Mechanism of remote vacancy emergence by a supersonic crowdion cluster in a 2D Morse lattice

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Abstract

The supersonic $M \times N$-crowdions are excited in a 2D lattice by giving sufficiently large initial velocity v to the $M \times N$ block of atoms along a close-packed direction, where N is the number of neighboring atoms in one close-packed row and M is the number of neighboring rows. In this study, dynamics of a pair of quasi-1D supersonic 1×2-crowdions moving in parallel close packed atomic rows separated by one non-excited atomic row (middle row) are investigated in 2D triangular Morse lattice by means of molecular dynamics simulations. We show that when a certain threshold excitation energy value is exceeded, the motion of these two 1×2-crowdions leads to creation of a remote vacancy in the middle row at a significantly long distance from the initiation point at

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the moment, when the supersonic stage of the crowdion propagation turns into subsonic one. This distance is directly proportional to the excitation energy of the 1×2-crowdion pair. The mechanism of vacancy formation is related to appearance of a Frenkel pair in the middle row, namely an immobile vacancy and an interstitial atom, which, together with the two interstitials in the outer rows, forms the stable subsonic 3×1-crowdion cluster. Thus, one can conclude that the crowdion propagation can be accompanied by not only mass transfer but also plays a role in the formation of atomic vacancies inside crystal lattices.

Keywords: crystal lattice, crowdion clusters, voidions, mass transfer, molecular dynamics simulations

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1. Introduction

Diffusion is responsible for many processes in materials such as defect structure evolution, phase transitions, etc. Generally there are two main mechanisms of lattice diffusion: motion of interstitial atoms and motion of vacancies. Both of these processes are thermally activated and associated with the lattice in a state of thermal equilibrium.

Non-equilibrium state of material caused by high energy external impacts is associated with enhanced diffusion. Under such conditions, new regimes of collective motion of atoms can emerge. These include rapid diffusion of atomic

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groups (islands) [1, 2] and one-dimensional motion of atomic groups characterized by movement of both compacted and rarefied lattice regions. The first case is related to motion of so-called crowdions and has been extensively studied in different crystal lattices [3, 4, 5, 6, 7, 8, 9, 10, 11, 12]. The case of sparsed one-dimensional region, i.e. a delocalized vacancy called *voidion*, has been studied much less in detail [13, 14, 15]. Molecular dynamics study of clusters in collision cascades has revealed the presence of both vacancy and interstitial clusters within the material, with the smaller fraction of vacancy clusters [16]. One-dimensional (1D) motion of such clusters turned out to be more energetically beneficial as compared to 3D one [17]. In the case of surface diffusion, the mechanism can change between hopping on the surface, direct exchange and crowdion-mediated exchange upon varying the surface biaxial strain state [18].

Different types of impact induced point defects simultaneously exist in a crystal lattice and can migrate, recombine and mutually affect each other. However, it is not always possible to unambiguously assess their contribution to the structure evolution. Vacancy formation as a result of surface exposure can significantly influence on the lattice dynamics in non-equilibrium conditions [19]. The presence of vacancy clusters near the surface has been experimentally revealed in Refs. [13, 20]. It has been demonstrated that voidions are quite mobile defects and their velocities can reach a significant fraction of the speed of sound in the material. This fact allows us to conclude that study of cooperative motion of vacancy-type defects is essentially important for understanding the fundamental issues of diffusion in lattices under non-equilibrium conditions.

The concept of supersonic $M \times N$-crowdion clusters in 2D lattices has been recently introduced and studied via molecular dynamics simulations [21, 22, 7, 5]. Such clusters are excited by giving sufficiently large initial velocity to a block of $M \times N$ atoms along a close packed direction. Here in the notation, N is the number of neighboring atoms in one close-packed row, and M is the number of neighboring atomic rows. In particular, it has been revealed that some crowdion clusters demonstrate stable dynamics and the distances traveled in supersonic mode can significantly exceed the distances of classical 1×1-crowdion [21]. The contribution of such supersonic $M \times N$-crowdions to mass transfer has been investigated in 2D triangular Morse lattices [21, 5, 7, 22].

The main purpose of this work is molecular dynamics study of the effects arising upon the excitation of two 1×2-crowdions in 2D Morse lattice in two parallel close packed atomic rows separated by a row where atoms are not initially excited.

