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Effect of surface curvature of an FCC crystal on the characteristics of localized vibrations of atoms

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Abstract. Localized states of discrete structures play an important role in energy transfer and reduction of potential barriers for local structure transformation. In this paper, we consider the influence of the surface curvature of the crystal with cylindrical symmetry on the possibility of excitation of surface localized modes. The study is performed by means of molecular dynamics method. A face-centered cubic crystal of composition A_3B with an $L1_2$ superstructure, where component A is Pt, B is Al is considered. The interaction of particles was described by the interatomic potential obtained by the embedded atom method. We demonstrate the fundamental possibility of the existence of localized modes on the surface under consideration. External oscillations, in turn, can imitate the boundary conditions corresponding to the dynamics of the crystal volume, thereby leading to the consideration of modes located far from the surface. The energy and dynamic characteristics of localized excitations are calculated as functions of the curvature and location of the atom on the crystal surface.

Keywords: localized states, surface, molecular dynamics

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Материалы конференции

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Влияние кривизны поверхности ГЦК кристалла на характеристики локализованных колебаний атомов

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Аннотация. Исследование проводится методом молекулярной динамики. Рассмотрен гранецентрированный кубический кристалл состава A_3B со сверхструктурой $L1_2$, где компонент A – Pt, B – Al. Взаимодействие частиц описывалось межатомным потенциалом, полученным методом внедренного атома. Показана принципиальная возможность существования локализованных мод на рассматриваемой поверхности. Рассчитаны энергетические и динамические характеристики локализованных возбуждений в зависимости от кривизны и положения атома на поверхности кристалла.

Ключевые слова: локализованные состояния, поверхность, молекулярная динамика

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Introduction

Dynamic discrete structures play an important role in a large number of processes in nature and technology. The possibility of supporting localized excitations by such structures expands the prospects for their application [1–5]. Localized states in a discrete system are possible with the manifestation of nonlinearity of connections. In the general case, this leads to the formation of various types of localized modes and states of the structure.

Local excitations of the atomic structure near the surface of crystals can lead to various nonlinear effects that affect the structural and energy transformations of the material at a significant distance from the surface [6–8]. In this case, the properties of localized excitations change depending on the energy relief of the surface. For simple cases, in [9], we considered oscillatory modes near the surface and their characteristics from the standpoint of the concept of discrete breathers [10]. In this case, it should be noted that we are talking about localized modes near inhomogeneities, because a nonlinear localized mode can be called a discrete breather if it exists in a medium with translational symmetry without distortion. The presence of any defects and inhomogeneities does not provide this condition. However, the possibility of energy transfer from the surface into the interior of such a system, shown by us in [9], indicates a direct relationship between these types of oscillations. Due to the high degree of DB localization in this type of crystal, one can speak of discrete breathers already at several interatomic distances from the surface. In addition, in the case of external influences on the crystal, which lead to the excitation of modes, it is possible to create conditions under which these oscillations will correspond to discrete breathers inside the crystal.

External periodic influences can lead to the manifestation of the effect of supratransmission. Which consists in the transfer of energy at frequencies outside the spectrum of the system [11, 12]. We have shown the possibility of manifestation of this effect in this crystal [13]. Noteworthy is the role of discrete breathers in the formation of conditions for energy transport through the crystal. They are a kind of accumulators that accumulate vibrational energy and ensure its further transmission.

In this work, high-amplitude vibrations of atoms on the surface of a crystal of cylindrical symmetry of various curvatures are studied by the method of atomistic simulation.



Materials and Methods

The model was an A_3B lattice with an $L1_2$ superstructure in the form of a cylinder of various diameters. Depending on the plane and diameter of the cylinder, the configuration of the crystal surface, including the energy relief, changed, which affected the conditions for the formation of the considered vibrational modes.

Cylinder-shaped models of Pt_3Al crystals have been created. The crystal lattice parameter $a = 3.876 \text{ \AA}$ was taken as the unit for measuring the dimensions of the models. So the height of the cylinders is $15a$, the radii vary from $1a$ to $10a$ in increments of $0.5a$. The number of atoms in the models varies from 195 to 18825. It is easy to see that the surface structure is repeated for cylinders with radii of 1, 3, 4, 5, 6, 7, 8, 9, 10. The axes correspond to the following crystallographic directions: $X - \langle 100 \rangle$, $Y - \langle 010 \rangle$, $Z - \langle 001 \rangle$. To simulate the interatomic interaction, the potential obtained by the embedded atom method (EAM) was used. Let us consider in more detail the process of constructing the EAM potential by the method proposed in [14]. The total energy E of the crystal can be expressed as

$$E = \frac{1}{2} \sum_{i,j,i \neq j} \varphi_{ij}(r_{ij}) + \sum_i F_i(\rho_i), \quad (1)$$

where φ_{ij} represents the pair energy between atoms i and j separated from each other by a distance r_{ij} , and F_i is the nesting energy associated with nested atom i at a local location with electron density ρ_i . For an alloy, the EAM potential contains not only the three functions φ , ρ , and F for each of the constituent elements, but also the pair energy φ_{ab} between different elements a and b ($a \neq b$). As a result, the functions φ , ρ , and F adapted for elemental metals cannot be directly applied to alloy or multilayer systems. However, by normalizing the EAM potentials and introducing an alloy model, a procedure for generalizing the EAM potentials and their cutoff distances was proposed by Zhou [15].

