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Dynamics of Discrete Breathers in the Pt_3Al Crystal

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Abstract. By method of molecular dynamics discrete breathers with soft and hard types of non-linearity in the Pt_3Al crystal are studied. Obtained graphs characterize the spatial localization of the discrete breathers, the dependence of the frequency on the oscillation amplitude and the amount of energy localized on the discrete breathers. It is shown that the collision of moving discrete breathers may lead to the energy exchange between the breathers with some portion of the energy given to the Pt_3Al lattice. The probability of excitation of discrete breathers in thermodynamic equilibrium is estimated.

Introduction

In this study, we consider discrete breathers (DB) in a bulk Pt_3Al crystal. DB is a nonlinear localized large-amplitude vibrational mode in a defect-free nonlinear discrete system [1]. However, in real crystals we should speak of quasi-breathers with a finite lifetime and non-strict periodicity of the oscillations in time [2]. Further, quasi-breathers will be called DB for brevity.

The possibility of localization of energy in the defect-free discrete ordered structures, which for the first time was predicted by the authors of [1], was confirmed experimentally. Discrete breathers have been found in the various physical systems [3-5].

DB can be divided into two types according to their dependence of frequency on the amplitude. For the discrete breathers of soft type (hereinafter DB1), the frequency decreases with increasing amplitude. DB1 can only exist in crystals with a gap in the phonon spectrum. Their frequency lies in the gap of the phonon spectrum and therefore they are called gap DB. For the discrete breathers of hard type (DB2) the relationship between amplitude and frequency isinverse. They can have frequencies in the gap or above the phonon spectrum. DB1 can be excited in the biatomic crystals, for example, NaCl [6-8], Pt_3Al [9-13], and also in the graphene and grafane [14-16]. DB2 exist in pure metals with fcc, bcc and hcp structure. Studies related to the DB, recently reached a higher level. The results of numerous recent studies suggest that the DB exist in virtually all crystals [6-17]. There is every reason to believe that the DB will be used to explain various physical phenomena in crystals.

The aim of this work is to study the dynamics of discrete breathers with soft and hard types of non-linearity in the Pt_3Al crystal, and their probabilities of excitation in the state of thermodynamic equilibrium.

The model and the experimental method

The model is a bulk crystal Pt_3Al with the superstructure $L1_2$ based on an fcc lattice, size $112.85 \times 97.73 \times 41.47$ Å, containing 28800 atoms. On thecellmodelwere imposedperiodic boundary conditions. Atoms interactvialong-rangepair potentialMorse:

$$\phi_{PQ}\left(r_{ij}\right) = D_{PQ}\beta_{PQ}\exp\left(-\alpha_{PQ}r_{ij}\right)\left(\beta_{PQ}\exp\left(-\alpha_{PQ}r_{ij}\right)-2\right), \quad (1)$$

where D - energy parameter corresponding to the depth of the potential well, α – parameter determining the stiffness of interatomic bonds, r_o – a certain average equilibrium distance for the

coordination spheres, which take into account the interaction between the atoms. For alloy Pt_3Al its parameters are taken from [17]: $D_{AlAl} = 0.318$ eV, $\beta_{AlAl} = 27.4979$, $\alpha_{AlAl} = 1.02658$ Å^{-1}, $D_{PtPt} = 0.710$ eV, $\beta_{PtPt} = 102.89$, $\alpha_{PtPt} = 1.582$ Å^{-1}, $D_{PtAl} = 0.5048$ eV, $\beta_{PtAl} = 63.124$, $\alpha_{PtAl} = 1.3501$ Å^{-1}, calculated by standard methods [17] of the conditions:

$$\frac{1}{2}\sum_{i=1}^{z}\eta_i\varphi_{V=V_0} = E_S,\ \frac{1}{2}\sum_{i=1}^{z}\eta_i\left(\frac{\partial\varphi}{\partial V}\right)_{V=V_0} = 0,\ -V_0\cdot\left(\frac{\partial P_S}{\partial V}\right) = K_0. \quad (2)$$

here E_S - the sublimation energy of the crystal atoms at zero Kelvin K_0 - the bulk modulus. Mass of the atoms of platinum and aluminum, as well $m_{Pt} = 195.23$, $m_{Al} = 26.97$ g/mol; lattice constant: $a_0 = 3.99$ Å.

