

DYNAMICS OF DISCRETE BREATHERS IN A Pt₃Al CRYSTAL**M. D. Starostenkov,² A. I. Potekaev,^{1,5} S. V. Dmitriev,^{3,4}
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UDC 538.913

The discrete breathers in a Pt₃Al crystal, which exhibit soft (DB1) and hard (DB2) nonlinearity, are shown to possess a number of principal differences. Unlike an immobile and stable DB1, a DB2 breather is mainly localized on four Al atoms and is stretched along one of the close-packed rows of crystals. On the other hand, DB2 can displace hundreds of nanometers along one of the directions of close packing. Having localized a considerable amount of energy, both DB1 and DB2 breathers slowly emit it during their lifetime. A collision of DB1 and DB2 results in part of their energy being released into the Al sublattice, the larger part lost by DB2 that is destroyed faster than DB1. The DB2 breather can effectively transport the energy throughout the crystal, and a collision of DBs results in its considerable localization in the crystal. A capability of transferring the energy can thus give rise to structural transformations far from the focus of excitation of such localized objects.

Keywords: discrete breather, energy localization, nonlinear dynamics, method of molecular dynamics.

INTRODUCTION

A good deal of attention has recently been given to investigations of a nonlinear object – a discrete breather representing a large-amplitude sustained oscillation localized in space in a defect-free discrete system [1]. In the case of crystals, we have to term them quasi-breathers having finite lifetimes and relaxed periodicity of oscillations in time [2]. The number of hypotheses on participation of DBs in different processes in solids has been increasing. It is believed that DBs can improve the catalytic properties of nanoparticles having disordered structure, give rise to radiation-stimulated pore growth in metals, contribute to the diffusion, transport the electric charge, result in the annealing of defects, lower the energy barriers of chemical reactions in crystalline solids, etc.

Discrete breathers have a long lifetime because their frequency lies outside the phonon spectrum of a crystal. They can be classified into two types by the character of their frequency dependence on the amplitude [3]. The frequency of DB1 decreases with increasing amplitude, hence, they can persist in the crystals with the energy gap in the phonon spectrum only, their frequency falling within this gap. The frequency of DB2 increases with the amplitude; their frequencies can both be found both within the energy gap (in case there is one) and above the phonon frequencies. Discrete breathers can be excited in biatomic crystals [4, 5] and in graphenes and graphanes [6]. Discrete breathers 2 persist in single-atom systems and pure metals [7–9].

The purpose of this work is to study the dynamics of DBs possessing mild and hard nonlinearity in the crystal of a Pt₃Al intermetallic compound and to estimate the possibility of their excitation in a state of thermodynamic equilibrium.

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THE MODEL AND EXPERIMENTAL PROCEDURE

As a model we selected a bulk aluminum FCC-alloy, Pt₃Al, with the L1₂ superstructure. The computational grid measures 225.71×29.32×20.73 Å and contains 14500 atoms. Axis *X* of the model corresponds to the crystallographic direction $\langle \bar{1}10 \rangle$, axis *Y* – $\langle 111 \rangle$, and axis *Z* – $\langle \bar{1}1\bar{3} \rangle$. Use was made of the periodic boundary conditions. Interatomic interaction is prescribed by the Morse potential as follows:

$$\phi(r_{ij}) = D\beta \exp(-\alpha r_{ij}) (\beta \exp(-\alpha r_{ij}) - 2),$$

where *D*, β and α are the parameters of the potential, r_{ij} is the spacing between atoms *i* and *j*.

Parameters *D*, β and α were determined from the following conditions:

$$\frac{1}{2} \sum_{i=1}^z \eta_i \phi_{V=V_0} = E_S, \quad \frac{1}{2} \sum_{i=1}^z \eta_i \left(\frac{\partial \phi}{\partial V} \right)_{V=V_0} = 0, \quad -V_0 \left(\frac{\partial P_s}{\partial V} \right) = K_0,$$

where E_S is the sublimation energy of the crystal atoms, K_0 is the bulk modulus of elasticity, P_s is the pressure induced by isentropic compression, V_0 and V are the relative volumes in the initial and deformed state, respectively, and η_i is the number of atoms in the *i*-th coordination sphere.

One can excite DB in a crystal by setting certain displacements or initial velocities in a group of *n* atoms. In this case, we are going to excite DB1 in the crystal center via deviating an Al atom along the $\langle 100 \rangle$ direction by 0.72 Å, i.e., without prescribing the exact DB profile. An excitation of DB2 is possible along the following directions:

$\langle 110 \rangle$, $\langle \bar{0}11 \rangle$, $\langle \bar{1}01 \rangle$, and $\langle \bar{1}10 \rangle$. In the model selected, a number of atoms of the “light sublattice” take part in the oscillations of DB2. In this case, DB2 can displace throughout the crystal by considerable distances, practically without dissipating any energy. In order to excite a mobile DB2, let us deviate two Al atoms from their equilibrium positions by 0.9 and 0.85 Å in the opposite directions along that of close packing.

