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Discrete Breathers in Biatomic Crystals of AB and A_3B Composition

P. V. Zakharov[a, b, *], M. D. Starostenkov[b], and S. V. Dmitriev[c, d, **]

[a] *Shukshin Altai State Humanities Pedagogical University, Biysk, 659333 Russia*
[b] *Polzunov Altai State Technical University, Barnaul, 656038 Russia*
[c] *Institute for Problems of Metal Superplasticity, Russian Academy of Sciences, Ufa, Bashkorstostan, 450001 Russia*
[d] *National Research Tomsk State University, Tomsk, 634050 Russia*
**e-mail: zakharovpvl@rambler.ru*
***e-mail: dmitriev.sergey.v@gmail.com*

Abstract—The conditions for the existence of discrete breathers (DBs) in biatomic crystals of AB and A_3B composition are established, and their properties are studied by means of molecular mechanics using the examples of CuAu and Pt_3Al, respectively. The phonon spectra of the crystals are analyzed, and a gap in the phonon spectrum of CuAu is obtained via considerable homogeneous elastic strain. There is a gap in the phonon spectrum of the Pt_3Al crystal at zero strain, due to the considerable difference between the atomic weights of its components. The frequencies at which discrete breathers can exist in the considered crystals are determined. The energy localized on different types of DBs is estimated. The propagation of a current pulse through Pt_3Al resulting in the excitation of DBs with mild nonlinearity is simulated.

Keywords: discrete breather, quasi-breather, nonlinear mode
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INTRODUCTION

Localized states of atoms and atomic groups in crystals remain poorly studied due to the complexity of full-scale experiments. The number of works dedicated to this problem and the study of different localized atomic states by means of atomistic simulation is steadily growing. The aim of this was to study a localized object in a crystal: a discrete breather (DB). A discrete breather is a nonlinear object that represents a space-localized, large-amplitude sustained vibration in a defect-free nonlinear discrete system [1]. Quasi-breathers in crystals are considered to have finite lifetimes and flexible temporal periodicity of vibrations [2]. Some authors believe that DBs can affect different processes in crystals. For example, it is suggested that DBs can improve the catalytic properties of nanoparticles with disordered structure, result in the radiation-stimulated growth of pores in metals, contribute to diffusion, carry an electrical charge, anneal lattice imperfections, and lower the energy barrier of chemical reactions in crystalline solids [3–8].

DBs have long lifetimes, since their frequency lies beyond the phonon spectrum of a crystal as a result of a nonlinear dependence of frequency on the amplitude of vibrations. There are two variants of this dependence. In the first, the frequency falls with an increase in amplitude. Such DBs display a mild type of nonlinearity; i.e., they have frequencies in the gap of the phonon spectrum of a crystal between the acoustic and optical modes. DBs with mild nonlinearity are mainly localized on one or two atoms and have no mobility. In the second, where the frequency of the DBs rises with amplitude, is associated with the hard type of nonlinearity. The frequencies of DBs with hard nonlinearity lie above the phonon spectrum of a crystal or can be in the gap of the phonon spectrum; such DBs can migrate over a crystal along close-packed rows of atoms. Gap DBs can be excited in biatomic crystals [9–12] and in grapheme and graphane [13]. DBs with hard nonlinearity have been detected in monoatomic systems and pure metals [14].

The main problem is determining the mechanism of DB excitation in crystals. The probability of DBs with mild nonlinearity being excited due to thermal fluctuations has been estimated for thermodynamic equilibrium. For an Pt_3Al crystal at 1000 K, it was found that 0.01% of the light sublattice atoms can be carriers of a nonlinear localized large-amplitude mode with an energy of around 0.8 eV [11]. However, the probability of DBs emerging should increase upon exposure to severe external factors. In [15] for example, it was shown via simulations that irradiating a crystal with high-energy particles can excite DBs with mild nonlinearity.

When metals are exposed to severe factors, a number of effects occur that cannot be explained in terms of classical theories. Many experimental works mention that the warming of a material cannot be

explained by the observed phenomena only, so the question arises as how to describe athermic mechanisms of interaction between a particle flux and a crystal lattice and its defects. Here, we cite only several examples. Ion-plasma treatment of the surfaces of high-purity germanium single crystals annealed imperfections at a depth of several microns [6, 16]. Plasma treatment was reduced to bombarding the crystal surface with ions having energies of 2 to 8 eV. It is interesting that simple heating did not result in similar annealing of imperfections in germanium.