2. Simulation details

Molecular dynamics has earlier proved to be a powerful tool for investigation of small scale phenomena associated with mass and energy transfer [23, 24, 25, 26, 27, 28, 29, 30, 31]. All atomistic simulations in the present study are carried out with the help of the Large-scale Atomic/Molecular Massively Parallel Simulator software package (LAMMPS) [32].

A well-known feature of the used simulation method is the quantitative and sometimes even qualitative dependences of the results on the interatomic potential [33, 8, 17]. In order to avoid this, in this study, the interatomic interactions are described via the classical pairwise Morse potential, allowing to mimic the main features that determine the defects dynamics, which can be expressed by the following formula:

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

where r is a distance between two atoms, and α, D, r_m are the parameters of the potential. The r_m determines the position of the minimum of the function $U(r)$ ($r = r_m$), D is the potential depth, and α is the bond stiffness. The units of energy, distance and time are chosen so that $D = 1$, $r_m = 1$ and atom mass $m = 1$. The value $\alpha = 5$ is fixed, and the cut-off radius is chosen to be $5a$. Thus all calculations in the present study are performed in dimensionless units.

Initially, before modeling crowdion excitation, the lattice is subjected to relaxation to obtain a minimum energy state and the equilibrium interatomic distance is found to be $a = 0.9655663$. The lattice dynamics is considered at zero temperature, i.e. in an absence of thermal vibrations. Calculations are performed with the use of the NVE thermodynamic ensemble presuming constant number of atoms, volume and energy in the system.

Due to the small spatial and temporal scale of the studied phenomena, the 2D computational cell containing 100×300 atoms arranged in a triangular lattice is chosen. Periodic boundary conditions are used along the two coordinate directions. The time step is $t = 0.001$ of dimensionless units.

The choice of initial conditions for the crowdion clusters excitation can drastically affect the path length, velocity and motion mechanism. For instance, an excitation of a crowdion by a molecule consisting of two and more atoms results in much more stable crowdion, which can travel longer distances as compared to one exited with a single atom [23, 27]. It should be noted that the dynamics of supersonic 1×1 and 1×2-crowdions is significantly different, although they both carry single interstitial atom. Supersonic propagation of classical 1×1-crowdion is accompanied by intense energy dissipation into the lattice and is energetically unfavorable. As a result, the crowdion rapidly slows down and quickly transforms into subsonic one. The movement of supersonic 1×2-crowdion is accompanied by much less energy dissipation, and the crowdion, even with a lower initial energy, can travel over longer distances as compared to supersonic 1×1-crowdion [21, 7]. In this connection, in the present work, 1×2-crowdions are considered and contrasted to the case of 1×1-crowdions addressed earlier in Ref. [15].

Initial conditions used in this study are as follows (see Fig.1). Two 1×2-crowdions are excited by applying initial velocities v to the two neighboring atoms in the top and bottom close packed rows along the rows (along the x-axis). The initial kinetic energy of each 1×2-crowdion is

$$E_0 = mv^2, \tag{2}$$

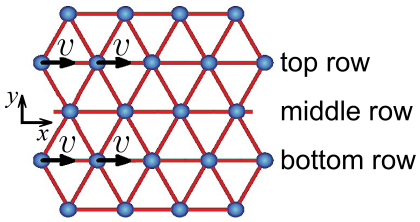

Figure 1: Schematic illustration of initial conditions for excitation of a pair of 1×2-solitons or 1×2-crowdions in 2D Morse lattice by giving velocities to the atom pairs in the top and bottom horizontal close-packed rows.

where $m = 1$ is the mass of the atom. All other atoms in the computational cell have zero initial velocities and all atoms have zero initial displacements.

3. Results and discussion

For sufficiently large excitation energy E_0, Frenkel pairs are formed in the top and bottom atomic rows. Two immobile vacancies and two supersonic 1×2-crowdions moving to the right in the top and bottom atomic rows emerge at the place of initiation. Interestingly, as will be shown below, a vacancy can appear in the *middle* row at a large distance from the point of initiation. Thus, the propagation of a pair of supersonic 1×2-crowdions in the top and bottom rows seemingly leads to a supersonic transport of a vacancy. The mechanism of vacancy generation in the middle row will be uncovered and it will be shown that it is different from the voidion mediated mechanism described in Ref. [15] for the case when supersonic 1×1-crowdions move in the top and bottom atomic rows.

If the excitation energy E_0 is insufficient for the creation of two Frenkel pairs then two compressive solitons are excited in the top and bottom rows. In this case, after the energy of initial kick is dissipated into the lattice, all the atoms return to their equilibrium positions and point defects do not appear in the lattice.

