Interaction of supersonic crowdions with point defects in BCC tungsten: molecular dynamics simulation

Yu. R. Sharapova · A. M. Kazakov · R. I. Babicheva · A. A. Isosimov · E. A. Korznikova

Received: 26 August 2024 / Accepted: 23 September 2024

Abstract
High mobility crowdions move in the lattice with subsonic and even supersonic velocity with the mass and energy transfer. This work studies the interaction between supersonic 1- and 2-crowdions with point defects in the tungsten crystal lattice. Molecular dynamics simulation shows that the presence of point defects in the row nearest to the crowdion motion path, strongly affects the crowdion dynamics. The mass and energy transfer of supersonic 2-crowdion is found to be more effective than that of the 1-crowdion.

Keywords Crowdion · Molecular dynamics · Point defect · Energy transfer · Tungsten

Introduction

The point defect migration in metals plays the key role in the mass and energy transfer during plastic strain, heat treatment, and irradiation processes. These defects are interstitial atoms and vacancies, having a significant influence on the material behaviour. Unlike vacancies, interstitial atoms are characterized by the higher energy and much higher mobility [1, 2]. The exceptions are crowdions embedding in close-packed atomic rows. These crowdions are characterized by high mobility and able to move along close-packed atomic rows, carrying the atomic mass with subsonic or even supersonic speed [3, 4].

Crowdions can result from the interaction between high-energy neutrons or ions, passing through the crystal lattice. These particles create vacancies and interstitials on their way that leads to the formation of crowdions. Interstitial atoms usually locate near vacancies, causing a localized distortion or "crowding" in the crystal lattice. It is important to study this type of defects because they affect mechanical, electrical, and thermal properties of materials. In addition, crowdions play a significant role in the radiation damage of materials, since they are formed by high-energy particles and can contribute to the accumulation of such damages.

It is important to study the crowdion behaviour in metals, as it can significantly affect the material performance. Understanding the formation and migration mechanisms of these defects helps to create new materials with improved properties and radiation damage resistance. For materials scientists and engineers engaged in high technology and nuclear power industry, it is therefore important to understand the migration of point defects and their influence on materials.

It is known that crystal lattices of refractory metals exhibit a high propensity to accumulate a multitude of defects, including vacancies, dislocations, and grain boundaries, when subjected to external influences. These defects give rise to internal stress fields, which inevitably affect the crowdion dynamics by influencing their velocity or displacing them from the axis of propagation. It is therefore important to understand the crowdion dynamics in the presence of internal stresses. At first, it is advisable to investigate the influence of point defects, as this represents the most straightforward case. The experimental identification of the crowdion motion has led to a widespread adoption of the molecular dynamics as a reliable and effective method for studying the crowdion behavior. This approach is an effective method to analyze the material structure, including surface voids [5],

 https://doi.org/10.1007/s11182-024-03335-6

Published online: 24 January 2025

discrete breathers [6], and recently discovered two-dimensional nanomaterials [7, 8]. Molecular dynamics is an appropriate method to investigate crowdions, as they are nanoscale that means multiple atomic spacing and high motion speed. This enables the use of relatively small computational cells and short simulation time.

Molecular dynamics simulation is successfully used to study the excitation of single crowdions in the niobium lattice, demonstrating its efficiency [9]. Since crowdions move along close-packed atomic rows, their motion can be considered as quasi-one-dimensional. This motion is described using chain models, e.g., the Frenkel-Kontorova model [10]. The supersonic crowdion motion is studied in two-dimensional triangular and face-centered cubic (FCC) crystal structures, providing valuable data on the defect behaviour in different crystal structures [11, 12, 13].

Nevertheless, the motion of supersonic crowdions in body-centered cubic (BCC) metals, remains underexplored. The aim of this work is to study the dynamics of 1- and 2-crowdions in the BCC crystal structure of tungsten. A deeper comprehension of the crowdion behaviour in this particular crystal structure may facilitate acquisition of novel insights into defect migration mechanisms and their impact on the material properties. Consequently, the molecular dynamics simulation of crowdions is a crucial step in the advancement of materials science and creation of novel technologies.

Molecular dynamics simulation

A three-dimensional BCC crystal structure of tungsten with 3.16 Å atomic spacing was considered to study the crowdion motion. As shown in Fig. 1, *X*-, *Y*- and *Z*-axes located along close-packed atomic rows parallel to <111>, <110> and <112> crystallographic directions, respectively. The atomic interaction in the tungsten crystal lattice was described by the many-body interatomic potential developed in [14]. The molecular dynamics simulation was conducted in the widely accepted LAMMPS program [15]. The computational cell included 80,000 atoms and had 543.7 Å × 51.3 Å × 44.4 Å atomic spacing. Periodic boundary conditions were imposed along three orthogonal axes, allowing to construct an infinite lattice.

The initial conditions for the crowdion motion included 137 eV pulse energy, 379 and 268 Å/ps initial atom velocity for 1- and 2-crowdion, respectively, and 5.2 km/s = 52 Å/ps sound velocity in tungsten [16]. The point defect (single vacancy) location in the 1st, 2nd and 3rd atomic row next to the 2-crowdion motion path, is schematically illustrated in Fig. 1. In the case with the 1-crowdion or divacancy, the number of initiated atoms and the defect configuration were changed accordingly. Divacancy was oriented along the *X*-axis. All other atoms had zero initial displacement and velocity, without external influences on the crowdion behaviour.

