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EXCITATION AND PROPAGATION OF 1-CROWDION IN BCC NIOBIUM LATTICE

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ABSTRACT

Crowdion is an interstitial atom found in a close-packed row of atoms in different crystals. These defects are efficient in transferring mass and energy into the crystal lattice because they are highly mobile. In recent years, it has been studied dynamics of various excitations in different types and sizes of lattices. In this article, we considered the motion of a classical 1-crowdion (a mode localized on a single atom has supersonic velocity in a close-packed row of atoms). Niobium has been chosen as material with bcc lattice and the analysis has been carried out for different initial velocities. It is shown that an excitation of the crowdion has the threshold character and can be induced only for sufficiently large initial velocity. If the latter is lower than this threshold than only soliton can be formed. It is also shown that crowdions play an important role in the formation of various mobile defects inside metals.

KEYWORDS

Molecular dynamics; point defects; crowdions; energy transfer; mass transfer; niobium.

ВОЗБУЖДЕНИЕ И РАСПРОСТРАНЕНИЕ 1-КРАУДИОНА В ОЦК РЕШЕТКЕ НИОБИЯ

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АННОТАЦИЯ

Краудион – это мобильная локализованная колебательная мода, распространяющаяся в плотно-упакованном ряду атомов в разных кристаллах. Эти моды представляют собой эффективный механизм массо- и энергопереноса в кристаллической решетке, поскольку они обладают высокой подвижностью. В последние годы была изучена динамика различных возбуждений в различных типах и размерах решеток. Рассмотрено движение классического 1-краудиона (режим, локализованный на одном атоме, имеет сверхзвуковую скорость в плотно упакованном ряду атомов). В качестве материала с ОЦК-решеткой был выбран ниобий, для которого был проведен анализ для различных начальных скоростей. Показано, что возбуждение краудиона имеет пороговый характер и может быть вызвано только при достаточно большой начальной

скорости. Если последнее ниже этого порога, то может быть сформировано только решение. Также показано, что краудионы играют важную роль в образовании различных подвижных дефектов внутри металлов.

КЛЮЧЕВЫЕ СЛОВА

Молекулярная динамика; точечные дефекты; краудионы; энергоперенос; массоперенос; ниобий.

Introduction

Single-layer materials composed of rigid, loosely bonded layers deserve a lot of attention in the modern community because they demonstrate the mechanisms of deformation due to the movement of interstitial atoms in close-packed directions. The high dynamics of the strain rate of these materials remains largely unexplored. In addition, many processes, such as the movement of a crowdion, oscillations of a nonlinear localized mode, or recombination of vacancies and interstitial atoms, occur at such a high rate that it makes it practically impossible to study such processes in a full-scale experiment [1–3]. Therefore, in many cases, the computer simulation method is relevant, which allows overcoming these obstacles [4–7]. Molecular dynamics is a method that allows you to study structural transitions, thermodynamic parameters, transport properties, as well as electronic states in complex systems that track the change in a system of interacting atoms or particles over time by numerically integrating their equations of motion. The method is based on mathematical modeling of the behavior of a system of particles or atoms with a given interaction condition. As a result of the numerical solution of the equations of motion, the dynamic trajectories of the particles are found, and then the averages of any dynamic variables.

Under certain conditions, an impact can be focused on a equally chain of equidistant atoms. The essence of this phenomenon lies in the fact that a moving particle transmits its momentum to the stationary atoms of a compact chain in such a way that it propagates along the chain at an angle to the chain axis, and this angle becomes smaller. at each collision. Focusing and crowdions collisions are closely related. The difference is that in focus collisions only momentum is transferred, while in mass collisions the substance, the interstitial, is also transferred.

Crowdions can move along a densely packed atomic row at subsonic or supersonic speeds [8–10]. In the first case, they are usually localized on half a dozen atoms, and in the second they are highly localized, so that only one or two atoms move at a time at high speed. Supersonic crowdions can carry not only mass, but also an electric charge. It turned out that a moving subsonic crowdion can carry a localized vibrational mode of relatively large amplitude with a frequency above the phonon spectrum; such dynamic excitation can be called a breather subsonic crowdion. This work is devoted to the analysis of the energy exchange of three crowdions propagating in parallel in neighboring close-packed atomic rows.

1. Model and methods

The main principle of the molecular dynamics method is the computer calculations of the dynamical behavior of each atom and their interaction [11, 12]. The use of computing systems of parallel architecture and multiprocessor computing systems made it possible to apply the method to systems containing many particles and various defects [6, 13–17]. The method is based on model concepts, such as the consideration of particles as material points bound by a covalent bond with a fixed mass, and the description of their motion by classical Newton's equations. Research takes place in a vacuum. To plot graphs, we will use the Cartesian coordinate system to plot graphs on which packed niobium atoms are located in the X and Y directions.