In [16], rolled magnesium alloy was subjected to electropulse treatment. The warming of the material during electropulse treatment was measured and calculated. The pulse current was shown to favor static recrystallization of the material, while simple heating to similar temperatures had no such effect. The contribution from thermal and athermal processes to the structure and properties of functionally graded titanium alloy subjected to electropulse treatment was discussed in [17]. The authors concluded that the phase and structural transformations observed in the alloy could not be explained only by the liberation of Joule's heat. The current traveling through the metal during its plastic strain favored an increase in plasticity and a reduction in flow stress [18–20]. An electrical current can be used simultaneously with the ultrasonic treatment of metals to improve their surface properties [21]. A reduction in flow stress after irradiation with an electron beam having an energy of 0.5 MeV was noted in [22] for polycrystalline aluminum and copper samples subjected to uniaxial tension. The migration of atoms upon the application of a high-density current can alter the morphology of the interface between two conductors [23–26].

Phenomenological approaches that provide no insight into the atomistic mechanisms of interaction between particle fluxes and crystal lattices are most often used to explain the above effects.

In this work, we consider the problem of DB generation in a Pt_3Al crystal upon the transmission of a high-density current pulse, along with the conditions for the existence of DBs in crystals of stoichiometric AB and A_3B composition.

EXPERIMENTAL

Molecular dynamics consists of solving Newton's classical equations of motion. The main problem is selecting the correct potential of interatomic interaction. In studying discrete breathers in crystals, we used both Morse's pair potentials and potentials obtained via the embedded atom method (EAM potentials). From the available data [4, 8–12, 14, 15], we may conclude that the use of one potential or another results in only some quantitative differences when solving the above problems, without touching on the qualitative components of phenomena. In this work, we therefore focused on interpreting the important aspects of observed phenomena in computer-aided experiments without emphasizing the interaction potential that was used.

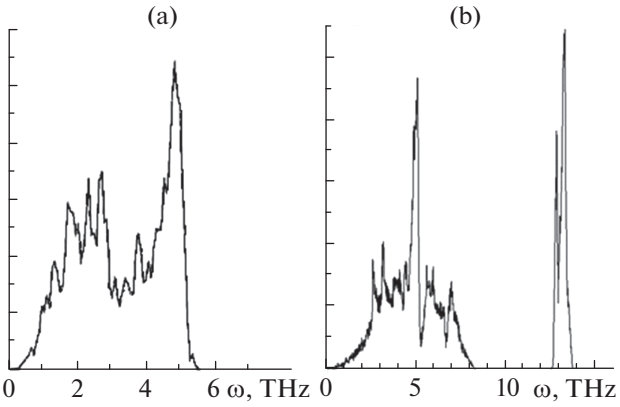

Fig. 1. Density of the phonon state of our (a) CuAu and (b) Pt_3Al crystals.

To study the possibility of DBs existing in certain crystals, we must consider the density of their phonon states. For example, a DB with mild nonlinearity can exist only in the range of frequencies in the gap of the phonon spectrum.

RESULTS AND DISCUSSION

Figures 1a, b show the densities of the phonon states of our CuAu and Pt_3Al crystals.

Analysis of Fig. 1 shows that DBs with mild nonlinearity can exist in a Pt_3Al crystal since there is a gap in its phonon spectrum. To excite DBs with mild nonlinearity, it suffices to displace one atom of the light crystal sublattice from equilibrium in a particular direction. Studies show that DBs with mild nonlinearity can exist in a Pt_3Al crystal along crystallographic directions [001], [010], and [100]. The vibrational frequency lies in the gap of the phonon spectrum in the 10–12.5 THz range of frequencies and depends on the amplitude of atomic vibrations. Such DBs can localize energies of around 1 eV.

The existence of a gap does not forbid that of DBs with hard nonlinearity. However, the search for such objects requires the selection of more specific initial conditions. For Pt_3Al, steady-state and dynamic DBs with hard nonlinearity localize on the Al atoms. To excite DBs with hard nonlinearity, we displaced two neighboring atoms of the light sublattice from equilibrium along the $[1\,\bar{1}0]$ direction (Fig. 2).

