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Mobility of Soliton-Like Waves in Cuau Crystal

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***Abstract*—Molecular dynamics is used in this work to study the energy transport through the CuAu crystal lattice by discrete breathers (DBs) with frequencies above the phonon spectrum. The DB moves along the close packed atomic row in the Cu sublattice. An asymmetry was introduced in the initial conditions used for DB excitation in order to set the DB in motion. The maximal distance travelled by the DB was calculated as the function of the asymmetry parameter. The results indicate a weak mobility of such objects in the considered CuAu crystal. Nevertheless, energy transport along the close-packed directions of the Cu sublattice is possible.**

Keywords— discrete breather; quasi-breather; phonon spectrum; nonlinear localized mode.

I. INTRODUCTION

Solitary waves are among the most interesting and important objects of nonlinear physics relevant for practical applications [1, 2]. Despite the fact that solitons were discovered more than 180 years ago, the number of studies devoted to their properties is still growing. Increasing interest to the investigation of discrete nonlinear systems supporting dynamic solitons stimulates new research in this field. High-amplitude, spatially localized time-periodic vibrational modes in nonlinear crystals with translational symmetry called discrete breathers (DBs) belong to the class of the above mentioned dynamical solitons [3].

Solitary waves can carry energy, momentum, mass, electrical and topological charge, other physical quantities, and even information in both continuum and discrete physical systems [4].

The possibility of energy localization in defect-free nonlinear discrete structures predicted by the authors of [5] has been confirmed experimentally later. Discrete breathers were detected in various physical systems including nonlinear optics [6], Josephson superconducting contacts [7] and antiferromagnets [8].

Establishing the physical nature of such DBs [1], mechanisms of their excitation and properties is currently performed by many scientific teams around the world. The main goal of the research is identification of possible role of DBs and other large amplitude vibrational modes in the evolution of structure and properties of crystals.

One should also mention the experimental attempts of DB identification in crystals. An active discussion on the experimental identification of DB in an alkali-halide NaI crystal by inelastic neutron scattering [1] can be found in the literature. Group of J. Archilla and M. Russell initiated the research on the origin of dark traces observed in mica crystal that were believed to be tracks of high-energy cosmic particles imitating systems of moving soliton-like modes (qudons). This problem has initiated new investigations of moving DBs. The same scientific group has experimentally observed the effect of annealing of defects in a germanium crystal at a large distance from the surface after the crystal surface was exposed to low-energy plasma discharge [6]. The authors hypothesized that the energy is transferred into the interior of the crystal by means of moving DBs resulting in defect annealing. One should note that the stationary DBs in germanium were excited and analyzed by means of molecular dynamics method in [7], and investigations of mobile DBs in this crystal are currently in progress.

The authors of [9] succeeded in excitation of DBs in a number of metals and alloys using the molecular dynamics approach. Intensive attempts of detecting DBs in metals and alloys by experimental methods face a number of difficulties, in particular, there is the problem of excitation of DBs and separation of their contribution to the vibrational spectrum from other types of lattice vibrations. Results of those studies will contribute to fundamental

understanding of condensed matter physics and realization of new approaches of governing structure and properties of the crystal for application in new technologies.

DB can be characterized by two types of nonlinearity. In the case of soft nonlinearity type DB frequency decreases with increasing amplitude, while hard type of nonlinearity is characterized by grow of frequency with increasing DB amplitude.

Decreasing of frequency of a soft nonlinearity type DB with growth of its amplitude can result in entering the gap of phonon spectrum, if it exists. This type of DB can only exist in crystals having more than one atom in the primitive translational cell, in particular, a biatomic crystals with sufficiently large difference in the atomic masses of the components providing a sufficient width of band gap. DBs with a soft type of nonlinearity can be excited in such biatomic crystals as alkali halide having NaCl structure [3] and in Pt_3Al [10-15]. Gap DBs were also reported to exist in strained graphene and in graphane [16-19].

For hard type nonlinearity modes the growing frequency can grow above the phonon spectrum. DBs with a hard type nonlinearity exist in pure metals with fcc, bcc, and hcp structures. Moving DB in metals is a special case of a hard type nonlinearity DB.