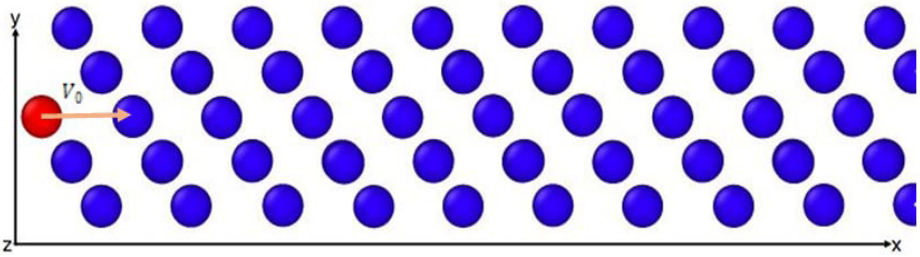


Fig. 1. Scheme of excitation of 1-crowdion in a niobium lattice with initial velocities v_0. Atom under external influence is marked in red; all other atoms are marked in blue

Рис. 1. Схематическое изображение возбуждения 1-краудиона в решетке ниобия с начальной скоростью v_0. Атом под внешним воздействием выделен красным цветом, остальные атомы – синим

For modeling and research, the method of molecular dynamics is used using the empirical potentials of interatomic interaction N in the LAMMPS software package [8].

With the Ovito visualization software for visualizing and analyzing atomic simulation data, you can see the structure of niobium and follow the formation of a crowdion and its dynamics through localization under external influence. Atomic mass m = 92.90638 amu. The crystal lattice of niobium consists of 82944 atoms with a size of 400×65×57. We use the eam potential [18] for describing the interatomic interaction.

2. Numerical results

In this paper, we study the dynamics of mass transfer by $N = 1$ crowdions induced in the niobium lattice by the set of directional impulse $p_0 = mv_0$, where m is a atomic mass and v_0 is the initial velocity, for a variation of v_0 within the range [7; 10] km/s. It is known that the crowdions in pure metals always propagate along the close-packed crystallographic direction, which is characterized by the minimal interatomic distance. Niobium has the bcc crystal lattice, and the <111> direction is characterized by the minimal distance. If the initial velocity is low, the external energy dissipates in the lattice through phonon oscillations. However, when the initial velocity exceeds a certain threshold level, the initial perturbation transforms to a soliton due to the nonlinear character of the interatomic interaction. This mode moves with the supersonic velocity and able to pass the energy in the long distances. The case of a soliton propagation is depicted by the shifts of the atomic of the close-packed row through which the soliton passes is shown in Fig. 2, *a* for the initial velocity v_0 = 6.9 km/s. Atoms shifts on the distance less than half interatomic distance a and relaxate back to initial sites after passing the crowdion. The soliton propagation is also accompanied by the intensive energy dissipation. The energy evolution of a soliton is represented in Fig. 3, *a*. It is seen that the soliton energy monotonically decreases in time. When the energy becomes lower than the threshold level, the soliton disappears and rest energy dissipates through phonons. But what happens if the initial impulse shifts an atom on the distance longer than a? In this case, the dynamic of a localized mode becomes significantly different. The dynamics of the localized mode for v_0 = 7.1 km/s are illustrated in the normalized atomic shifts in Fig. 2, *b* and the corresponding energy evolution in Fig. 3, *b*. It is shown that now the atoms through which the wave moves do not return back to the initial position but slowly replace the sites of the next atoms, which also begin to shift and replace the following atoms, and so on. This vibration mode is called by a crowdion, which present the wave passing not only energy, but also additional mass. Note that the crowdion is characterized by two stages, namely supersonic and subsonic ones. At the first stage the crowdion propagates with the supersonic velocity, but its energy quickly dissipated. As a result, the energy becomes insufficient for overcoming the potential barrier and the supersonic crowdion transforms to a soliton. However, the crowdion carries also

the interstitial atom and new mobile localized vibrational mode is formed around this atom. It is so-called the subsonic crowdion, which able to propagate in a very long with subsonic velocity. Comparison of the energy evolutions for the soliton and crowdions shown in Fig. 3, *a* and *b* demonstrates that the energy losses is very similar for them. However, there is a new increase in the energy in the plot, which corresponds to the subsonic crowdion formation. An increase in the initial velocity leads to elongation of a way which the crowdion overcomes during the supersonic stage. This case is exemplified by the normalized atomic replacements for $v_0 = 10$ km/s in Fig. 2, *c*. The energy evolution plotted in Fig. 3, *c* shows that at the initial stage of crowdion propagation the energy losses is very intensive, but noticeably decrease with $t > 0.1$ ps.

