating physicochemical experiment. This allows one to replace expensive long physicochemical experiments with computer imitation modeling. The computer simulation of real chemical and physical systems based on the methods of molecular simulation is a promising direction for the near future [3–8]. Methods of computer simulation in physics, chemistry, and other fields of knowledge require very large calculation resources and have requirements to the characteristics of the computer technologies used.

In this work, algorithms and results of the computer molecular-dynamics simulation of SiC crystal system are given.

BRIEF CHARACTERISTICS OF METHODS OF CONVENTIONAL MOLECULAR DYNAMICS

Success in using the methods of conventional molecular dynamics depends primarily on the use of adequate chemical potentials that describe the interaction of bonds in molecules all possible intra- and intermolecular degrees of freedom. Assuming the corresponding contributions, the value of potential energy can be written as follows [9, 10]:

\[ U = U_{\text{imb}} + U_{\text{ang}} + U_{\text{tors}} + U_{\text{el}} + U_{\text{emp}}, \]  

where \( U_{\text{imb}} \) is the potential of intramolecular bond, \( U_{\text{ang}} \) is potential of angular bond, \( U_{\text{tors}} \) is torsion poten-
tial, $U_q$ is electrostatic potential, and $U_{\text{emp}}$ is empirical part of full potential.

Calculation of the values of coordinates and velocities of atoms in molecular system is performed with the use of calculation scheme of integration of the equations of motion according to the simplest Werle scheme [11]:

$$r(t + \Delta t) = r(t) + \Delta t \cdot v\left(t + \frac{1}{2} \Delta t\right),$$

$$v\left(t + \frac{1}{2} \Delta t\right) = v\left(t - \frac{1}{2} \Delta t\right) + \Delta t \cdot \frac{f_j(t)}{m},$$

where $f_j(t)$ is the force that acts on the $j$ atom and is determined by the following equation:

$$f_j = -\frac{1}{r_{ij}} \frac{\partial}{\partial r_{ij}} U(r_{ij}) r_{ij}.$$  \hspace{0.5cm} (3)

It should be noted that, when using calculation scheme (2) and (3), the trajectories of atoms in molecular system should be generated in the given assembly in accordance with the thermodynamic conditions of the system under study [12]. Furthermore, various algorithms of integration can be used to simulate the evolution and dynamics of the system (from simple atomic to complex molecular at various assemblies and values of physical parameters (NVT, at constant number of particles, volume, and temperature; NPT, constant particle number, pressure, and temperature; and others). Temperature $T$ and particle number $N$ are almost always maintained constant. We can choose the condition of constant volume (NVT) or the condition of constant pressure (NPT) for system. In NVT assembly, volume of system $V$ is definite. In contrast with NVT, NPT assembly enables one to change the volume, acquire its optimal value; therefore, most studies are performed in this assembly.

During the physicochemical experiment, the molecular system under study is exposed to the action of external physical parameters. In order to keep the temperature of the molecular system near the required value, special calculation schemes are used, such as calculation thermostats [9, 13]. In our calculations, the Nose–Hoover calculation thermostat is applicable, which allows one to simultaneously multiply the velocities of all particles on $k$ coefficient, as a result of which the average kinetic energy of the system decreases or increases to the given temperature. In the Nose–Hoover calculation scheme, the assumption of the heat exchange of the system with a heat reservoir is performed such that the equation of motion is modified to the following form:

$$\frac{dr(t)}{dt} = v(t),$$

$$\frac{d\dot{v}(t)}{dt} = \frac{f(t)}{m} - \mu(t) \cdot v(t),$$

where $f(t)$ is the force acting on individual atoms, $m$ is mass of atom, and $\mu(t)$ is friction coefficient.

The Werle method of integration for calculating intramolecular bonds in the simulation of polyatomic molecules with all possible interactions was implemented as the SHAKE algorithm [9, 13]. The SHAKE algorithm is widely used to calculate the characteristics of complex molecular systems and is used almost in all known programs of molecular dynamics (AMBER, GROMOS, X-PLOR, DL_POLY, and others).

The numerical analysis of the displacement of atoms and the estimation of the structures of molecules using the SHAKE algorithm is performed at two stages.

1. Coordinates of atoms are calculated based on the Werle difference scheme assuming the complete absence of bonds. It is natural that new positions of atoms would not retain the bond lengths and the coordinates of atoms should be corrected.

2. The estimation of deviations of bond lengths from exact values (initial values is performed and bond strengths required to retain the atomic-bond lengths in the molecule are calculated [14–17].

In general case, the SHAKE algorithm is an iterative procedure for calculating the atomic displacements and corrections of all possible bond lengths in molecular system. The exactness of the calculation of bond lengths (within $10^{-6}$–$10^{-8}$ Å) depends on the type of molecules and specifics of the study. At intrinsic bond lengths on the order of 1 Å, this precision means the retention of six to eight signs and is required in order to estimate the stability of the calculations. A higher precision of $10^{-8}$ Å is usually used to simulate molecules with large numbers of bonds.

**BRIEF CHARACTERISTICS OF DL_POLY PROGRAM OF MOLECULAR DYNAMICS**

In our studies, we used the multipurpose DL_POLY program (version 2.20) designed by the molecular-simulation group at Daresbury Laboratory (Great Britain) with the support of the Research Council of Engineering and Physical Sciences for the simulation of condensed phases [10].

The DL_POLY program is used to simulate macromolecules of polymers and ionic systems, as well as other molecular systems, including simple atoms and compounds, i.e., Ne, Ar, and Kr; simple nonpolarized ions, i.e., NaCl and KCl; polarized ions and molecules, i.e., MgO and H$_2$O; simple rigid molecules Cl$_2$, SF$_6$; solid molecular ions with charge KNO$_3$ and (NH$_4$)$_2$SO$_4$; polymers with rigid bonds and charge proteins; macromolecules and biological systems; simple metals and alloys Al, Ni, and Cu; and covalent systems C, Si, Ge, and SiC. A simplified block scheme of architecture of DL_POLY program is given in Fig. 1 [10, 12, 13].

The block of input information involves the following files: CONFIG, including cell sizes, key for period-