https://doi.org/10.26160/2474-5901-2021-27-21-23

МАТЕМАТИЧЕСКОЕ МОДЕЛИРОВАНИЕ ФИЗИЧЕСКИХ ПРОЦЕССОВ В КРИСТАЛЛИЧЕСКИХ СТРУКТУРАХ МЕТАЛЛОВ И СПЛАВОВ

Семёнова М.Н., Бебихов Ю.В.

Ключевые слова: математическое моделирование, металл, потенциал взаимодействия, кристаллическая решетка, энергия.

Аннотация. Смоделировано хаотическое движение атомов в двумерной и трехмерной кристаллических решетках. Показано распределение энергии по расчетной ячейке и выход за её пределы. Определено соотношение энергий связи в реальных металлах и расчетной модели, а также определен потенциал взаимодействия, который получился положительным. Построены амплитудно-фазочастотные характеристики, прошедшие проверку на устойчивость.

MATHEMATICAL MODELING OF PHYSICAL PROCESSES IN THE CRYSTAL STRUCTURES OF METALS AND ALLOYS

Semenova M.N., Bebikhov Yu.V.

Keywords: mathematical modeling, metal, interaction potential, crystal lattice, energy.

Abstract. The chaotic motion of atoms in two-dimensional and three-dimensional crystal lattices is modeled. The energy distribution over the computational cell and going beyond its limits is shown. The relationship between the binding energies in real metals and the computational model was determined, and the interaction potential was determined, which turned out to be positive. Amplitude-phase-frequency characteristics are constructed that have passed the stability test.

Using the MatLab software package, the behavior (chaotic movement) of the *N* number of atoms in the crystal lattice was simulated by the molecular dynamics method. Previously, for such purposes, the authors used directly MD modeling programs, for example, the LAMMPS package [1-3]. To implement the calculations, we chose the Verlet high-speed scheme. In general, the formulas are as follows:

$$\begin{cases} \vec{r}(t+\Delta t) = \vec{r}(t) + \vec{v}\Delta t + \vec{a}\Delta t^2/2 \\ \vec{v}(t+\Delta t/2) = \vec{v} + \vec{a}\Delta t/2 \\ \vec{a}(t) = -grad(U(\vec{r}(t)))/2 \\ \vec{v}(t+\Delta t) = \vec{v}(t+\Delta t/2) + \vec{a}\Delta t/2 \end{cases}. \quad (1)$$

Here *U* is the Lennard-Jones potential, which was selected from a variety of other pair potentials, as optimal for the conditions of our problem:

$$U = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right], \quad (2)$$

where σ is the value of the interatomic distance at which $\varphi(\sigma)=0$, ε is the depth of the potential well located at a distance.

The modeling was carried out in two-dimensional (2D) and three-dimensional (3D) spaces, so the gradient in the third formula was taken first in two and then in

three directions. The transformation of the potential *U(r(t))* into *U(x(t), y(t))* and *U(x(t), y(t), z(t))* was carried out according to the formulas:

$$\begin{cases} \vec{r}_{2D} = x\vec{i} + y\vec{j} \\ \vec{r}_{3D} = x\vec{i} + y\vec{j} + z\vec{k} \end{cases}. \quad (3)$$

The initial data were 100 atoms with a crystal lattice (cell) size of 10x10 for 2D modeling and 1000 atoms with a cell size of 10x10x10 for 3D modeling.

In Fig. 1 (a) shows a two-dimensional calculated crystal lattice with parameters *L*x*W*. A typical form of the Lennard-Jones potential is shown in Fig. 1 (b). To speed up the calculations, we will cut off the potential at a distance $r_c=2.5\sigma$. This choice is due to the fact that at this distance the value of the interaction energy is only ≈0.0163 of the depth of the well ε. The parameters ε and σ can be found through the Joule-Thomson coefficient, or by comparing the experimental value of the viscosity coefficient with the value obtained from the formula for the potential energy.

