Hard-Type Nonlinearity Moving Discrete Breathers in Crystals and Their Interaction with a Vacancy

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Abstract—Molecular dynamics study of moving discrete breathers (DBs) in pure vanadium is carried out. The following properties of the DBs are estimated: the frequency as the function of amplitude, the degree of spatial localization and the maximum propagation velocity. Interaction of DBs with a vacancy is studied in frame of the two-dimensional model of crystal with Morse interatomic potentials.

1. Introduction

The works [1, 2] have contributed to the development of the nonlinear lattice dynamics by discovering that the large-amplitude, spatially localized vibrational modes can exist in the absence of the lattice defects. Such modes are called discrete breathers (DBs) or intrinsic localized modes [3].

According to a number of experimental [4, 5, 6, 7, 8] and numerical [9, 10, 11, 12, 13, 15, 16, 17, 18, 20] studies, crystals can support DBs. In the recent years, the number of works where DBs are used to explain various physical effects in crystals has been growing [6, 21, 22, 23, 24].

DBs do not radiate their energy in the form of small-amplitude waves because they vibrate at frequencies outside the phonon spectrum of crystal. DB frequency can leave the phonon spectrum when its amplitude is sufficiently large because the frequency of a nonlinear oscillator is amplitude-dependent. There are two types of nonlinearity, the hard-type and the soft-type. In the former (latter) case the DB frequency increases (decreases) with increase in its amplitude. In the case of the hard-type nonlinearity the DB frequency can be above the phonon spectrum. For the soft-type nonlinearity DBs can exist only if the phonon spectrum possesses a gap.

Soft type nonlinearity DBs with the frequencies within the gap have been studied in the crystals with the NaCl structure [6, 7, 8, 9, 10], in strained graphene and graphene nanoribbons [17, 18, 19], in graphane [20]. DBs with frequencies above the phonon spectrum have been identified in Si and Ge [11], in graphene [12], and more recently in pure metals with fcc lattice (Ni) and bcc lattice (Nb, Fe) [13, 14]. The latter study has inspired the development of an ansatz for the initial conditions to excite DBs with hard-type nonlinearity [25].

In the present study, using the ansatz offered in [25] for setting the initial conditions to excite moving DBs with hard-type nonlinearity, the properties of DBs in bcc V are analyzed numerically. The ansatz is also used to simulate the interaction of DBs with a vacancy in the 2D close-packed crystal with Morse interactions.

2. Simulation Setup

The simulations are performed using the LAMMPS package [26, 27] with the embedded atom method (EAM) interatomic potentials for V [28]. The lattice parameter of bcc V is equal to $a = 3.024$Å.

Hard-type nonlinearity DB in monatomic lattices is extended along a close-packed atomic row [25]. In bcc lattice the close-packed atomic rows have $\langle 111 \rangle$ crystallographic orientation. Taking this into account, the computational cell in the form of a cuboid is chosen so that the x, y and z axes are oriented along the $\langle 111 \rangle$, $\langle \bar{1}2\bar{1} \rangle$ and $\langle \bar{1}01 \rangle$ crystallographic directions, respectively. The size of the computational cell is $130 \times 74 \times 64$Å^3. Total number of atoms in the computational cell is 45000.

Two-dimensional close packed lattice with the interatomic distance equal to b is considered. Interatomic interactions are described by the classical pairwise Morse potential

$$U(r) = D(e^{-2\alpha(r-r_m)} - 2e^{-\alpha(r-r_m)}), \qquad (1)$$

where r is the distance between two atoms, D, α, r_m are the potential parameters. The function $U(r)$ has a minimum at $r = r_m$, the depth of the potential (the binding energy) is equal to D and α defines the rigidity of the bond. In the following, the dimensionless units of time, energy and distance are used such that $D = 1$, $r_m = 1$ and the atom mass is unity. We take $\alpha = 5$, for which the equilibrium interatomic distance is $b = 0.98813$. The cut-off radius is chosen to be $r_c = 5$.