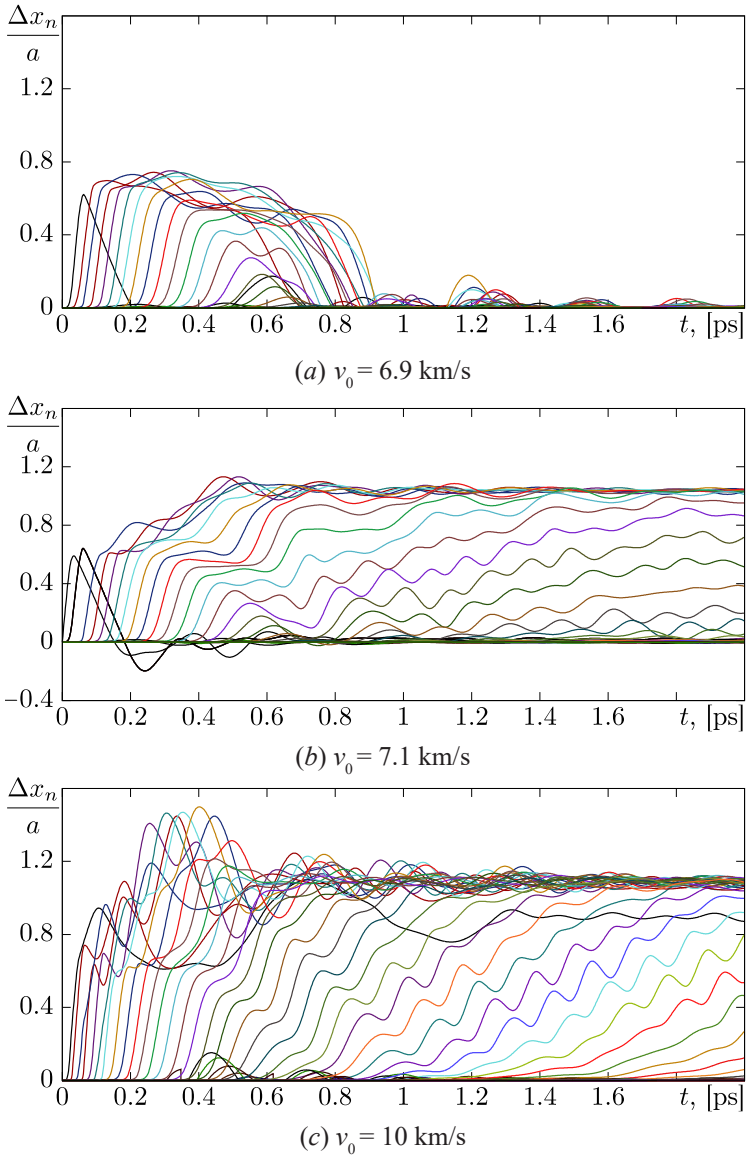
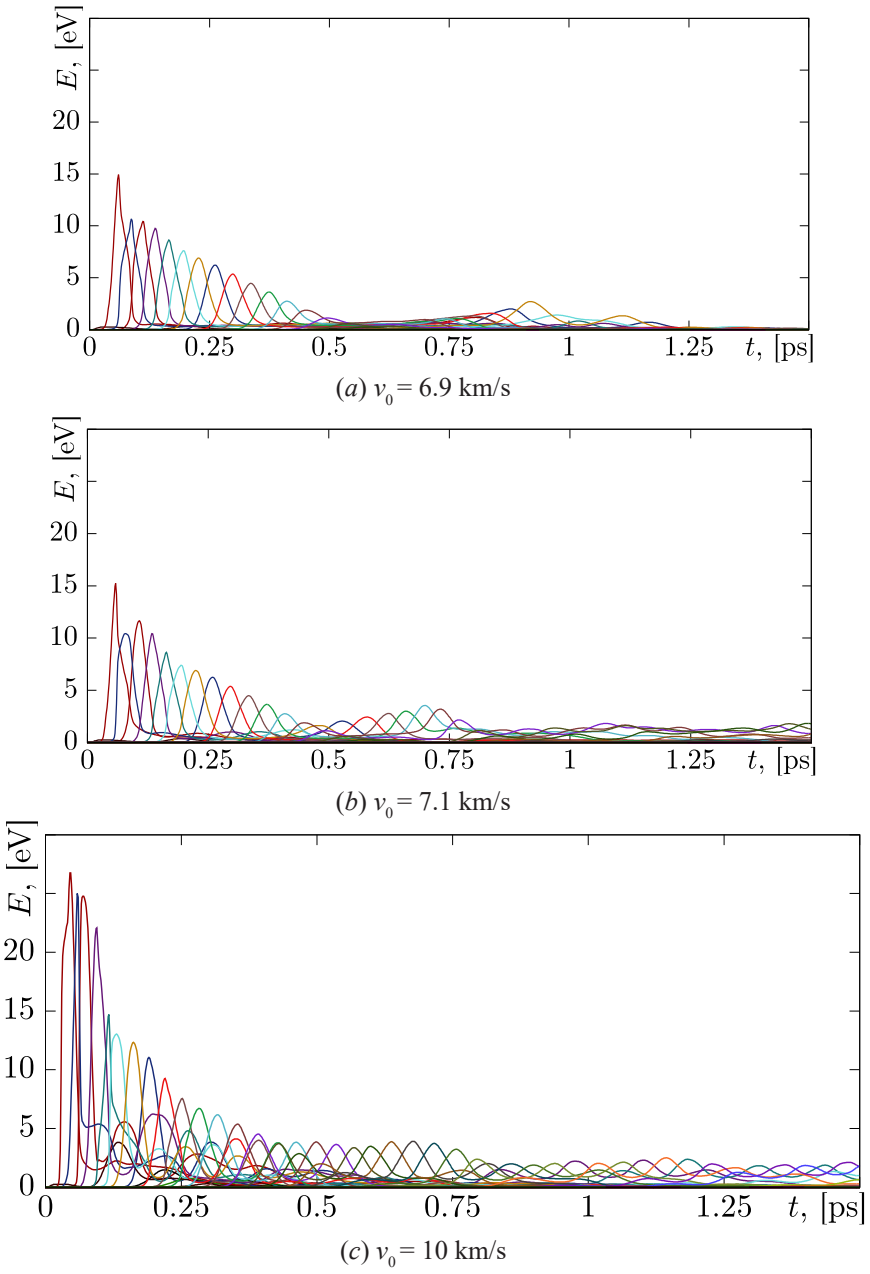