As a result, the vibrational energy was redistributed to 4–6 neighboring atoms, after which this localized mode could exist for more than 1000 periods of vibrations and migrate along the abovementioned direction with asymmetry of the displacement profile. The

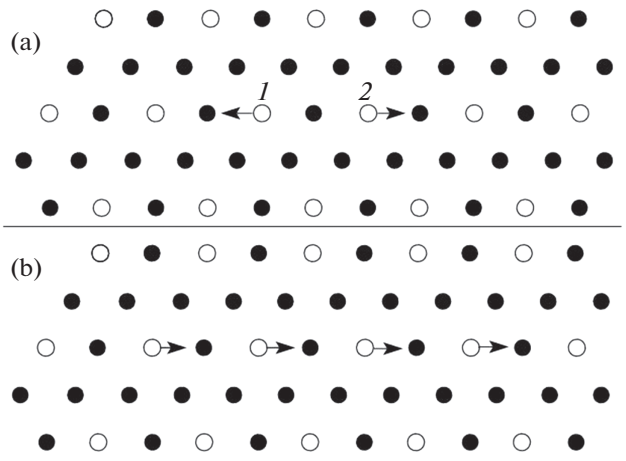

Fig. 2. Plane (111) of our Pt_3Al crystal: (a) initial conditions for the excitation of DBs with hard nonlinearity and (b) the redistribution of vibrational energy.

vibrational frequency lay above the phonon spectrum of the crystal and depended on the amplitude of vibrations as well. Such discrete breathers can localize energies of more than 2.5 eV.

We examined close-packed rows of atoms when searching for DBs with hard nonlinearity in our CuAu crystal. Our selection of conditions for the excitation of DBs produced the bell-shaped function

$$f(x) = A_0 e^{-\frac{x^2}{2C^2}}, \quad (1)$$

where A_0 is the initial amplitude of the central atoms of a discrete breather, x is the relative coordinate of an pair of atoms in a row, and C is the degree of spatial localization of a discrete breather. Varying values A_0 and C, we selected the profile of a discrete breather and thus specified the initial deviations from equilibrium for the atoms comprising the DB (Fig. 3).

The resulting discrete breather was localized on 6–8 Cu atoms. It had a vibrational frequency of more than 5.6 THz and could accumulate a total energy of up to 2.1 eV.

Some works [27, 28] have shown that a discrete breather with mild nonlinearity can be obtained in a crystals via strain that forms a gap in its phonon spectrum and thus provides the necessary consitions for the existence of DBs.

We strained a CuAu crystal with allowance for the Poisson principle; i.e., the volume of the model unit cell did not change. The characteristic index for crystals with tetragonal structure is the ratio of lattice parameters c/a; under normal conditions, this value for CuAu is 0.92. We obtained the densities of the phonon states of the crystal by straining it along the [001] crystallographic direction corresponding to lattice parameter c and allowing for the change in lattice parameter a in order to preserve the volume of the model under consideration.

A fairly wide gap in the crystal's phonon spectrum was obtained at $c/a = 0.8$, which was 9.5% of the compression strain along the [001] direction (Fig. 4).

To search for a discrete breather with mild nonlinearity, one of the Cu atoms was displaced from equilibrium along different crystallographic directions. As a result, we succeeded in obtaining a discrete breather along the [100] direction. The frequency of the resulting DB with mild nonlinearity lay within the gap of the

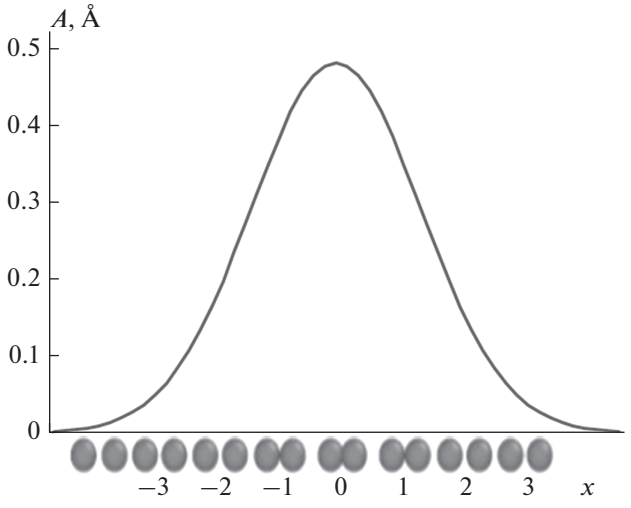

Fig. 3. Initial profile of the discrete breather defined by function (1) for a copper row along the [110] plane.

