

# Scenarios of mass transfer in fcc copper: the role of point defects

A M Bayazitov<sup>1</sup>, E A Korznikova<sup>2</sup>, I A Shepelev<sup>3</sup>, A P Chetverikov<sup>3</sup>,  
S Kh Khadiullin<sup>4</sup>, E A Sharapov<sup>4</sup>, P V Zakharov<sup>5</sup>, S V Dmitriev<sup>2,6</sup>

<sup>1</sup> Bashkir State University, 32 Zaki Validi st., 450000 Ufa, Russia

<sup>2</sup> Institute for Metals Superplasticity Problems of RAS, 39 Stepan Khalturin st.,  
450001 Ufa, Russia

<sup>3</sup> Saratov Chernyshevsky State University, 83 Astrakhanskaya st., 410012 Saratov,  
Russia

<sup>4</sup> Ufa State Aviation Technical University, 12 K. Marx st., 450008 Ufa, Russia

<sup>5</sup> Altai State Humanitarian and Pedagogical University, 53 Korolenko st., 659333  
Biysk, Russia

<sup>6</sup> National Research Tomsk State University, 36 Lenin Ave., 634050 Tomsk, Russia

E-mail: elena.a.korznikova@gmail.com

**Abstract.** It is well known that mass transfer in crystalline materials in most cases is assisted by the motion of point defects. Interstitial atoms are highly mobile, because they have relatively small migration energy as compared to vacancies. Crowdion is a type of interstitial defect being an extra atom inserted in a closely packed atomic row and having even smaller migration energy than an interstitial atom occupying a pore. In this work, we study scenarios of collisions of supersonic  $N$ -crowdions in Cu by means of molecular dynamics simulation. It was found that 2-crowdions collide leading to the emergence of two new 2-crowdions, which is an example of the soliton-type interaction.

## 1. Introduction

The mass transfer by the point defects in crystalline solids facilitates structure transformations occurring during plastic deformation, heat treatment and irradiation [1-3]. In thermal equilibrium, vacancy migration is the main mechanism of diffusion, while in nonequilibrium conditions, interstitials also contribute noticeably to the mass transfer [1]. The interstitial atoms occupying the pore are relatively immobile, while those located in a closely packed atomic row, called crowdions, are highly mobile. Interestingly, crowdions usually have a lower potential energy than immobile interstitials [4]. Crowdions can be at rest, and they can move both with subsonic and supersonic velocities. Standing or subsonic crowdions have a kink profile, the width of which is typically half a dozen of atoms. Often they can bear a vibrational mode with a frequency above the phonon spectrum [5,6]. In this case, one can speak about a combination of a discrete breather and a crowdion, which is an object of particular importance because discrete breathers can localize energy [7-18], thus promoting the generation and/or migration of defects. Supersonic crowdions are strongly localized on a single atom. Recently, the notion of supersonic  $N$ -crowdions has been introduced [4-6], where not one, but  $N$  atoms move simultaneously at high speed along a close-packed atomic row. It has been

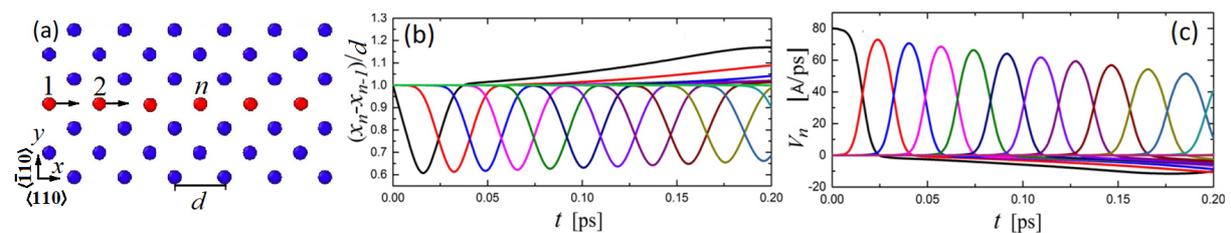


shown that  $N$ -crowdions are very mobile and much more efficient in the mass transfer as compared to classical 1-crowdions [4-6].

Interest in the study of moving crowdions in crystals is stimulated by recent experimental observation of annealing of defects deep inside a germanium crystal after surface plasma treatment [19], and also in connection with the study of tracks visible in mica crystals with the naked eye [20-22]. Crowdions can make a significant contribution to the mass transfer observed in metals and alloys during severe plastic deformation [1-3]. It has been shown that severe plastic deformation even at room temperature can stimulate phase transformations occurring in the absence of deformation at much higher temperatures [1,4]. These phase transitions occur very quickly and are accompanied by accelerated mass transfer, which cannot be explained only by conventional mechanisms, such as bulk and grain boundary diffusion, even in the presence of a high concentration of vacancies [1]. Direct experimental observation of crowdions moving at supersonic speed is a serious technical problem, so atomistic modeling can be extremely useful for studying them. The aim of this work is to study the motion and collisions of supersonic  $N$ -crowdions in a fcc Cu crystal.