Fig. 2. Atomic displacements Δx_n normalized on interatomic distance *a* illustrate the propagation of soliton/crowdion along the close-packed atomic row in <111> crystallographic direction. The localized wave is excited for the initial velocity $v_0 = 6.9$ km/s (*a*), $v_0 = 7.1$ km/s (*b*) and $v_0 = 10$ km/s (*c*)

Рис. 2. Смещения атомов Δx_n, нормированные на межатомное расстояние *a* показывают распространение солитона/краудиона в плотноупакованном ряду в <111> кристаллографическом направлении. Локализованная волна возбуждается для $v_0 = 6{,}9$ км/с (*a*), $v_0 = 7{,}1$ км/с (*b*) и $v_0 = 10$ км/с (*c*)



(*a*) v_0 = 6.9 km/s

(*b*) v_0 = 7.1 km/s

(*c*) v_0 = 10 km/s

Fig. 3. Temporal evolution of the total energy E of atoms of the close-packed atomic row in <111> crystallographic direction, through which soliton/crowdion propagates. The localized wave is excited for the initial velocity v_0 = 6.9 km/s (*a*), v_0 = 7.1 km/s (*b*) and v_0 = 10 km/s (*c*)

Рис. 3. Временная эволюция полной энергии E атомов плотно упакованного атомного ряда в кристаллографическом направлении <111>, через которое распространяется солитон/краудион. Локализованная волна возбуждается при начальной скорости v_0 = 6,9 км/с (*a*), v_0 = 7,1 км/с (*b*) и v_0 = 10 км/с (*c*)

Conclusion

In this work, methods of molecular dynamics have been used to study the 1-crowdion in the crystal lattice of niobium subjected to high-speed impact. It is shown that crowdions can be formed by applying an initial impulse to one atom. It has been established that the crowdion propagates faster than the speed of sound in the material under study up to 0.5 ps, then transforms into subsonic crowdion. The mechanism of mass

transfer in the lattice at the zero temperature has been studied. Plots of the dependences of the normalized atomic displacement on time and the dependence of the total energy on time are calculated. It has been found that the intensity of energy dissipation through phonons increases with growth of the initial velocity.

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