The aim of this work is the revealing the possibility of existence of mobile DBs in CuAu system able to move along close packed crystallographic directions. Existence of such objects was previously demonstrated in [20].

II. Sumulation Details

Investigation was performed by means of well-known molecular dynamics method. This method was implemented using the LAMMPS package of molecular dynamics simulation, which uses well-tested many-body interatomic potentials built according to the embedded atom method (EAM-potentials). We considered a three-dimensional crystal containing 48000 atoms (Fig. 1). Periodic boundary conditions were imposed along all directions.

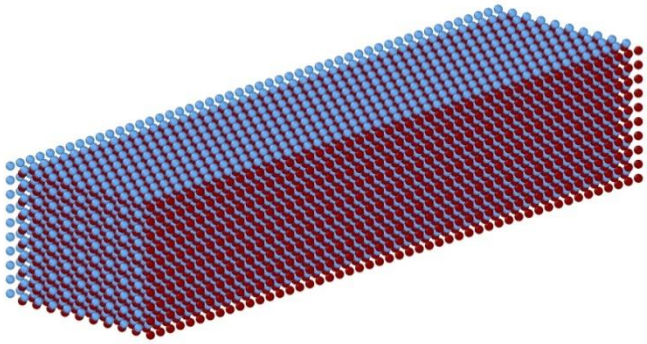

Fig. 1. The view of a 3D CuAu crystal containing 48000 atoms

The potential obtained by the method described in [21] for the Cu-Au system was used in the calculations. The process of selecting the interatomic potentials is an important task worth a detailed consideration. The home-made software [21] generates EAM-potentials of alloys using the rapid fitting procedure by combining the previously developed elemental potentials. More precisely, we have considered the Finnis-Sinclair potentials for the alloy determining the energy of each atom in the system, using the expression:

$$U_i = F_\alpha\left(\sum_{i\neq j}\rho_\alpha\beta\left(r_{ij}\right)\right) + \frac{1}{2}\sum_{i\neq j}\varphi_\alpha\beta\left(r_{ij}\right). \quad (1)$$

This equation consists of three types of functions: embedding functions (F), electron density functions (ρ), and pair functions (φ). In this formula there is an embedding function for each element type, one electron density function for each permutation of two types of atoms (a, p), and a pair function for each combination. For binary potentials, there are only three functions that need to be selected in case of using elementary conditions from existing potentials: $\rho_{\alpha\beta}$, $\rho_{\beta\alpha}$, and $\varphi_{\alpha\beta}$. Since there are no triple conditions in the Finnis-Sinclair formula, potentials with more than two elements can be created by combining all the information contained in the binary files. The method proposed by the authors of the article allows to combine elemental EAM potentials and to establish the potentials for the alloy using the density functional theory (DFT) data.

Firstly, the approach of simple "rule of mixtures" is used for compensation of the difference between the lattice parameters and elasticity modulus predicted by the DFT and measured experimentally. The elastic moduli and lattice parameters calculated for intermetallic compounds are defined with the effective correction factor, being the average of the elementary correction factors taken in the proportion of elements fractions. Secondly, single-element potentials are adapted to improve compatibility in binary and multicomponent potentials in such a way as to preserve all the initial states of the system. Thirdly, in the case of bonding of two elemental potentials, the maximum cut off distance is adopted for the binary potential. The electron density functions and the interaction of the original pair potentials are defined as equal to 0 at the distances greater than the cut off radius. Since most of interatomic potentials are available in a tabular format with functions defined at discrete points, this implementation uses cubic spline interpolation in order to calculate the values of functions in between the tabulated points.

The next step was the installation of cross-potentials. The Finnis-Sinclair composition for the EAM potential is used for every alloy potential considered. For a binary system, two embedding functions (F_α, F_β), four electron density functions ($f_{\alpha\alpha}$, $f_{\alpha\beta}$, $f_{\beta\alpha}$, $f_{\beta\beta}$) and three pair interaction functions ($\phi_{\alpha\alpha}$, , $\phi_{\beta\beta}$) are used. Similarly to the case of single-component potentials, two-component ones are combined by converting the embedded function so that it exists on the same interval and assumes the maximum cut off radius. While the "pure" elemental potentials are used to create each double file, the electron density and interaction functions of the pair contained in the original binaries are sufficient to create higher-order potentials without any additional equipment. In addition, the properties of each binary system and the original pure elements remain in these new potentials. The potentials created with the proposed technique were confirmed by comparison with the experimental results and the existing potentials for the alloys. In addition, the dependence of the accuracy of binary potentials on the source of elementary potentials was estimated.