In this paper, DB1 was excited at the center of the crystal by displacing Al atoms along the <100> direction by 0.72 Å, i.e., does not give the exact profile of discrete breathers. DB1 in the Pt_3Alcrystal lacks mobility and can not move through the crystal. In more detail the conditions of excitation of DB1 were considered in [11-13].

Excitation of DB2 is possible along the close-packed directions <110>, $<0\bar{1}1>$, $<\bar{1}01>$, $<\bar{1}10>$.In vibrations DB2 attended by several atoms of light sublattice. DB2 can move through the crystal over long distances, almost without dissipating its energy.To excite the mobile DB2 deviated from the equilibrium position two Al atoms on the value of 0.9 and 0.85 Å in opposite directions along one of the possible directions, for example, $<\bar{1}10>$. Result of the transient processes is the energy redistributed to the 4 atoms of Al. Vibrations occur with a frequency above the phonon spectrum of the crystal. DB2 has obtained some initial momenta in the direction of an atom with a smaller initial deviation.

Characteristics of discrete breathers and their interaction

The most important parameters of DB1 and DB2 may include the time of their life in the crystal, the amount of energy they can localize, spatial localization, as well as the dependence of the frequency of the oscillation amplitude. Consider these characteristics in more detail for the objects of study in the crystal Pt_3Al.

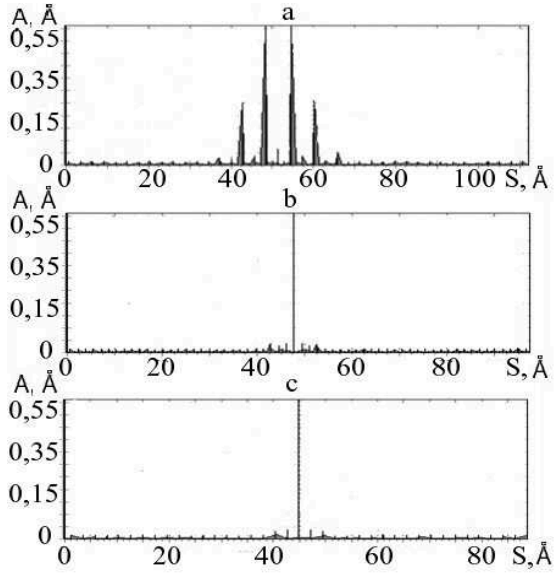

Fig.1. Oscillationamplitudesof atoms in the vicinity of discrete breather with a hard type of nonlinearity: a) projection on the (111) plane, b) on the $(\bar{1}10)$ plane, c) on the $(11\bar{3})$ plane. Along the abscissa the distance along certain direction is shown in Angstroms.

The factor of spatial localization plays a significant role in the study of the stability of discrete breathers to various kinds of impacts. For example, an increase in temperature significantly reduces the lifetime of the DB. It was found that DB1 is localized practically on one Al atom (this atom holds up to 85% of the total energy of discrete breathers), while neighboring atoms vibrate with much smaller amplitudes. This leads to immobility of DB1 and its robustness, e.g., it survives the collision with DB2.

In turn, DB2 is localized mainly on four Al atoms and it is extended along the close-packed atomic row of the crystal. The atoms oscillate along this atomic row. DB2 is less stable because its degree of spatial localization is smaller than that of DB1.

