Regimes of mass transfer in a 2D crystal in nonequilibrium states

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Abstract. A variety of new technologies associated with the severe impact on materials have been developed recently. The promotion of these technologies is, in turn, associated with the stability of the structure and properties of materials under nonequilibrium conditions. It is well known that under such conditions new mechanisms of structure evolution can occur. The study of these mechanisms is an important task of modern materials science. In our work, we present the results of an analysis of possible scenarios of impact induced mass transfer in a two-dimensional crystal with a Morse interaction potential including a topological compression soliton, a crowdion complex and a moving vacancy – a voidion. The influence of the initial impact energy distribution is analysed. The obtained results contribute to the fundamental understanding of mass transfer processes under nonequilibrium conditions.

1. Introduction

Diffusion is a process basically responsible for all processes occurring in a material, including the evolution of a defect structure, phase transition, and others. Enhancement of diffusion-type processes is often observed in the case of a nonequilibrium state of materials associated with extreme external impacts. Generally, there are two main mechanisms of diffusion – the motion of vacancies and the motion of interstitial atoms; the first being more energy demanding [1]. However, both of these processes are discrete and can be related to the equilibrium state of the lattice. In case of nonequilibrium conditions associated with high energy impacts, new modes of collective atomic motion can be activated. Among them, one can recall the rapid diffusion of atomic clusters (islands) [2] and one-dimensional (1D) motion of atomic groups that can be realized by the motion of both compacted and rarefied lattice regions.

The case of a sparsed one-dimensional region, being a delocalized vacancy, is called a voidion, and this object has been less studied [3]. Recent studies have revealed that the mass transfer efficiency of the mentioned dynamic point defects depends essentially on their initial configuration and can increase considerably when not a single but several atoms are involved in one dimensional motion [4–7]. It was also demonstrated that when several crowdions propagate in neighboring parallel rows, they exchange energy with each other that inevitably influences the scenario of the evolution of the defect structure [8–
This work is devoted to the analysis of the influence of the initial impact energy on the propagation scenario of crowdion ensemble excited in three parallel crystallographic rows.

2. Simulation details

The investigation was performed by the method of atomistic simulation due to the small spatial and temporal scale of the phenomena studied. Molecular dynamics has earlier been proved to be a powerful tool for the investigation of small scale phenomena associated with mass and energy transfer [4,7–9], nonlinear dynamics of the lattice [11–14], and the evolution of mechanical characteristics of the material upon external loading [15–20], analysis of phase transformations [21–24] and many other applications [25-26]. The calculations were done for the calculational cell forming a 2D lattice with a size of 100 x 300 interatomic distances. Boundary conditions are periodic in all directions. A Cartesian coordinate system is used, with the X-axis coinciding with one of the densely packed directions. The interaction between particles in a triangular lattice is determined using the Morse potential, described elsewhere [5,10].

The main attention is paid to the processes associated with the transfer of mass and energy in the crystal by means of the M-crowdion, which is initiated by applying the initial velocities simultaneously to three atoms in three adjacent closely packed crystallographic atomic rows, i.e. M = 3 (see figure 1 a). We have analyzed the development of the defect structure evolution scenario for several course groups of initiation velocity combinations resulting in different types of relaxation path. Thus, the major groups of principally different cases can be distinguished as follows (1) \( v_1 = v_3 < v_2 \); (2) \( v_1 = v_3 > v_2 \), (3) \( v_1 = v_3 >> v_2 \), (4) \( v_2 > 0, \ v_1 = v_3 >> v_2 \), (5) \( v_2 < 0, \ v_1 = v_3 >> v_2 \) marked hereinafter as A,B,C,D and E modes respectively. Each of these modes results in different combination of point defects emerged as the result of the initial impact.

3. Results and discussion

The main purpose of this work is the investigation and analysis of the effects arising upon the excitation of an M-crowdion cluster with different initial velocities in adjacent atomic rows. The initial kick of the atom results in its shift from the equilibrium position. The resulting scenario of both the excitation propagation dynamics and the resulting defect structure depends on two main parameters, namely the initial velocity of the kick and the ratio of initial velocities of the atoms involved in the M-crowdion (3 atoms in the considered case). The former defines the ability of the affected atoms to overcome the potential barrier of vacancy formation and initiation of a moving soliton type object with 1D locally increased density (crowdion). If the energy provided at the initial moment is below the potential barrier threshold, one can expect the formation of a topological soliton. Thus, due to the presence of inevitable cone type radiation, the crowdion motion is a subject of the permanent complicated self-regulated process of energy exchange defining the motion dynamics and corresponding stress-strain state in local areas affected by the impact. The major issue concerns the difference between the values of energy provided to atoms located in the middle and edge rows.