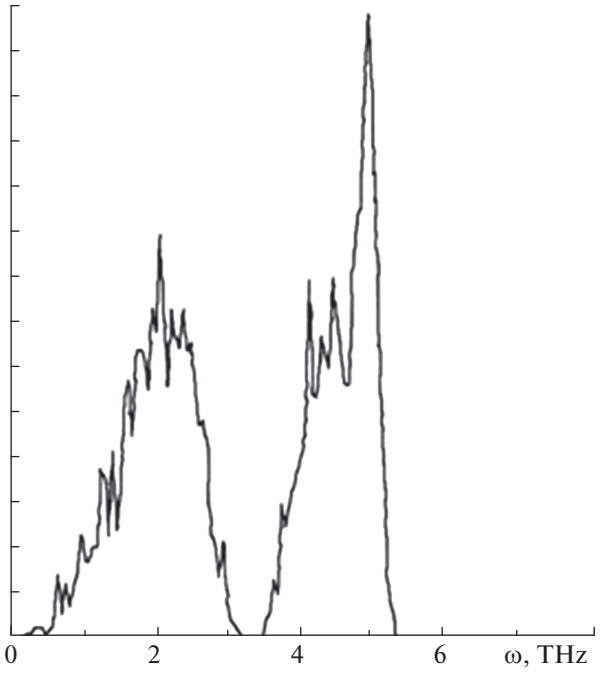

Fig. 4. Density of the phonon states of our CuAu crystal upon compression strain corresponding to a ratio of $c/a = 0.8$.

phonon spectrum and was 3.5 THz. The lifetime of the resulting localized vibrations was around 2 ps (more than 15 periods of vibrations), due to the narrow gap in the phonon spectrum and the negligible spread in the weights of the alloy components. Such DBs are localized mainly on one Cu atom and accumulate energies of around 0.8 eV.

Since Pt_3Al was the only one of the considered crystals that supports the existence of DBs in the unstrained state, we studied the generation of DBs with mild nonlinearity in the crystal without artificial underestimates of the weights of alloy components.

We simulated the interaction between the crystal's atoms and the flow of particles (electrons) with energies of up to 2.5 eV by considering particle collisions to be perfectly inelastic; i.e., an electron transfers all of its energy to an atom when they collide. To simulate collisions between electrons and the atoms of Pt_3Al alloy upon a current pulse, a certain percentage (0.025 to 1.5%) of the atoms receiving the pulse was randomly selected from the entire array. The pulses were transferred to atoms along the axis corresponding to the [100] crystallographic direction. The density of the current passing through the model unit cell was thus controlled:

$$J = \frac{Ne}{tS}, \tag{2}$$

where N is the number of electrons traveling through area S in time t, and e is the electron charge. By controlling the number of atoms receiving the pulse and the time in which secondary collisions occur, we can estimate the current density. In our case, it varied from 10^4 to 10^6 A cm^{-2}.

The generation of DBs requires the Al atoms to acquire a velocity of around 50 Å ps^{-1}. Let us assume that one collision between an electron and an atom transfers 20% of this energy or more to the latter. In other words, the atom, being immobile acquires a velocity of 10 Å ps^{-1} or more. Let us calculate the minimum energy an electron should have, based on the law of the conservation of energy. The energy gained by the atom is determined by the formula $E = \frac{m_a v_a^2}{2}$, and is around 0.14 eV per collision. The velocity of an electron with such energy is determined by the formula $v_e = \sqrt{\frac{2E}{m_e}}$, so we obtain a value of around 2×10^5 m s^{-1}. To accelerate an electron almost at rest to this velocity requires the free path voltage determined from the formula $\frac{m_e v_e^2}{2} = eU$. Then $U = \frac{m_e v_e^2}{2e} = 0.139$ V. We thus estimate the values that can be reached in a full-scale experiment and are observed during industrial processes.