Discrete breathers are able to localize significant energy. This energy can trigger the structural transformations occurring in the crystal. In addition, DB2 can move through the crystal over hundreds of nanometers, transporting energy. Fig 2 shows the discrete breather energy as the function of time for (a) DB2 and (b) DB1. During the whole period of life DB slowly radiate energy. DB cannot exist if its energy is smaller a threshold value. The minimal energy for DB1 is 0.8eV, while for DB2 it is 1.8 eV. The maximal DB energy observed in our simulations is 1.0 eV for DB1 and 2.7 eV for DB2. When DB disappears, certain amount of energy is released and this energy can lead to activation of various processes, such as movement of dislocations.

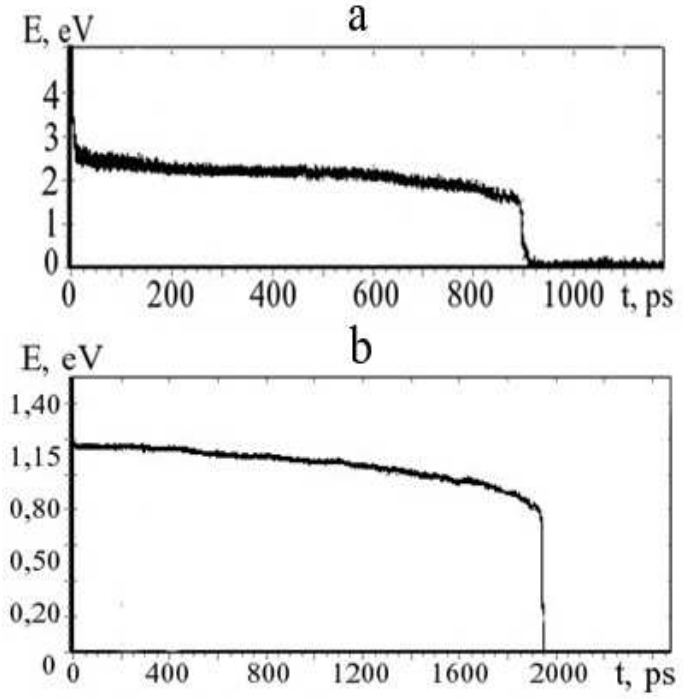

Fig. 2.The dependence of the discrete breather energy on time,
a) for DB2, b) for DB1.

As already noted, DB1 may exist in the gap of the phonon spectrum of the crystal, and DB2 - discrete breathers with a hard type of nonlinearity, in this case there above the phonon spectrum of the crystal. Analyzing the dynamics of DB1 and DB2 are obtained depending on the amplitude of the oscillation frequencies shown in Fig. 3.

Turning to the issue of interaction of discrete breathers in the three-dimensional crystal Pt_3Al, we note that the process is complicated because of the large number of atoms to oscillate. In the theory of solitons discrete breathers in the collision of elastic repel each other, but as in this work, in fact, considered quasi-breathers. Absolutely elastic interactions are absent.

Consider the interaction between of two DB2, moving towards each other along one direction. On their first encounter of DB2 there occursthe elastic repulsion from each other. In the collision partly scattering of their energy in the sublattice Al takes place. Second encounter DB leads to the destruction of one of them. In this process not only the reduction of the oscillation amplitude DB2 plays a role, but also heating Al sublattice in the process of their movement through the crystal.

For collision of two or more DB2 it is important their mutual configuration. If breathers moving along different crystal directions, reach the rendezvous point simultaneously, as in the case of movement in one direction, of their mutual repulsion occurs with loss of energy, but the second collision in this case is not possible due to their different atomic rows motion along. If one of the breathers reaches the point of the meeting DB2 earlier, the collision leads to its destruction and the second DB2 changes its direction of movement to the opposite.