First, we consider the case of relatively small E_0 at which compressive solitons are excited, and then we focus on the case of the formation of topological defects, when the initial energy E_0 is sufficiently large.

3.1. Compressive solitons

The propagation of two 1×2-solitons excited with the energies $E_0 = 25$ in the top and bottom close packed rows is illustrated in Fig. 2. In (a), the distribution of total (kinetic plus potential) energies over the atoms is shown at time $t = 1.3$. Dark blue atoms have ground (minimal) energy and red color corresponds to maximal energy. The initiation point is close to the left end of the figure. Panels (b) and (c) show the time evolution of the normalized horizontal displacements of atoms, X/a, in the top and middle rows. The displacements of atoms in the

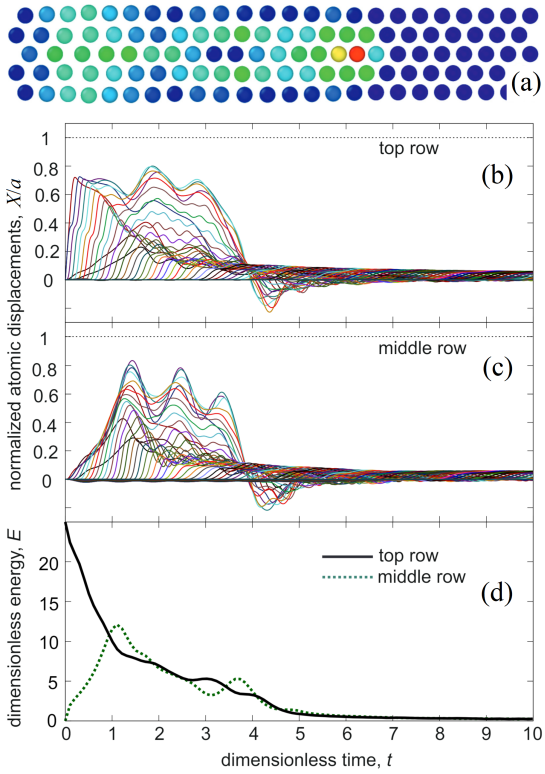

Figure 2: Propagation of two 1×2-solitons in the top and bottom layers excited with the initial energies of $E = 25$. (a) Crystal structure at $t = 1.3$ where atoms are colored according to their total (kinetic plus potential) energy. Dark blue corresponds to the ground energy and red to maximal energy. (b,c) Normalized atomic displacements along the x-axis from equilibrium lattice sites, X/a, for the top and the middle atomic rows, respectively. (d) Total energy of the atoms in the top row (solid line) and in the middle row (dashed line) as the functions of time.

bottom row are not shown because they coincide with the top row due to the symmetry of the initial conditions. Panel (d) shows net total energies in the top (same with the bottom) and in the middle rows as the functions of time.

As seen from Fig. 2(b) and (c), initially, the solitons run only in the outermost rows with the supersonic velocity. After a while, the soliton energy in the middle row begins to increase [see in (d)], while the energy in the outermost rows starts to decrease. In (c), one can see that the atomic displacements in the middle row increase as energy of the atoms in this row increase. The energy of the middle row reaches its maximal value at $t \approx 1.2$, and becomes even greater than in the outermost rows. This is the clear evidence of the energy exchange between the atomic rows, which can be explained by the Cherenkov radiation [34] occurring during propagation of the 1×2-solitons. Namely, part of the energy from the outermost atomic rows is pumped into the middle row,

which is thus accelerated. It is interesting to note that the displacements of atoms in the top, middle and bottom rows grow above $a/2$, but eventually they are pushed by the lattice to the initial positions. It can be seen that the maxima of atomic displacements in the middle row correspond to minima in the outermost rows. This phenomenon can be explained as follows. Firstly, the atoms of the outermost rows are maximally displaced from the equilibrium positions, while the atoms in the middle row keep them from moving into the adjacent sites. After that, the middle row atoms are accelerated, while the outermost atoms hold them. This process is repeated several times, as seen in Fig. 2(b) and (c). Eventually, the energy of the initial kick is dissipated into the lattice and the energies of the middle and outermost rows approach zero value [see in (d)].