The computational cells of the 3D bcc lattice of vanadium and the 2D Morse lattice are subjected to the periodic boundary conditions. The microcanonical, or NVE ensemble, is used, meaning that the system is isolated from

changes in moles (N), volume (V) and energy (E). The velocity Verlet scheme with the time step of 1 fs is employed to integrate the equations of atomic motion.

Atoms in a close-packed atomic row with the ⟨111⟩ crystallographic direction oriented along x axis are numbered by the index n. To excite a moving DB in the close-packed row of atoms the following ansatz is used [25]

$$x_n(t) = \cos[\omega t + \varphi_0 + \delta n] X_n^0, \quad y_n(0) = 0, \quad \dot{y}_n(0) = 0, \tag{2}$$

where ω is the DB frequency, φ_0 is the initial phase, δ is the parameter that defines the phase difference for neighboring atoms, X_n^0 are defined as follows

$$X_n^0 = (-1)^n T_n^0 + S_n^0, \quad T_n^0 = \frac{A}{\cosh[\beta(n - x_0)]}, \quad S_n^0 = \frac{-B(n - x_0)}{\cosh[\gamma(n - x_0)]}, \tag{3}$$

where A is the DB amplitude, B defines the amplitude of displacements of the vibration centers of the atoms, β and γ define the degree of spatial localization of DB, x_0 is the DB initial position. For $x_0 = 0$ the DB is centered on a lattice site, while for $x_0 = 1/2$ in the middle between two neighboring lattice sites.

For all atoms in the atomic rows where DB is not excited we set $x_n(0) = y_n(0) = 0$ and $\dot{x}_n(0) = \dot{y}_n(0) = 0$.

The DB velocity depends on δ, and for $\delta = 0$ it is equal to zero.

The functions T_n^0 and S_n^0 in (3) describe the amplitudes and the displacements of the vibration centers of the atoms at $t = 0$, respectively. These quantities will be calculated for each period of DB oscillation as

$$T_n = \frac{x_{n,\max} - x_{n,\min}}{2}, \quad S_n = \frac{x_{n,\max} + x_{n,\min}}{2}, \tag{4}$$

where $x_{n,\max} > 0$ and $x_{n,\min} < 0$ are the maximal and minimal values of the (quasi)periodic function $x_n(t)$ that describes the motion of nth atom of the close-packed atomic row.

It should be noted that the ansatz (2), (3) is not an exact solution to the equations of motion for the considered bcc crystals. That is why, a part of energy given to the system at $t = 0$ is radiated in the form of small-amplitude extended waves and then a stable and robust moving DB emerges, if the parameters in (2), (3) are properly chosen.

3. Standing and Moving DBs in V

In Fig. 1 the profile of standing DB in V is presented by the functions (a) T_n and (b) S_n (4) at $t = 3.5$ ps. The DB is centered in between two neighboring lattice cites by setting $x_0 = 1/2$ in (3). Other parameters are as follows: $A = 0.35$Å, $B = 0.14$Å, $\beta = 0.7$, $\gamma = 0.9$, $\delta = 0$. One can see that in the presented example the DB amplitude (maximal T_n) is about 0.38Å. Maximal shift of the atoms' vibration centers, S_n, is 0.1Å. DB in V is localized on 6 atoms. It was found that the degree of localization of the DB does not change much with its amplitude.