In order to analyze the possibility of the existence of DBs in CuAu crystal, the density of the phonon states of the crystal was calculated (see Fig. 2). The absence of a gap in the CuAu phonon spectrum dictates the impossibility of DB

with soft nonlinearity type in this system. [16, 17]. This was confirmed in [20].

There exist several ways of DB excitation including application of anzats [22], applicaiton of localization of short wavelength phonon modes [23, 24] and modulational instability [25]. First two approaches set the initial atomic displacements from the equilibrium position and initial velocities for a group of atoms involved in the DB.

For pure metals or alloys with a small difference in the atomic masses of the components, the excitation of DBs with a hard type of nonlinearity has some peculiarities. Thus, the authors of [18] proposed an ansatz for excitation of DBs in pure fcc and bcc metals, setting the DB profile in a closely packed atomic row by setting atomic displacements and velocities according to physically motivated functions. The displacements of the atoms were realized in such a way that the neighboring atoms oscillated in antiphase [18].

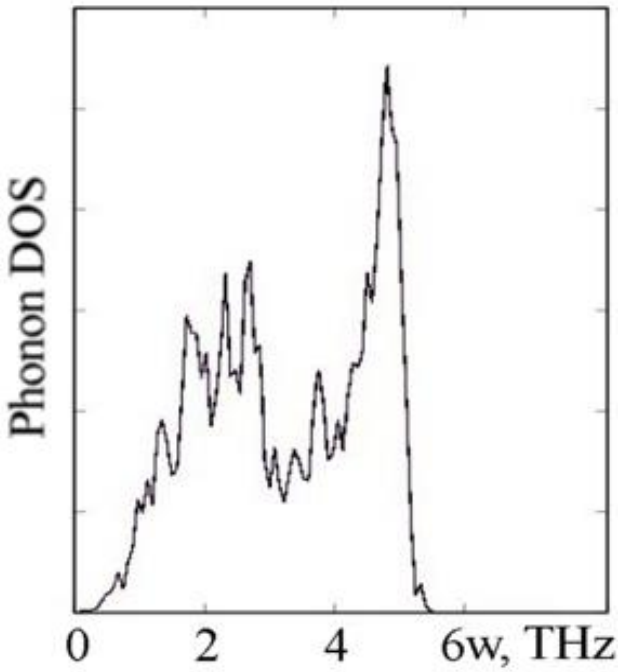

Fig. 2. The density of phonon states of CuAu crystal

The Gaussian function (2), adapted for crystal conditions was used to excite a DB in the CuAu crystal

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

where A_0 defines the initial amplitude of the central atoms of a DB, x is the relative coordinate of a pair of atoms in a row, and parameter C is the degree of spatial localization of DB. Varying the values A_0 and C, we select the profile of the discrete breather, thereby setting the initial deviations from the equilibrium position for the atoms included in the DB oscillations (see Figure 3).

III. RESULTS AND DISCUSSION

To set the initial conditions for a moving DB it is necessary to introduce asymmetry into the DB profile. For this purpose, a factor γ was introduced as a multiplier of C to redefine one of the branches of the function (2), the second branch was calculated for the case of $\gamma = 1$:

$$f(x) = A_0 e^{-\frac{x^2}{2\gamma C^2}}. \quad (3)$$

In Fig. 2. The initial profile of the moving (γ >1) and stationary (γ = 1) DB is presented. Choosing a value of γ factor for the right branch, one can obtain a DB with a different initial velocity along the crystal. The obtained results show that the velocity of such DB is much lower than the speed of sound in the considered crystal. The motion of a DB with a non-symmetrical profile occurs toward the steeper branch of the function (2). DB can overcome several tens of interatomic distances in a crystal along a close-packed direction during its lifetime. As initial parameters for a moving breather, the parameters of equation (2) were chosen for which the DB existed in a steady state for a maximum time. The values of these parameters are as follows: $A_0 = 0.48, \quad C = 0.75$