3.2. Crowdions and vacancies

If the initial energies used for excitation exceed a certain threshold level of $E_0 \approx 27$, then the dynamics of propagation of a pair of 1×2-crowdions differs greatly as compared to that for 1×2-solitons. In Fig. 3, the case of $E_0 \approx 27.2$ is presented. In (a) the crystal structure and the energy distribution over atoms is shown, with the interstitial atoms marked with crosses. In (b) and (c), the time evolution of the normalized component of horizontal displacements of the atoms in the top and middle rows are shown. In (d), one can see the net energy of the atoms in the top and middle rows. The supersonic stage of the crowdion motion occurs in the outermost rows up to $t \approx 1.2$, while only low-amplitude oscillations are observed in the middle row. The energy exchange between the rows takes place similar to that for the solitons. In the supersonic stage, the crowdion energy in the outermost rows decreases intensively (crowdions decelerate), while the energy in the middle row increases. At $t \approx 1.2$ the two supersonic 1×2-crowdions in the outermost rows become subsonic, but the structure with two slowly moving interstitials in the outermost rows is energetically unfavorable and a new Frenkel pair appears in the middle row. As a result, an immobile vacancy appears in the middle row and the third interstitial together with the interstitials in the outermost rows create a subsonic 3×1-crowdion moving to the right. Subsonic motion of the 3×1-crowdion can be seen in (b) and (c), where atom trajectories raise from $X/a = 0$ to $X/a = 1$. Oscillations of the curves indicate that the subsonic crowdion carry the internal vibrational mode [35]. It is clearly seen in Fig. 3(d) that after the supersonic stage the energies of the outermost and the middle rows become practically the same. Moreover, after formation of subsonic 3×1-crowdion, the energy slightly decreases in a fairly short time and further remains almost constant and equal to about 5. Thus, propagation of a pair of supersonic 1×2-crowdions in the outermost rows is accompanied by a birth of a vacancy at a distance from the initiation point, more precisely, at the point where the supersonic motion of the crowdions transforms into subsonic. That is why, the distance at which the formation of the vacancy in the middle row occurs is determined by the duration of the supersonic stage of initially excited 1×2-crowdions.

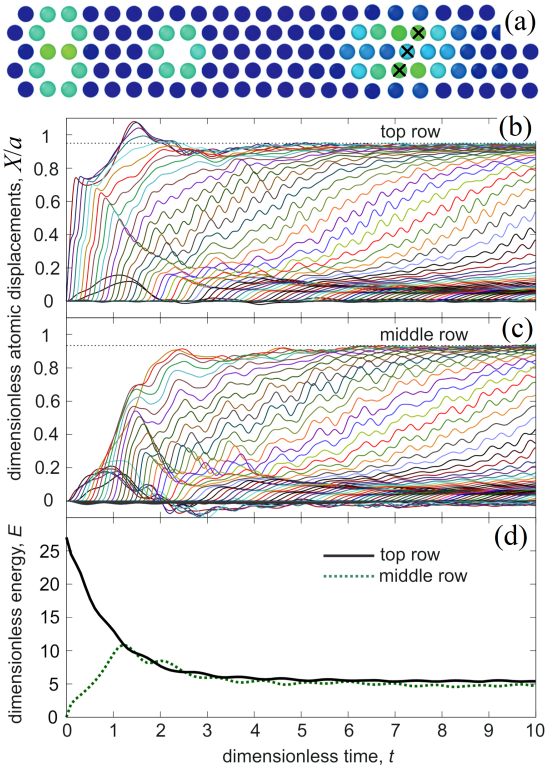

Figure 3: Propagation of two supersonic 1×2-crowdions in the outermost rows excited with the initial energies of $E_0 = 27.2$ and formation of a vacancy in the middle row and a subsonic 3×1-crowdion. Interstitial atoms are shown by crosses. In (a) atoms are colored according to their total energy with dark blue (red) color used for minimal (maximal) energy. (b) and (c) Normalized atomic displacements along x-axis, X/a, as the functions of time for the top and the middle atomic rows, respectively. (d) Net energy of the atoms in the top (solid line) and middle (dashed line) rows as the functions of time.