## 2. Simulation details

In this paper, the fcc lattice of copper with the lattice parameter  $a = 3.615 \text{ \AA}$  and the interatomic distance  $d = a/\sqrt{2} = 2.556 \text{ \AA}$  is considered. Simulations are carried out using the LAMMPS package, which includes the EAM many-body interatomic potential for Cu. The  $x$  and  $y$  axes are oriented along the close-packed crystallographic directions  $\{110\}$  and  $\{\bar{1}10\}$ , respectively, and the  $z$  axis is oriented along the  $\{001\}$  direction (figure 1a). The number of translational cells along the  $x$ ,  $y$  and  $z$  axes was equal to 20, 4 and 2, respectively. The total number of atoms in the simulation cell was equal to 1280. Note that supersonic crowdion produces perturbations only in a certain cone behind it. Periodic boundary conditions are used. Thermal vibrations were not introduced, which means that simulations were carried out at 0 K.  $N$ -crowdion is excited by giving equal initial velocity  $V_x$  to  $N$  neighbouring atoms in a close packed atomic row along the row. The initial velocities of all other atoms and the initial displacements of all atoms are equal to zero. Thus, the total energy of the system is equal to the kinetic energy of the atoms excited at  $t=0$ .



**Figure 1.** (a) Simulation setup. Cu atoms projected to  $\{001\}$  plane. Atoms of one close-packed atomic row are shown in red, they are numbered by index  $n$ .  $N$ -crowdion is excited by giving initial velocities to  $N$  neighbouring atoms along the row (the case of  $N=2$  is shown). (b) Interatomic distances normalized to equilibrium distance  $d$  and (c)  $x$ -component of velocities for the atoms in the row where classical 1-crowdion moves, as a functions of time.

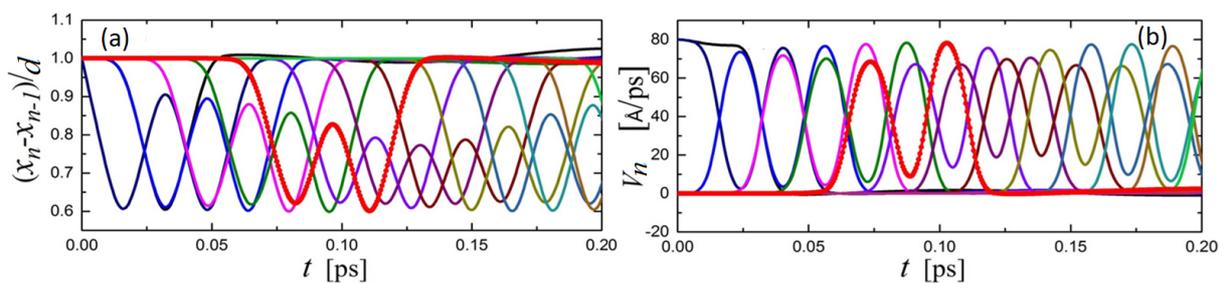
## 3. Simulation results and discussion

First, we show the dynamics of 1-crowdion moving along the  $x$  axis in the close-packed row (figure 1 a). The initial velocity  $V_x$ , given to a single atom, was  $80 \text{ \AA/ps}$ . The distances between neighbouring atoms normalized to equilibrium distance  $d$  as a function of time are shown in figure 1 b. One can see that the minimal distance between two atoms, normalized to  $d$ , is about 0.6, so that the condition of self-focusing motion,  $(x_n - x_{n-1})/d > 1/2$ , is satisfied [4]. Under this condition, 1-crowdion is able to propagate a relatively long distance. Figure 1 b also shows that the distance between neighboring atoms may exceed the equilibrium value  $(x_n - x_{n-1})/d = 1$  due to the oscillations of atoms behind the