The technique for studying vibrations of surface atoms consisted in the initial analysis of possible configurations of atoms on the surface. Next, the atoms of the light sublattice, Al, were chosen, because namely, they can be carriers of localized modes in the bulk of the crystal. After that, such atoms were removed from the equilibrium position and their dynamic parameters were calculated as a function of time. The cylinder model was previously minimized in energy at zero Kelvin. The entire modeling process was carried out in the LAMMPS environment [16]. Visualization was performed using OVITO [17].

Results and Discussion

Initially, the state of the model as a whole was analyzed. This is how the potential energy per atom was calculated for models with different radii. The corresponding dependence is shown in graph in Fig. 1, *a* for both components of the alloy, and the distribution of potential energy in the cylinder section is also shown. This makes it possible to estimate the contribution of the free surface to the specific binding energy for each type of crystal atoms and to take this into account in the presence of differences in vibrations for different vibrational modes.

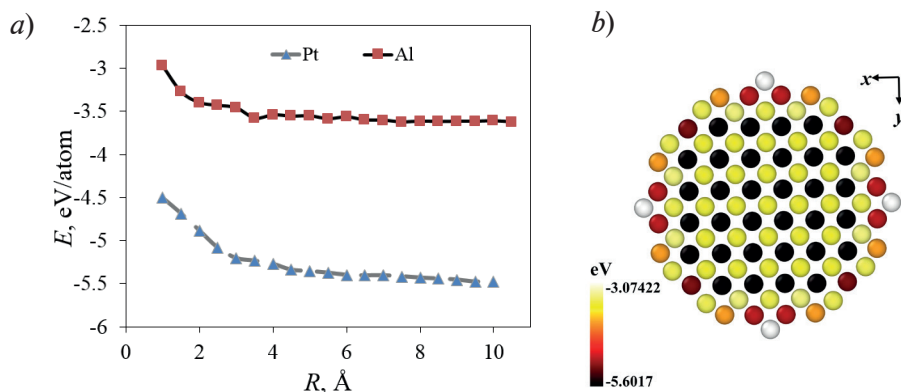


Fig. 1. Energy parameters of the model: potential energy per atom vs the radius of the cylinder model (*a*), visualization of the potential energy distribution on the example of a model with a radius of 4 lattice constants (*b*)

Next, we consider the dependence of the energy of the most loosely bound Al atom on the distance from the crystal surface (Fig. 2). The atom (indicated by the number I in Fig. 3) was removed at a distance S from the perpendicular surface, and the binding energy was calculated. The figure shows two results for the minimum cylinder size and for a cylinder with a radius of $5a$. The difference is not significant, which may indicate that the curvature of the surface does not play a significant role when considering single atoms. However, the shape of the curve indicates possible features of oscillations for different initial amplitudes.

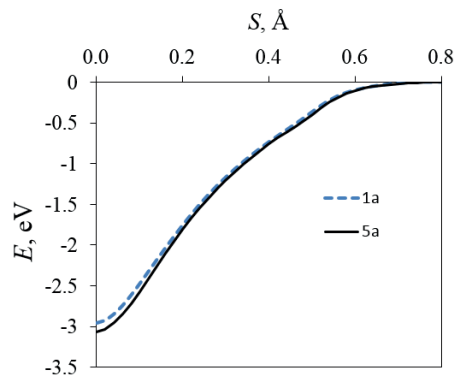


Fig. 2. Dependence of the binding energy of the Al atom on the distance S as it moves away from the surface of the cylinder for two cases: radius $1a$ and $5a$