An increase of the excitation energy up to $E_0 = 40$ results in a significantly longer (up to $t \approx 2.3$) supersonic stage of motion of 1×2-crowdions in the outermost rows, as illustrated in Fig. 4(b). Firstly, the supersonic crowdions move only in the outermost rows. During the supersonic stage, the crowdions propagate emitting the energy into the crystal and into the middle row, see Fig. 4(d). When the crowdion energy is no longer enough to overcome the potential barrier, the fast front parts of both crowdions transform into the solitons, and the subsonic crowdion is formed. This is accompanied by the formation of an additional Frenkel pair in the middle row. The interstitial atom forms the middle part of the subsonic 3×1-crowdion and it runs to the right moving away from the immobile vacancy. The distance from the initiation point, at which formation of the vacancy in the middle row occurs, becomes significantly longer, compare Figs. 3(a) and 4(a'). As seen in Fig. 4(b), the supersonic crowdion

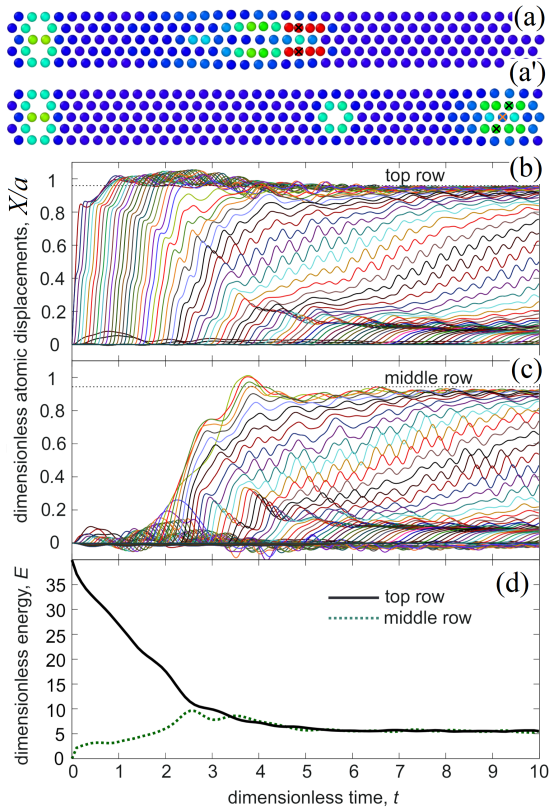

Figure 4: Same as in Fig. 3, but for $E_0 = 40$. Panels (a) and (a') show the crystal structures at $t = 1.6$ and 6.0, respectively.

(in the outermost row) constantly decelerates (distance between the trajectories increases). The energy exchange between the outermost and the middle rows in in Fig. 4(d) takes longer time in comparison with the case presented in Fig. 3(d). This means that the faster 1×2-crowdions moving in the outermost rows interact weaker with the middle row.

The distance which the 1×2-crowdions pass during the supersonic stage as a function of the initial excitation energy E_0 is depicted in Fig. 5. It is seen that there is the threshold level of the initial excitation energy above which a vacancy appears in the middle row. The distance L/a almost linearly increases with increase of initial excitation energy E_0. Thus, the distance between the initiation point and the vacancy formed in the middle row can exceed 100 interatomic distances if the initial excitation energy is high enough.

3.3. Mechanism of vacancy formation in the middle atomic row

Our studies show that the propagation of two subsonic crowdions with interstitial atoms in the top and bottom atomic rows is impossible because this defect

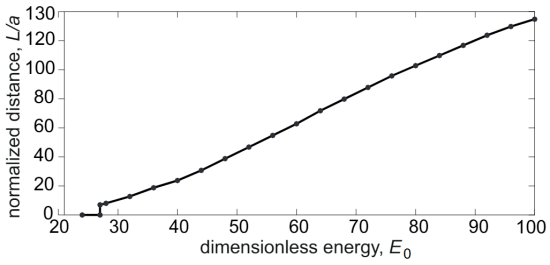

Figure 5: Dependence of the normalized distance between the crowdion initiation point and the vacancy formed in the middle row on the initial excitation energy in the outermost atomic rows.

configuration has relatively high energy. There are two ways of structure transformation that lead to the reduction of the potential energy. In order to study these transformations, let us excite two subsonic crowdions in the outermost atomic rows. Single crowdion can be excited using the ansatz [35]

$$\begin{array}{l} x_n(t) = \frac{a}{2}\{1 - \tanh[\beta(n - x_0 - Vt)]\}, \\ y_n(0) = 0, \quad \dot{y}(0) = 0. \end{array} \tag{3}$$

Here n is the index numbering atoms in a close-packed row, β is the inverse width of crowdion (anti-kink) and V is the crowdion propagation velocity. Initial position of the subsonic crowdion is x_0. All other atoms in the computational cell have zero initial displacements and velocities. It should be pointed out that the ansatz Eq.(3) gives not exact, but *approximate* initial conditions for crowdion excitation. The parameter β for given crowdion velocity V was defined earlier by the try and error method [31] to achieve a propagating crowdion with low energy dissipation.