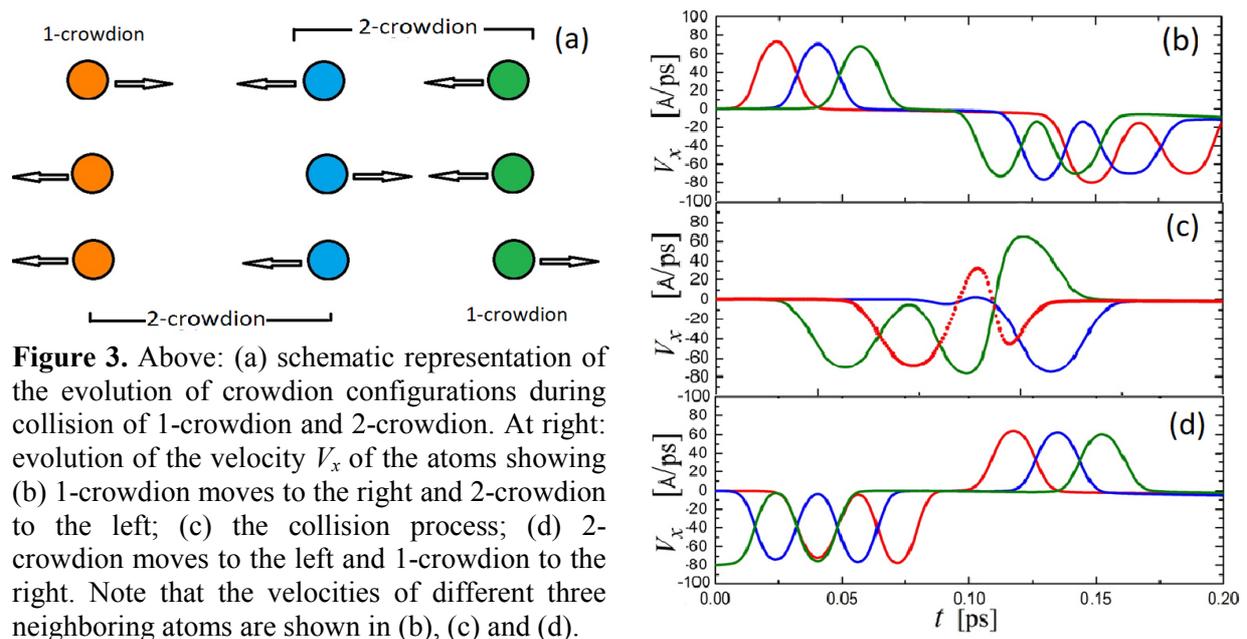
crowdion. The velocities of atoms in the row where 1-crowdion moves are shown in figure 1 c (the  $x$ -component of the velocity is shown). It can be seen that 1-crowdion continuously radiates its energy, and the velocities of atoms gradually decrease with time, starting from the initial value of 80 Å/ps.

In figure 2 a, b we plot the same as in figure 1 b, c, but for 2-crowdion propagating along the close-packed row in fcc Cu. Here again, the condition of self-focusing motion,  $(x_n - x_{n-1})/d > 1/2$ , is satisfied [4] because  $(x_n - x_{n-1})/d$  is not smaller than 0.6. However, the dynamics of energy radiation by 1- and 2-crowdions differs considerably. The function  $V(t)$  for the case of 2-crowdion, plotted in figure 2 b demonstrates the same average level of  $V$  during the simulation time, while for 1-crowdion (figure 1 c), a noticeable decrease in velocity is observed within the same simulation time. Thus, 2-crowdion demonstrates a more robust propagation as compared to 1-crowdion.

The next step of our study is to analyze the collision scenarios between 1- and 2-crowdion, moving toward each other from the left and right, respectively. Figure 3 a schematically shows the collision process. At the first stage, the 1-crowdion collides with the first atom of the 2-crowdion, resulting in their repulsion and momentum exchange. Then the two atoms, which initially belonged to the 2-crowdion, collide and exchange by the momentum. As a result, at the end of the collision we have 1-crowdion moving to the right and a new 2-crowdion moving to the left, as if they passed through each other.



**Figure 2.** (a) Interatomic distances normalized to the initial distance  $d$  and (b) velocities of the atoms along  $x$ -axis as functions of time, showing propagation of 2-crowdion in a close-packed atomic row of Cu. The curves for one particular atom are highlighted by dots both in (a) and (b).



**Figure 3.** Above: (a) schematic representation of the evolution of crowdion configurations during collision of 1-crowdion and 2-crowdion. At right: evolution of the velocity  $V_x$  of the atoms showing (b) 1-crowdion moves to the right and 2-crowdion to the left; (c) the collision process; (d) 2-crowdion moves to the left and 1-crowdion to the right. Note that the velocities of different three neighboring atoms are shown in (b), (c) and (d).

To provide additional information on the collision between 1- and 2-crowdion, in figure 3 b-d we plot the  $x$ -component of the velocity for the atoms in the close-packed atomic row where the collision takes place. In figure 3 b the three nearest atoms which are to the left of the collision point are shown. In figure 3 c the three nearest atoms at the collision point are shown. Finally, in figure 3 d the three nearest atoms which are to the right of the collision point are shown. Thus, in figure 3b, first the 1-crowdion passes through the three nearest atoms with positive velocity and then the 2-crowdion, generated as a result of the collision, passes through these atoms with a negative velocity. The results shown in panels c and d are interpreted in a similar way.