RESULTS AND DISCUSSION

The Morse potential parameters for the model Pt₃Al alloy were taken elsewhere [10–12]:

$$D_{\text{AlAl}} = 0.318 \text{ eV}, \quad \beta_{\text{AlAl}} = 27.4979, \quad \alpha_{\text{AlAl}} = 1.02658 \text{ \AA}^{-1},$$

$$D_{\text{PtPt}} = 0.710 \text{ eV}, \quad \beta_{\text{PtPt}} = 102.89, \quad \alpha_{\text{PtPt}} = 1.582 \text{ \AA}^{-1},$$

$$D_{\text{PtAl}} = 0.5048 \text{ eV}, \quad \beta_{\text{PtAl}} = 63.124, \quad \alpha_{\text{PtAl}} = 1.3501 \text{ \AA}^{-1}.$$

It was assumed that the masses of platinum and aluminum were equal to $m_{\text{Pt}} = 195.23$ a.m.u. and $m_{\text{Al}} = 26.97$ a.m.u., respectively, and the lattice constant was $a_0 = 3.99$ Å.

Let us consider the characteristics of discrete breathers and their interaction. Among the most important characteristics of DB 1 and DB2 are the following: their lifetime in a crystal, value of their localized energy, degree of spatial localization, and frequency dependence on oscillation amplitude.

As far as the degree of DB localization is concerned, it was established that the nearest neighbors of the Al atom possess much lower oscillation amplitudes and hence energy. This suggests that the energy in DB1 is nearly completely localized on a single Al atom (85 % of the total DB energy). This makes DB1 immobility and highly resistant to perturbations. The situation is different in the case of DB2. Because of the transition process, the energy is redistributed over 4 Al atoms of the close-packed direction. The oscillation frequency is now 13.8 THz, i.e., it is above

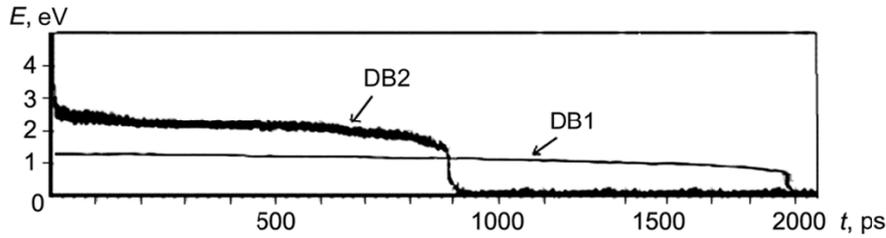


Fig. 1. Energy of discrete breathers versus their lifetime.

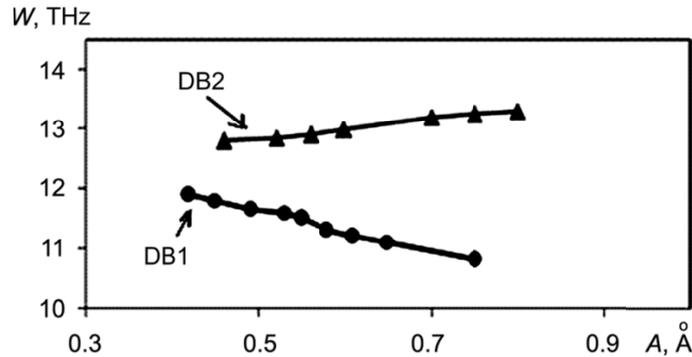


Fig. 2. Frequency of DB1 and DB2 versus their oscillation amplitudes.

the phonon spectrum of the crystal. It should be noted that the atoms oscillate about the close-packed row in which a DB2 has been excited. The resulting DB2 possesses a certain initial momentum towards an atom with the lowest initial deviation. Being mobile, this DB2 is less stable compared to a DB1 due to its lower localization.

Thus, unlike the immobile and stable DB1, the DB 2 discrete breather is mainly localized on four Al atoms and stretched along one of the close-packed crystal rows.

It is well known that discrete breathers can localize a considerable amount of energy. Figure 1 shows the DB1 and DB2 energy versus time. It is evident that the breathers slowly radiate their energy during their lifetime. Recall that the lifetime of DB1 is twice longer than that of DB2, while the energy of the latter is nearly twice higher than of the former. The temporal dependence depicted reveals that with time the DB energy reaches a certain minimum value and then rapidly dissipates, resulting in the destruction of this DB. Note that the threshold values of the energy for DB1 and DB2 are ~ 0.8 and ~ 1.8 eV, respectively. We might expect that a release of this energy into the lattice would activate a variety of processes, e.g., dislocation motion.