Two standing crowdions placed at $t = 0$ in the top and bottom rows with the use of the ansatz Eq. (3) with $\beta = 0.3$, $x_0 = 80$ are shown in Fig. 6(a). Interstitials in the figures are marked with the crosses and the two vacancies are far to the left of the interstitials and do not affect the transformation of the structure. If the crowdions in the top and bottom rows have zero initial velocities ($V = 0$), then structure relaxation results in the transformation of the initial configuration into a 2×1-crowdion in the close-packed rows inclined to the horizontal ones, as shown in Fig. 6(b). Crowdions with initial velocity $V = 0.2$ transform into a vacancy in the middle row and a subsonic 3×1-crowdion, as presented in Fig. 6(c). The subsonic 2×1- and 3×1-crowdions in (b) and (c), respectively, are stable and highly mobile, being able to move along the close-packed direction [7]. These defects can be regarded as the small prismatic dislocation loops.

In our simulations presented in Sec. 3.2, the supersonic crowdions moving in the top and bottom rows transformed into the subsonic ones and then they evolved into a vacancy in the middle row and a 3×1-crowdion, as shown in Fig. 6(c).

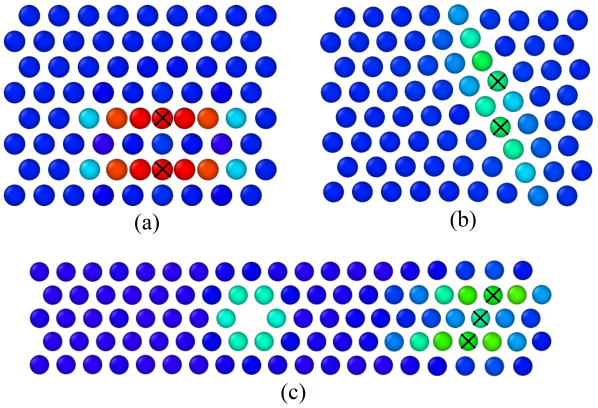

Figure 6: (a) Two subsonic crowdions at $t = 0$ induced in the top and bottom rows using the ansatz Eq. (3) with $\beta = 0.3$ and $x_0 = 80$. Atoms are colored according to their total energy. Two possible scenarios of structure relaxation are shown in (b) for zero initial velocities $V = 0$ at $t = 15$ and in (c) for $V = 0.2$ at $t = 5$. Interstitials are marked with crosses. Two vacancies are located far to the left of the interstitials and do not affect the transformation of the structure.

4. Conclusions

Employing molecular dynamics simulations, we have performed the study of propagation of two supersonic 1×2-crowdions in the two parallel close-packed rows separated by one row in triangular Morse lattice. The main conclusions are as follows.

- If the initial energy E_0 given to the system in a way shown in Fig. 1 is sufficient for excitation of two Frenkel pairs, then two supersonic 1×2-crowdions are excited and mass transfer takes place, see Fig. 3 or 4. If the energy is insufficient, then a pair of compressive solitons appear and, after the initial energy is dissipated by the lattice, all atoms return to their equilibrium positions, see Fig. 2.

- Supersonic 1×2-crowdions moving in the top and bottom rows give a part of their energy to the atoms of the middle row and the rate of the energy transfer is faster for crowdions moving with a smaller supersonic speed.

- Due to energy radiation, the supersonic 1×2-crowdions slow down and eventually transform into subsonic ones. At the point of transformation, a new Frenkel pair appears in the middle row. The newly born vacancy is immobile, while the new interstitial together with the two existing ones form a subsonic 3×1-crowdion, see Fig. 3(a) or 4(a').

- The distance between the newly born vacancy and the initiation point is nearly proportional to the excitation energy E_0 and can be greater than hundred of interatomic distances, see Fig. 5.

The final important remark is that the mechanism of the appearance of a vacancy far from the initiation point described here is very much different from that reported in the work [15], although in both works it looks like a supersonic vacancy jump along the middle row takes place. In Ref. [15], not supersonic 1×2-crowdions but supersonic 1×1-crowdions were excited in the top and bottom atomic rows. The 1×1-crowdions create an extended vacancy called *voidion*, which can give birth of a normal localized vacancy at any point along the voidion. The mechanism of vacancy generation in the middle row reported in the present study is not related to the voidion formation.

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