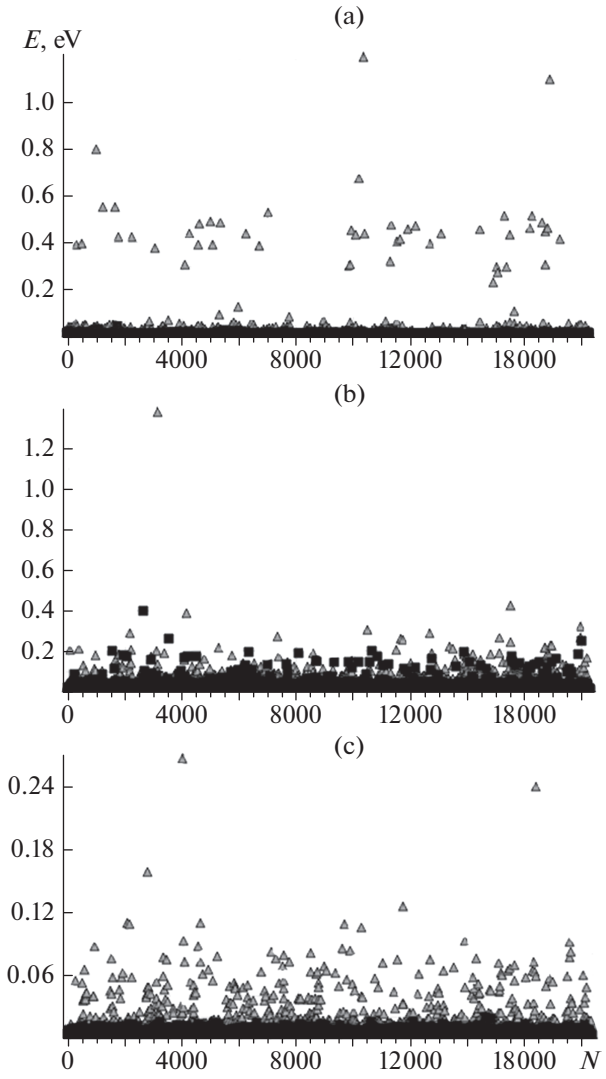

Fig. 5. Distribution of energy in a calculated unit of our Pt_3Al crystal. The kinetic energy per atom is plotted along the vertical axis, while the atomic number of the atom in an unit cell is plotted along the horizontal axis (Al atoms are denoted by triangles; Pt atoms, by squares) at current densities of (a) 10^6 A cm^{-2}, (b) 10^5 A cm^{-2}, and (c) 10^4 A cm^{-2}.

Having performed a number of computer-aided experiments in the abovementioned ranges of electron–atom interaction energies and current densities, we found that one act of interaction is not enough to excite DBs. An atom must collide with electrons several consecutive times to accumulate the energy required for the formation of DBs with mild nonlinearity.

Figure 5 shows the results from a series of consecutive experiments with different initial conditions when the energy of interaction was held constant (0.5 eV) and the current density was reduced from 10^6 to 10^4 A cm^{-2}. The probability of several consecutive collisions pumping energy is obviously higher at the max-

imum current density (Fig. 5a). As a result, we observe in the calculated unit cell (Fig. 5a) three atoms with energies higher than 0.8 eV that are carriers of a nonlinear localized large amplitude mode, in addition to the entire group of light sublattice atoms, which can accumulate sufficient energy in the next collision. Reducing the current density (Fig. 5b) to 10^5 A cm^{-2}, we were able to detect only one atom with sufficient energy, and the number of potential DBs fell considerably. At current densities of 10^5 A cm^{-2} and below, we failed to detect DBs at these electron energies. Reducing the energy of interaction raised the probability of DBs being excited at lower current densities as well.

CONCLUSIONS

Such nonlinear objects as discrete breathers and conditions of their existence in the AB and A_3B crystals with a face-centered cubic lattice were studied by means of molecular dynamics. Two types of discrete breathers (ones with mild and hard types of nonlinearity) were considered. A necessary condition for the existence of DBs with mild nonlinearity is a gap in the phonon spectrum of a crystal. The considered DBs with hard nonlinearity were localized on ten atoms in a close-packed lattice row. Strain in a CuAu crystal produces a gap in its phonon spectrum, providing conditions for the excitation of DBs with mild nonlinearity that have frequencies in the spectral band gap. Due to slight differences between the weights of the components of CuAu alloy, the lifetime of such DBs is several tens of periods of vibration.

The search for mechanisms of the excitation of discrete breathers in crystals is of great importance. A simplified model was proposed for the flow of particles through a Pt_3Al crystal, which results in the generation of DBs with mild nonlinearity. The range of current densities and particle energies that might be achieved in real experiments and indistrial processes was considered.

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