It should be noted that the frequency of DB1 with a mild type of nonlinearity falls within the phonon spectrum of a crystal, while that of DB2 lies above this spectrum. Shown in Fig. 2 are the plots of dependence of the oscillation frequencies of DB1 and DB2 on their amplitudes.

Let us now deal with the interaction of discrete breathers. Since we focus on quasi-breathers, there are no elastic interactions between DBs.

Assume that two mirror-symmetrical DB2s are moving towards each other along the $\langle 110 \rangle$ direction. Figure 3 depicts their interaction dynamics 4 (a), 8 (b) 10 (c), and 16 ps (d) after the beginning of the experiment. On the axis of abscissas, we have their position along the $\langle 110 \rangle$ direction, and on the axis of ordinates – the amplitude of atomic vibrations.

It is clear from Fig. 3 that in the initial stage the interaction of discrete breathers is elastic. Further interaction is accompanied by the energy dissipation by transferring a part of their energy to the Al sublattice atoms. This becomes evident from a sequential comparison of the maxima in Fig. 3, where the maximum values in the sequence do not exceed 0.60, 0.55, 0.50 and 0.45. Whenever the oscillation amplitudes prior to a collision were ~ 0.6 Å, then afterwards

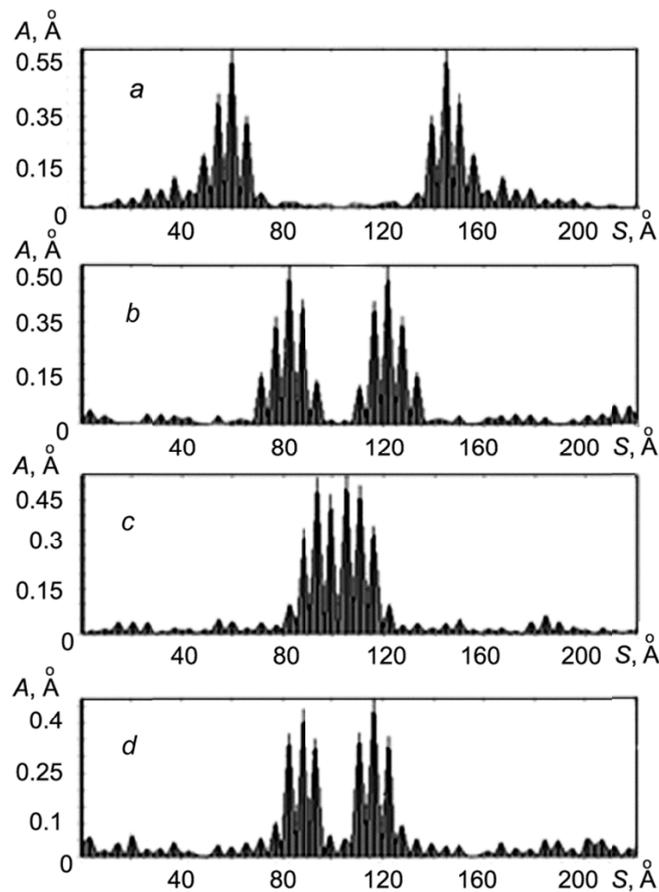


Fig. 3. Collision of two DB2s along the $\langle 110 \rangle$ direction: DB2 formation 4 ps after the beginning of the experiment (a), their approach 8 ps after (b), collision 10 ps after (c), and separation after collision in 16 ps (d).

they were $\sim 0.45 \text{ \AA}$. A repeated collision of DBs results in the destruction of one of them. This is likely to be associated with the use of periodic boundary conditions. Thus, in addition to a decrease in the DB2 oscillation amplitude (energy dissipation) during interaction of two mirror-symmetrical DB2s, a certain role is played by the ‘heating’ of the Al sublattice in the course of DB motion throughout the crystal and continuous energy dissipation.

When considering a collision between DB1 and DB2, let us note the stability of DB1, whose atomic vibrations are polarized along the $\langle 100 \rangle$ direction. As a result of this collision, the oscillation amplitude in DB2 is reduced from 0.60 to 0.55 \AA . This suggests a considerable energy loss by the breather. Repeated collisions do not result in such a marked decrease in the oscillation amplitude and, hence, the energy losses by DB2. As this goes on, the lifetime of DB2 is as low as 350 ps, while DB1 does not virtually lose any of its energy as a result of collision and can persist for 2000–2500 ps.