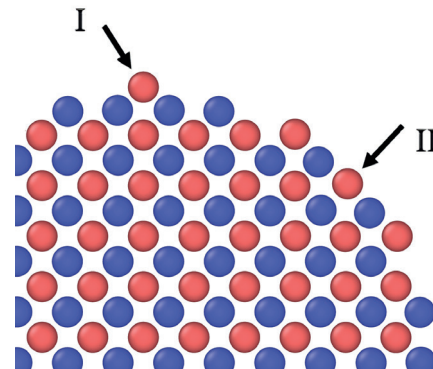


Fig. 3. Atoms whose modes were studied in the work

Two Al atoms were considered, shown on the cut of the cylinder in Fig. 3. In Fig. 3 shows the characteristic position of such atoms, however, all variants of the cylinder diameter indicated in the model description section were considered. For models with a small radius, i.e. the first two points on the graph in Fig. 1, a for the Al atom, there were no stable oscillations. A significant gradient in energy led to the fact that the oscillatory system was not stable, and the slightest imbalance in the system led to the destruction of the oscillations. With an increase in the size of the model, the oscillations showed greater stability and the radius of curvature did not have a significant effect on the duration of the oscillations. In the case of consideration of vibrations of atom I, they remained stable in the range of amplitudes $0.2\text{--}0.55\text{ Å}$. The upper limit corresponds to the inflection of the function on the graph of Fig. 2. In this case, the oscillations are harmonic in nature, and their modulation was also observed, depending on the initial amplitude of the deviation of the atoms (Fig. 4). In fact, modulation indicates a displacement of the center of oscillation relative to the surface and does not affect the amplitude or frequencies. In this case, it makes sense to talk about complex oscillations of the system.

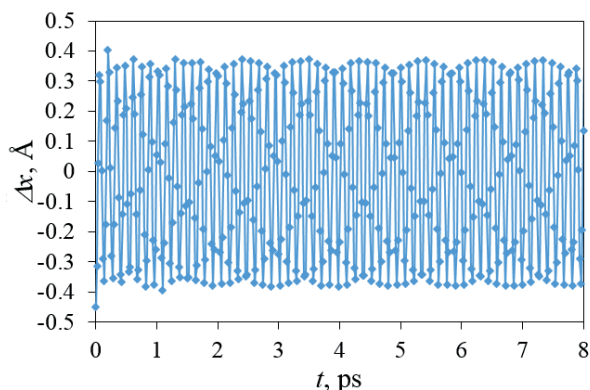


Fig. 4. Time dependence of the atomic coordinate, with an initial deviation of 0.45 Å , for a cylindrical surface with a radius of $6a$

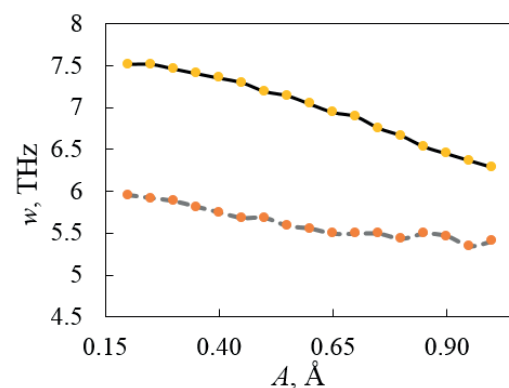


Fig. 5. The dependence of the frequency on the amplitude for the considered configurations of atoms on the surface



One of the main characteristics of discrete breathers is the type of amplitude-frequency dependence. In the bulk part of the crystal, we observe a soft type of nonlinearity, i.e. with decreasing frequency with increasing amplitude.

Similar behavior is observed in Fig. 5 for both variants of atomic position on the surface. Surface effects, in turn, have an influence, and the frequency in this case lies in the range characteristic of the acoustic branch of the phonon spectrum of the crystal.

The obtained results qualitatively correlate with [9] where it was shown that differences of the lattice in the bulk part and on the edge of the crystal result in considerable shift of amplitude-frequency characteristics of discrete breathers. A stronger decrease of the $A(\omega)$ dependence in Fig. 5 can be attributed to the higher curvature in the vicinity of the atom location where the bond length can be higher. This fact of the dependence of nonlinear localization properties on its location with respect to the crystal surface is an important issue, since in most real crystals there are a large number of surface defects, such as grain boundaries [18], where the characteristics of discrete breathers are also likely to be different from those in an ideal lattice. It can also be noted that in such cases the implementation of highly symmetrical breathers can be difficult due to the variable lattice parameter [19] and can reveal some properties of breathers in 2D structures [19–21]. In the future, it is planned to study the dynamics of the modulation instability of delocalized modes [22–25] in such crystals in order to understand the effect of the presence of a surface on the formation of discrete breathers because of the decay of delocalized nonlinear modes.

Conclusion

Various surface configurations and directions of displacement of atoms from the equilibrium position are considered by means of computer experiments. The influence of the potential relief on the possibility of stable localized excitations is analyzed. It is shown that for small radii of the considered cylindrical surfaces, stable excitations do not occur: localized oscillations are rapidly destroyed. The obtained numerical results within the framework of the considered model of interatomic interaction show the possibility of sufficiently long oscillations on the surface of the model, the curvature of which has more than four lattice parameters. The study contributes to fundamental understanding of the behavior of discrete breathers in the vicinity of the surface crystal, having a potential effect on the macroscopic characteristics of the considered material [26].

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