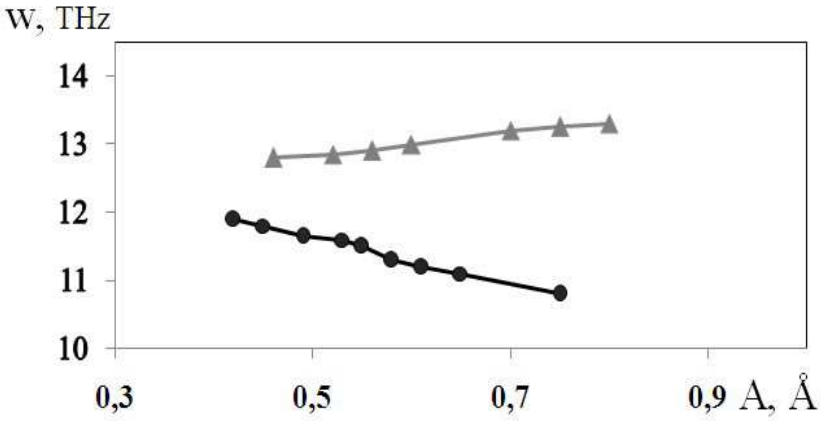

Fig. 3.The dependence of the frequency on the oscillation amplitude for DB1 (circles) and DB2 (triangles)

Considering the collision DB2 DB1 note the greater stability of DB1 polarized along the <100> direction. As a result of the collision, amplitude decreased from DB2 0.6 Å to 0.55 Å. Repeated collisions do not lead to a significant loss in the same DB2 energy, but its lifetime did not exceed 350 ps. DB1 almost don't lose its energy by collisions and could exist during 2000 - 2500 ps.

Estimating the probability of excitationof discrete breathers

In the experimental work [9] to study the phonon spectra of NaI, authors obtained the peak in the band gap of the phonon spectrum of the crystal in thermodynamic equilibrium at a temperature of 555 K. These results were interpreted as the possible presence in the gap of phonon spectra of the crystal discrete breathers.

Let us estimate probability of excitation of the DB1 and DB2 in the crystal Pt_3Al. As it is known, the probability for atoms and molecules to stock large energy is negligible. This requires a large number of consecutive collisions, as a result of which the atom is gaining energy, almost losing it. Therefore, for many processes only a tiny fraction of the atoms have enough energy to overcome the barrier. This proportion, in accordance with the Arrhenius theory, in this case can be determined by the following formula:

$$D = e^{\frac{-E_a}{kT}} \quad (3)$$

where k - Boltzmann constant and T - temperature of the crystal, E_a the activation energy of the process. From the formula the share of active collision D depends very much from the energy of activation and the temperature

For DB1 E_a is of the order 0.8 eV. Based on this value of D at a temperature of 1000 K the crystal was of the order of 10^{-5}, which means that up to 0.001% of the atoms of the crystal model at the temperature of 1000 K can be carriers of DB1. In turn, DB2 has a higher activation energy than DB1.

The minimum energy at which DB2 can stably exist equals to 1.8eV. In this case, the probability of excitation of DB2 in thermal equilibrium at a temperature of 1000 K is about 10^{-9}. The values obtained indicate that the probability of excitation of DB2 in thermodynamic equilibrium is rather small and spontaneous excitation of DB2 is hardly possible. However, such DB can be readily formed in various non-equilibrium processes.

Summary

By the method of molecular dynamics, discrete breathers with soft (DB1) and hard (DB2) types of nonlinearity were studied in the Pt_3Al crystal. The possibility of motion of the DB2 over hundreds of nanometers in the directions <110>, $<0\bar{1}1>$, $<\bar{1}01>$, $<\bar{1}10>$ was demonstrated.

The characteristics of discrete breathers, such as their lifetime, the amount of energy they can localize, degree of spatial localization, as well as dependence of the oscillation frequency on the amplitude were obtained. The estimation of the concentration of discrete breathers in the crystal in the state of thermodynamic equilibrium was made. The interaction of discrete breathers with each other was studied.

These results indicate that DB2 can effectively transport the energy through the crystal, and DB collision leads to even greater energy localization in the crystal. The possibility of the energy transfer through the crystal over long distances can lead to structural transformation away from the point of their excitation.

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