Table 1. Summarization of possible scenarios of crowdion propagation for different ratios and amounts of emerging energies.

| Mode | Scenario |
|------|----------|
| A | Propagation of a compression soliton (without the appearance of atomic vacancies) or a crowdion (with the appearance of prismatic vacancies in 3 adjacent atomic rows) |
| B | Propagation of a soliton \( \Rightarrow \) the appearance of a vacancy at a certain distance from the starting point in the median row (voidion) and of a quasi-1D subsonic crowdion |
| C | Propagation of a supersonic crowdion with the emergence of two vacancies at the starting point in the edge rows \( \Rightarrow \) the appearance of a vacancy remote from the starting point in the median row (voidion) and of a M = 3-subsonic crowdion |
| D | Propagation of a supersonic crowdion with the emergence of two vacancies at the starting point in the edge rows \( \Rightarrow \) the appearance of a voidion and a M = 3-subsonic crowdion \( \Rightarrow \) their... |
subsequent merger ⇒ forming a $M = 2$-subsonic crowdion propagating in another close-packed direction

E Propagation of a supersonic $M = 3$-crowdion ⇒ the appearance of a voidion (V1), $M = 3$-subsonic crowdion (Cr1) and of the additional Frenkel pair (voidion (V2) + a quasi-1D subsonic crowdion (Cr2)) ⇒ subsequent merger of V1 with Cr1 and of V2 with Cr2 ⇒ forming a $M = 2$-subsonic crowdion propagating in the same or another close-packed direction

F The same as for regime E but merging of V2 and Cr2 is absent. V2 remains at the same place, while Cr2 moves to the starting place, loses their stability and transforms to an interstitial.

Figure 1. (a) Scheme of the initial crowdion complex excitation, propagation of the M-crowdion induced by the initial impact with velocities for the initial velocities (b) $v_{1,3} = 10$ and $v_2 = 8$ (regime A) (c) $v_{1,3} = 9$ and $v_2 = 0.5$ (regime B) (d) $v_{1,3} = 12$ and $v_2 = 4$ (regime C) (e) $v_{1,3} = 11$ and $v_2 = 3$ (regime D). (f) Summarizing map of modes and propagation distances of the voidion on the plane of initial velocities ($v_2$, $v_1$). The A mode on the mode map corresponds to the propagation of the M-soliton without the formation of a voidion, and the B - F modes correspond to the voidion propagation. The crowdion propagation distance is indicated by the color scale bar on the bottom panel.

Table 1 presents the summarization of the possible scenarios of crowdion propagation for different ratios and amounts of emerging energies. The values of the applied velocities are presented in the regime map in figure 1 f. Thus, one can see that the region of small velocities corresponds to the propagation of the compression soliton because the initial energy in this case is insufficient to overcome the potential barrier of bond breaking. An increase in velocity results in a switch to regimes B and C where the propagation of a supersonic crowdion with the emergence of two vacancies takes place (figure 1 c-d). One of the most interesting cases in this study is the situation of $v_1 = v_3 >> v_2, v_2 < 0$. In this case, due to energy exchange due to Cherenkov radiation 27, a vacancy is formed in the middle row, which, under the influence of the stress field of adjacent rows, moves forward, forming a voidion (figure 1 d-e). The reason for the emergence of a voidion with sufficiently large propagation distances is an open question and requires a detailed analysis.

4. Conclusions
We have performed a molecular dynamics study of the propagation regimes of the triple crowdion complex with variable initial velocities in all three rows. It was revealed that the scenario of the point defect evolution strongly depends on the velocities value and ratio. Three general scenarios, each having several features can be distinguished, namely (i) propagation of a topological compression soliton, (ii) propagation of a 3-crowdion complex with a triple vacancy at the initiation site and (iii) propagation of two crowdions and a voidion in the middle row in case of zero or negative initial velocities. The obtained
results contribute to a fundamental understanding of the defect structure evolution under nonequilibrium conditions.

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