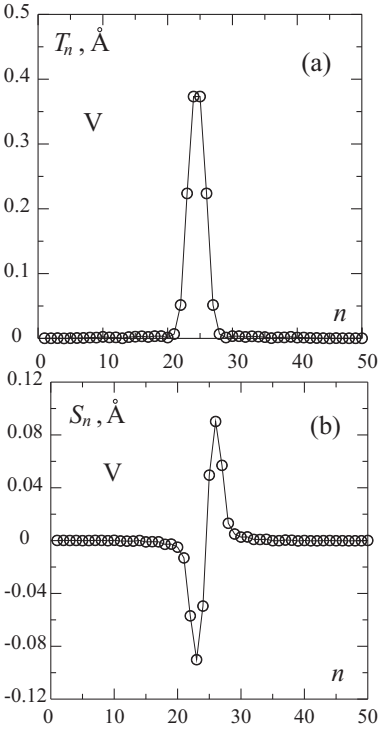

Figure 1: Standing DB in V presented by the functions (a) T_n and (b) S_n (4) at $t = 3.5$ ps. The DB is centered in between two neighboring lattice cites by setting $x_0 = 1/2$ in (3). Other parameters are: $A = 0.35$Å, $B = 0.14$Å, $\beta = 0.7$, $\gamma = 0.9$, $\delta = 0$.

DB moving in V is presented in Fig. 2 by the functions $\Delta x_n(t)$. The DB was excited with the following parameters: $\delta = 0.3\pi$, $A = 0.45$Å, $B = 0.14$Å, $\beta = 0.7$, $\gamma = 0.9$. It can be seen that DB in V demonstrates a robust motion along the lattice.

In Fig. 3 the frequency of standing DB in V is presented as the function of DB amplitude. The horizontal line indicates the upper edge of the phonon band for vanadium. It can be seen that the DB frequency is above the phonon spectrum and it increases with increase in DB amplitude. Vanadium supports DBs in a wide range of amplitudes from 0.25 to 0.55Å.

In Fig. 4 the DB velocity as the function of the parameter δ in the ansatz (2,3) is given for V. Values of the other parameters are: $A = 0.45$Å, $B = 0.14$Å, $\beta = 0.7$, $\gamma = 0.9$. Speed of sound for V is 45.6 Å/ps. The maximal DB velocity we could observe is equal to 14.0 Å/ps, which is 0.31 of the speed of sound.

4. Interaction of DBs with a Vacancy

We now turn to the simulation of the interaction of a moving DB with a vacancy in 2D Morse crystal.

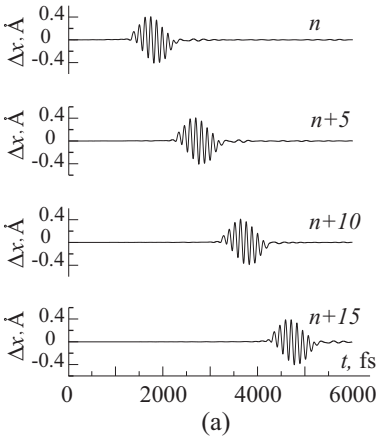

Figure 2: Moving DB in V presented by the functions $\Delta x_n(t)$. The DB was excited with the following parameters: $\delta = 0.3\pi$, $A = 0.45$Å, $B = 0.14$Å, $\beta = 0.7$, $\gamma = 0.9$.

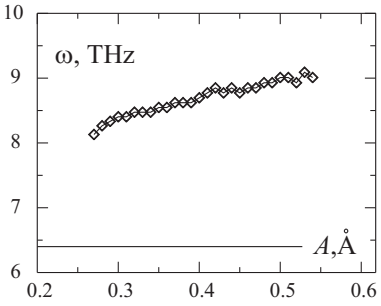

Figure 3: Frequency of standing DB in V as the function of DB amplitude. The upper edge of the phonon band is shown by the horizontal line.

Two examples of the interaction of the DB with a vacancy are shown in Fig. 5. The functions T_n for the close-packed atomic row along which the DB moves are shifted vertically for different times t_j with the interval of $\Delta t = 5$. Vacancy position is shown by the vertical dashed line. Parameters of the ansatz (2,3) used for setting the initial conditions are the following: (a) $A = 0.2565$, $B = 0.015$, $\beta = \gamma = 0.25$, $\omega = 19.52$, $x_0 = 1/2$, $\delta = 0.02\pi$; (b) the same except for $\delta = 0.04\pi$. Thus, in (a) the DB has velocity two times smaller than in (b). In (a) almost elastic repulsion of DB from the vacany is observed, while in (b) the DB is destroyed as a result of interaction with the vacancy. It was found that for DBs initiated with $\delta \leq 0.035\pi$ ($V_{DB} \leq 4.51$), elastic repulsion of the DB from the vacancy takes place and for $\delta > 0.04\pi$ ($V_{DB} > 5.15$) DB is destroyed by the vacancy.