#### 4. Conclusions

The investigation of the motion and collision of supersonic 1- and 2-crowdion in Cu was performed by means of molecular dynamics. The simulation results can be summarized as follows:

(i) Supersonic crowdions in Cu can propagate for long distances along a close-packed atomic row with the velocities of atoms satisfying the self-focusing condition [4].

(ii) 2-crowdion propagates a longer distance and radiates less energy than 1-crowdion.

(iii) The collision of 1-crowdion and 2-crowdion results in their passing through each other, demonstrating soliton-like interaction.

#### Acknowledgement

For A.M.B., I.A.Sh. and A.P.Ch. the research was supported by the Russian Science Foundation, grant no. 16-12-10175 (obtaining numerical results). E.A.K. and S.V.D. were supported by the Russian Foundation for Basic Research, grant no. 17-02-00984-a (design of the research and writing the paper). P.V.Z. gratefully acknowledges the support of Russian Foundation for Basic Research, grant no 18-42-220002 r\_a (discussion of results). The work was partly supported by the State Assignment of IMSP RAS.

#### References

- [1] Korznikova E A, Schafner E, Steiner G and Zehetbauer M 2006 *TMS Annual Meeting* **2006** 97
- [2] Konkova T, Mironov S, Korznikov A, Korznikova G F, Myshlyaev M and Semiatin S 2015 *J. Alloys Compd.* **629** 140
- [3] Wang L, Wang Y, Zhilyaev A P, Korznikov A V, Li S, Korznikova E A and Langdon T 2014 *Scripta Mater.* **77** 33.
- [4] Dmitriev S V, Medvedev N N, Chetverikov A P and Zhou K 2017 *Phys. Status Solidi RRL* **11** 1700298
- [5] Chetverikov A P, Shepelev I A, Korznikova E A, Kistanov A A, Dmitriev S V and Velarde M G 2017 *Comput. Condens. Matt.* **13** 59
- [6] Dmitriev S V, Korznikova E A and Chetverikov A P 2018 *J. Exp. Theor. Phys.* **126** 347
- [7] Dmitriev S V, Korznikova E A, Baimova Y A and Velarde M G 2016 *Physics-Uspokhi* **59** 446
- [8] Korznikova E A, Fomin S Yu, Soboleva E and Dmitriev S V 2016 *JETP Lett.* **103** 277
- [9] Barani E, Lobzenko I, Korznikova E A, Soboleva E, Dmitriev S V, Zhou K and Marjaneh A 2017 *Phys. Lett. A* **381** 3553
- [10] Murzaev R T, Bachurin D V, Korznikova E A and Dmitriev S V 2017 *Phys. Lett. A* **381** 1003
- [11] Evazzade I, Lobzenko I P, Korznikova E A, Ovid'ko I, Roknabadi M and Dmitriev S V 2017 *Phys. Rev. B* **95** 035423
- [12] Barani E, Lobzenko I P, Korznikova E A, Soboleva E G, Dmitriev S V, Zhou K and Marjaneh A 2017 *Eur. Phys. J. B* **90** 38
- [13] Murzaev R T, Babicheva R I, Zhou K, Korznikova E A, Fomin S Yu, Dubinko V I and Dmitriev S V 2016 *Eur. Phys. J. B* **892** 168
- [14] Barani E, Korznikova E A, Chetverikov A P, Zhou K and Dmitriev S V 2017 *Phys. Lett. A* **381** 3553
- [15] Zakharov P V, Korznikova E A, Dmitriev S V, Ekomasov E G, Zhou K 2019 *Surface Sci.* **679** 1

- [16] Kistanov A A, Murzaev R T, Dmitriev S V, Dubinko V I and Khizhnyakov V V 2014 *JETP Lett.* **99** 353
- [17] Baimova J A, Korznikova E A, Lobzenko I P and Dmitriev S V 2015 *Rev. Adv. Mater. Sci.* **42** 68
- [18] Dmitriev S V, Chetverikov A P and Velarde M G 2015 *Phys. Status Solidi B* **252** 1682
- [19] Archilla R, Coelho S, Auret, D, Dubinko V I and Hizhnyakov V 2015 *Physica D* **297** 56
- [20] Russell F 1967 *Nature* **217** 51.
- [21] Russell F, Archilla J, Frutos F and Medina-Carrasco S 2017 *Europhys. Lett.* **120** 46001
- [22] Archilla J and Russell F 2016 *Letters on Materials* **6** 3