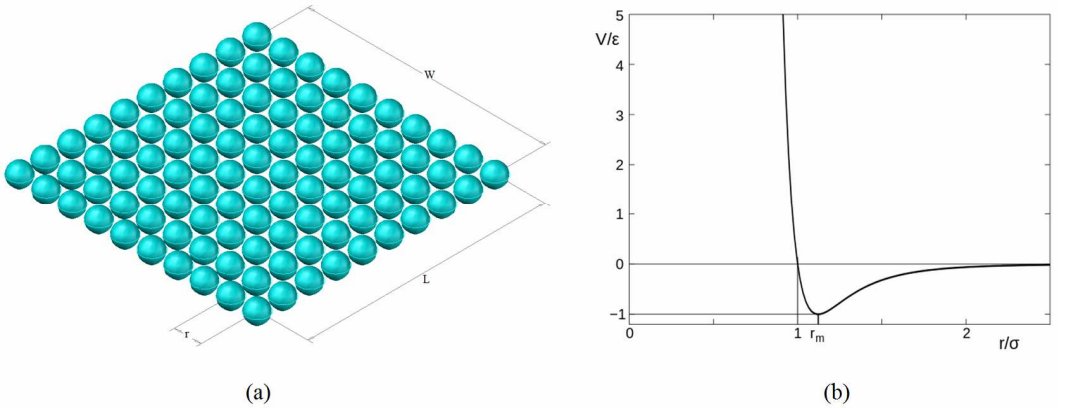

Fig. 1. The structure of the computational cell for modeling (a) and the characteristic form of the Lennard-Jones potential (b)

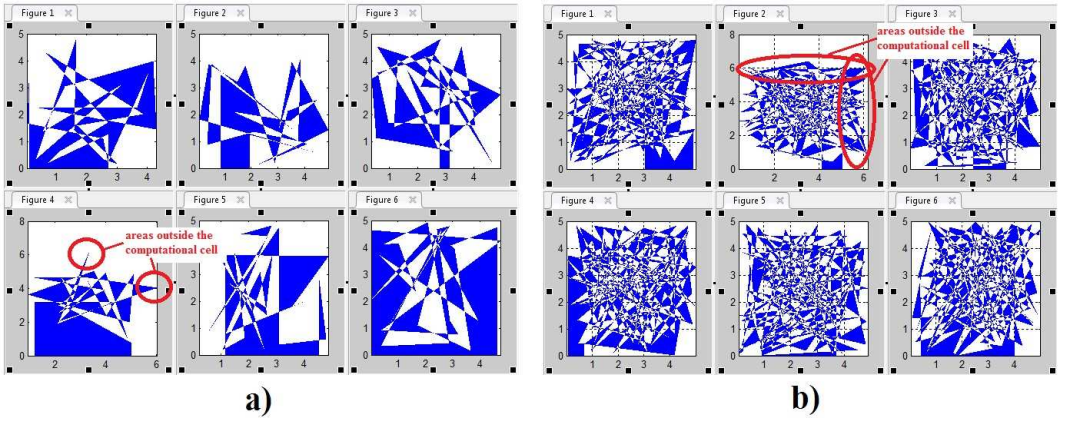

Fig. 2. Atom Migrations Beyond the Computational Cell for 2D (a) and 3D (b) Simulation

The main results of modeling are: obtaining a graphical dependence of the bond energies between the present model and standard data for a metal hcp cell;

obtaining stable amplitude-phase-frequency characteristics; identifying the positive value of the Lennard-Jones potential and calculating its sample mean; identification of isolated cases of atoms leaving the computational cell zone as a result of chaotic displacement (Fig. 2).

Список литературы / References

1. Abdullina D.U., Semenova M.N., Semenov A.S. Korznikova E.A., Dmitriev S.V. Stability of delocalized nonlinear vibrational modes in graphene lattice // European Physical Journal B. 2019. Vol. 92. Is. 11. No. 249.
2. Shepelev I.A., Korznikova E.A., Bachurin D.V., Semenov A.S., Chetverikov A.P., Dmitriev S.V. Supersonic crowdion clusters in 2D Morse lattice // Physics Letters A. 2020. Vol. 384. Is. 1. No. 126032.
3. Krylova K.A., Lobzenko I.P., Semenov A.S., Kudreyko A.A., Dmitriev S.V. Spherically localized discrete breathers in bcc metals V and Nb // Computational Materials Science. 2020. Vol. 180. No. 109695.

Семёнова Мария Николаевна – кандидат физико-математических наук, старший преподаватель, mariya_semyonova86@mail.ru	**Semenova Maria Nikolaevna** – candidate of physical and mathematical sciences, senior lecturer, mariya_semyonova86@mail.ru
Бебихов Юрий Владимирович – кандидат физико-математических наук, доцент, bebikhov.yura@mail.ru	**Bebikhov Yuriy Vladimirovich** – candidate of physical and mathematical sciences, assistant professor, bebikhov.yura@mail.ru
Северо-Восточный федеральный университет им. М.К. Аммосова, Якутск, Россия	Ammosov North-Eastern Federal University, Yakutsk, Russia

Received 07.12.2021