Conclusions. Molecular dynamics based on the EAM many-body interatomic potentials was used to study properties of standing and moving DBs in bcc vanadium. It was found that DBs in V are robust and can move with the velocity equal to 0.31 of the speed of sound.

The molecular dynamics method was also used to study

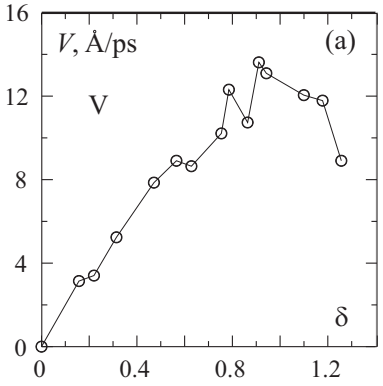

Figure 4: Velocity of DB in V as the function of the parameter δ in the ansatz (2,3). Values of the other parameters are: $A = 0.45$Å, $B = 0.14$Å, $\beta = 0.7$, $\gamma = 0.9$.

the effect of the velocity of the moving DB on the result of its interaction with a vacancy. It was shown that if the DB velocity is less than a threshold value, elastic repulsion of DB by the vacancy takes place. At higher velocities DB is destroyed as the result of the collision with the vacancy. Duration of the interaction of the DB with the vacancy in all cases is of the order of 10^2 periods of DB vibration.

The question how DBs influence mechanical and physical properties of metals is yet to be fully answered.

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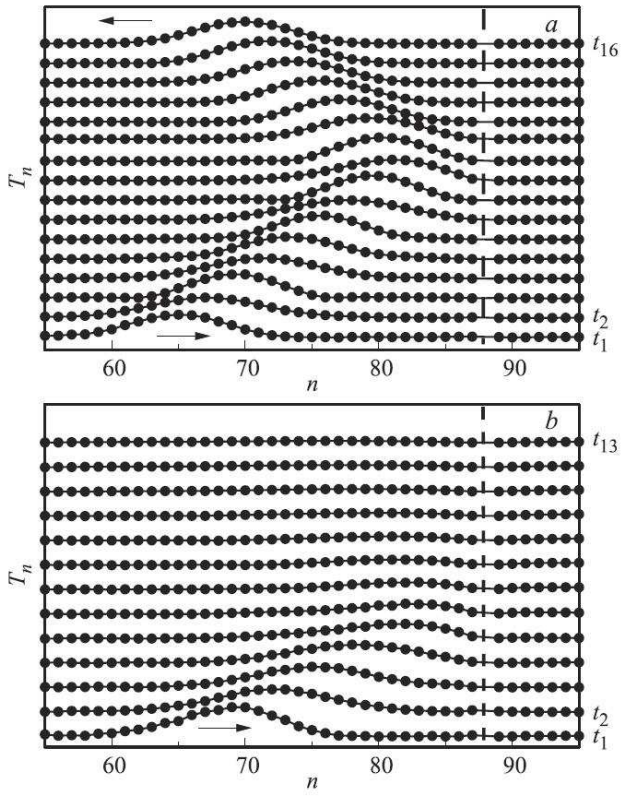

Figure 5: Examples of DB interaction with a vacancy the position of which is shown by the vertical dashed line. In (a) the speed of DB is two times smaller than in (b). In (a) DB is reflected by the vacancy almost elastically, while in (b) DB is scattered on the vacancy. DB excitation parameters are given in the text.

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