a

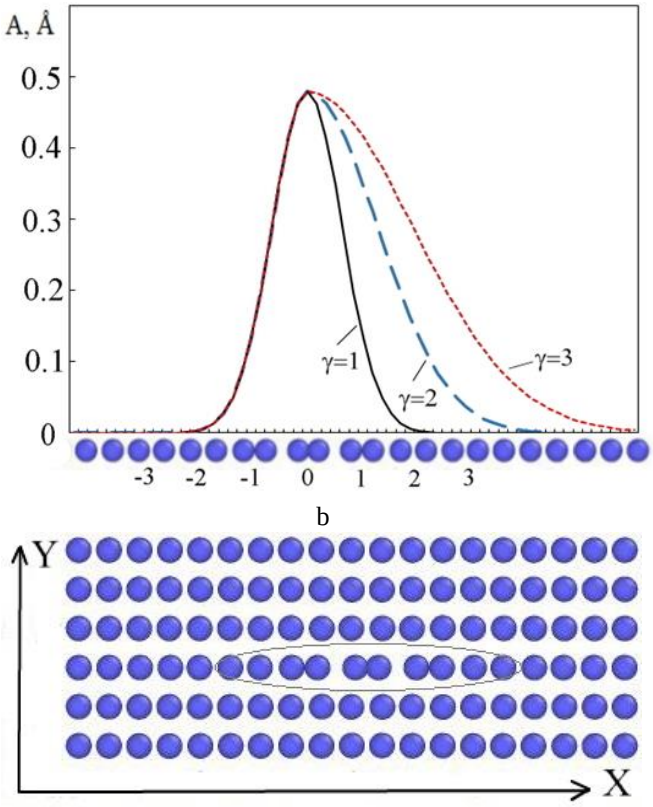

Fig. 3. a) Setting the profile of initial atomic displacements for the DB by imposition (2) and (3) functions. b) Visualization of atomic displacements in the plane of Cu atoms, the X axis is directed along the <110> crystallographic direction, the Y axis along the <001> crystallographic direction.

Further, the variation of parameter γ for the right-side of the DB profile was performed. The dependence of the distance traveled by the DB from the value of the parameter γ is shown in Fig. 4. One can notice that the dependence S(γ) is not monotonous and maximal

distances of the DB motion correspond to the interval of γ values between 0.4 and 0.5.

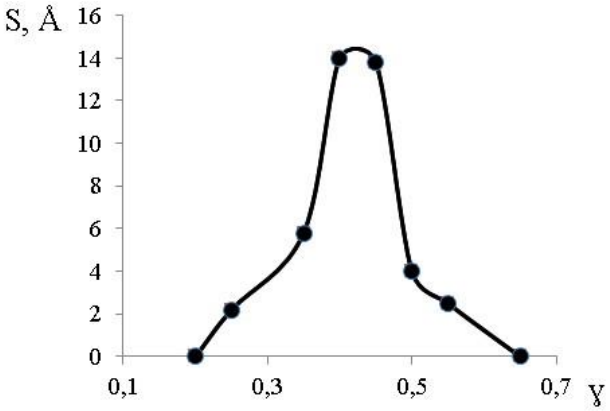

Fig. 4. Dependence of the distance traveled by the DB on the parameter γ

The results indicate a weak mobility of such objects in the considered CuAu crystal. Nevertheless, energy transport along the close-packed directions of the Cu sublattice is possible.

IV. CONCLUSIONS

The possibility of excitation of a mobile DB with hard nonlinearity type in CuAu crystal in the copper sublattice was demonstrated by means of molecular dynamics method. General characteristics of the DB are analyzed, the possibility of movement, the travelled distance as well as the influence of the initial conditions on the DB lifetime have been analyzed. The results obtained in the present study are important in frames of the concept of new mechanisms of energy transport by DBs having frequencies above the phonon spectrum.

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