Let us estimate the probability of exciting discrete breathers DB1 and DB2. According to the Arrhenius theory, the fraction of atoms capable of overcoming the energy barrier of the process is equal to

$$D = e^{\frac{-E_a}{kT}},$$

where k is the Boltzmann constant, T is the crystal temperature, and E_a is the activation energy of the process. For DB1, the value of E_a falls within the range 0.8–1.0 eV. An estimation of the percentage of atoms, capable of overcoming the energy barrier at the temperature 1000 K, demonstrates that up to 0.01% atoms could be carriers of DB1s. A DB2

breather requires higher activation energy than does DB1. The minimum energy, at which DB2 could stably exist, is found to be ~ 1.8 eV. In this case, the probability of exciting a DB2 in the state of thermodynamic equilibrium at the temperature 600 K would be $7.6 \cdot 10^{-19}$. This implies that the probability of exciting a DB2 in the state of thermodynamic equilibrium is extremely low; hence, a spontaneous excitation of a DB2 without an external action on the crystal is impossible.

SUMMARY

An investigation of discrete breathers with mild (DB1) and hard (DB2) nonlinearity in a Pt₃Al crystal has demonstrated a number of principal differences. In DB1, the energy is nearly completely localized on a single Al atom (up to 85 % of the total DB energy). This results in immobility of DB1 and its stability towards external disturbances. This is not the case with DB2. As a result of a transition process, the energy is redistributed over four Al atoms in the close-packed direction. Possessing higher mobility, DB2 is less stable than DB1, due to its lower localization. Thus, unlike an immobile and stable DB1 localized on one atom, a DB2 breather is mainly localized on four atoms of aluminum and stretched along one of the close-packed rows of the crystal. On the other hand, DB2 can displace by hundreds of nanometers along close-packed directions.

Having localized a considerable amount of energy, DB1 and DB2 slowly dissipate it. It has been noted that the lifetime of DB1 is twice as long as that of DB2, while the energy of the latter is twice that of the former. A temporal dependence of the energy reveals that in the course of time the DB energy reaches a certain minimum value and then dissipates rapidly, resulting in DB annihilation. A collision of DB1 and DB2 causes part of their energy to be emitted into the Al sublattice, with DB2, which annihilates faster than DB1, losing its larger part. It is not only a decrease in the DB2 oscillation amplitude (energy dissipation), which plays an important role, but also a so-called heating of the Al sublattice in the course of DB motion throughout the crystal during continuous energy dissipation.

The DB2 breathers can effectively transfer the energy throughout the crystal, and their interaction can give rise to its considerable localization in the crystal. One could assume that a release of this energy into the lattice would result in activation of a variety of processes. A possibility of the energy transfer throughout the crystal could thus bring about structural transformations at a certain distance from the focus of excitation of such localized objects.

This study has been performed within the framework of a scientific project No. 166 of the RF Ministry of education and science The Formation of State Terms of Reference for Higher Educational Establishments as concerns the Scientific Research Procedure; the financial support from the RFBR has been granted within project No. 15-58-04033 Bel_mol_a.

REFERENCES

1. A. J. Sievers and S. Takeno, *Phys. Rev. Lett.*, **61**, 970 (1988).
2. G. M. Chechin, G. S. Dzhelauhova, and E. A. Mehonoshina, *Phys. Rev. E*, **74**, 036608 (2006).
3. S. V. Dmitriev, *Pis'ma Mater.*, **1**, Iss. 1, 78–83 (2011).
4. L. Z. Khadeeva and S. V. Dmitriev, *Phys. Rev. B*, **81**, 214306 (2010).
5. N. N. Medvedev, M. D. Starostenkov, and M. E. Manley, *J. Appl. Phys.*, **114**, 213506 (2013).
6. B. Liu, Yu. A. Baimova, S. V. Dmitriev, *et al.*, *J. Phys. D*, **46**, 305302 (2013).
7. R. T. Murzaev, A. A. Kistanov, V. I. Dubinko, *et al.*, *Comp. Mater. Sci.*, **98**, 88–92 (2015).
8. Yu. A. Baimova, S. V. Dmitriev, and A. A. Kistanov, *Russ. Phys. J.*, **56**, No. 2, 180–191 (2013).
9. A. I. Potekaev, S. V. Dmitriev, V. V. Kulagina, *et al.*, *Low-Stability Long-Period Structures in Metallic Systems [in Russian]*, Tomsk, NTL Publ. (2010).
10. N. N. Medvedev, M. D. Starostenkov, A. I. Potekaev, *et al.*, *Russ. Phys. J.*, **57**, No. 3, 387–395 (2014).
11. A. I. Potekaev, V. V. Kulagina, A. A. Chaplygina, *et al.*, *Russ. Phys. J.*, **55**, No. 7, 1248–1257 (2012).
12. A. I. Potekaev, V. V. Kulagina, A. A. Chaplygina, *et al.*, *Russ. Phys. J.*, **56**, No. 6, 620–629 (2013).