Results and discussion

Let us consider cases when the introduced vacancy was one to three atomic rows away from the row along which the crowdion moves. We thus can evaluate the vacancy effect on the crowdion motion. In particular, we analyze the dynamics of the 1- and 2-crowdion propagation in ideal lattice. Figure 2 shows the crowdion motion in the form of the relative atom displacement along which the crowdion propagates. Different colors indicate trajectories of successive atoms locating in the row of the motion path to trace their displacement. The maximum atom displacement $\Delta x/h \approx 0.6$ corresponds to overcoming the energy barrier, while the atom is slowly drawn into the next lattice site. In this case, the energy dissipation leads to a shorter atomic range, and some time later, the atom returns to a position matching a supersonic-to-subsonic transfer of the crowdion.

In the case with the 2-crowdion (Fig. 2b), two consecutive jumps of two atoms enable the atom motion, and the process continues. The mass transfer is much longer than in the case with the 1-crowdion. For a more thorough investigation of the crowdion behaviour in different situations, it is important to count on the higher initial velocity of the 1-crowdion than of the 2-crowdion.

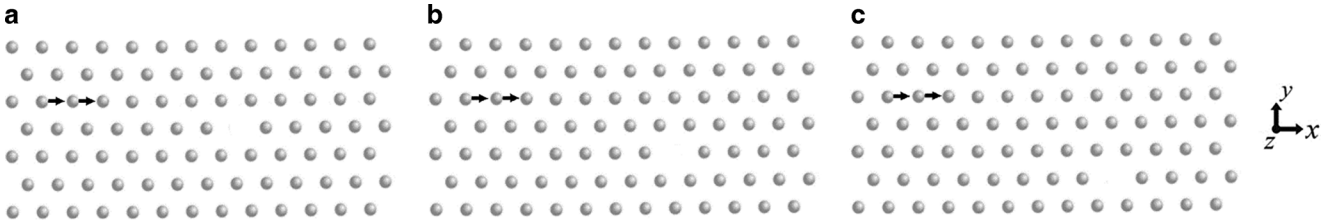

Fig. 1 Supersonic 2-crowdion motion initiated by pulses applied to atoms in the tungsten lattice with single vacancy in different rows: **a** 1st, **b** 2nd, **c** 3rd atomic rows next to the motion path. Arrows indicate pulses

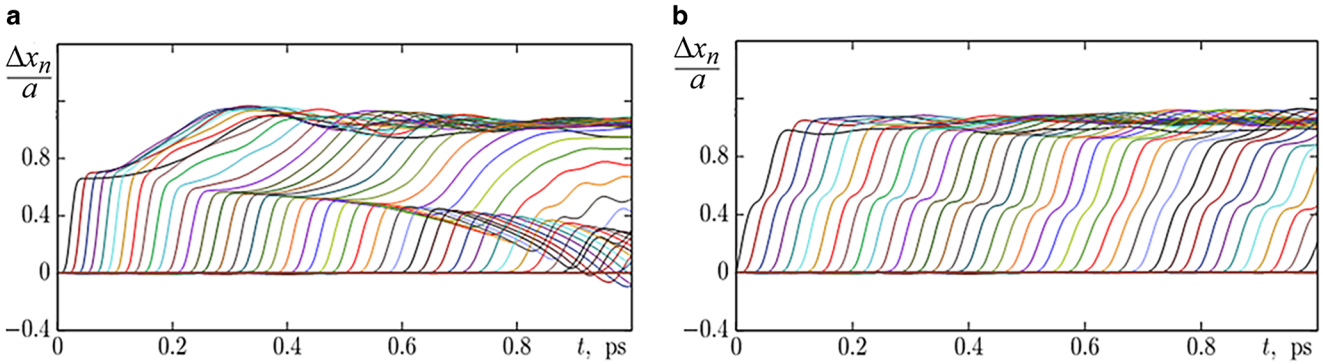

Fig. 2 Relative atom displacement in <111> crystallographic direction in BCC tungsten during supersonic crowdion motion: **a** 1-crowdion, **b** 2-crowdion. Initial pulse energy: 137 eV

The obtained results show that the vacancy locating in the atomic row nearest to the motion path, has the greatest influence on the crowdion dynamics. This influence significantly reduces with increasing distance between the vacancy and the row nearest to the motion path. In order to quantify the vacancy influence, the energy difference is computed for ideal lattice and lattice with a defect. It is found that when the vacancy locates one row away, this difference is much larger than when it moves by two rows. If the vacancy locates two or more rows away from the row the crowdion moves in, its influence becomes insignificant, and the motion dynamics almost does not change.

In addition, it was investigated how the initial crowdion velocity affected the energy difference when the vacancy located in the adjacent atomic row. It was found that this dependence was nonlinear, i.e., at the higher initial velocity, the energy loss by the 1-crowdion monotonically increased, reached its maximum, and then reduced. At the same time, the supersonic 2-crowdion turned out to be much less sensitive to the point defect, and the energy loss was much lower.

The main reasons for the crowdion energy loss are as follows. When the crowdion moves near the vacancy, velocity vector components perpendicular to the main direction of motion, appear in its velocity vector. This effect can be clearly demonstrated by the atom displacement in the direction perpendicular to the crowdion motion path. Figure 3 shows time dependences of the atom displacement along *X*- and *Y*-axes for the supersonic 1-crowdion.

It is worth noting that in ideal defect-free lattice, the atom displacement along *X*- and *Y*-axes is absent during the crowdion motion. In the lattice with defects, the situation is different. Figure 3 clearly shows that the atom displacement along the *X*-axis occurs in the presence of a vacancy in the nearest-neighbor row, and almost completely disappears when the vacancy locates at a longer distance. At the same time, significant displacements are observed along the *Y*-axis. Up to six atoms shift noticeably from their equilibrium positions when the crowdion passes near the vacancy.

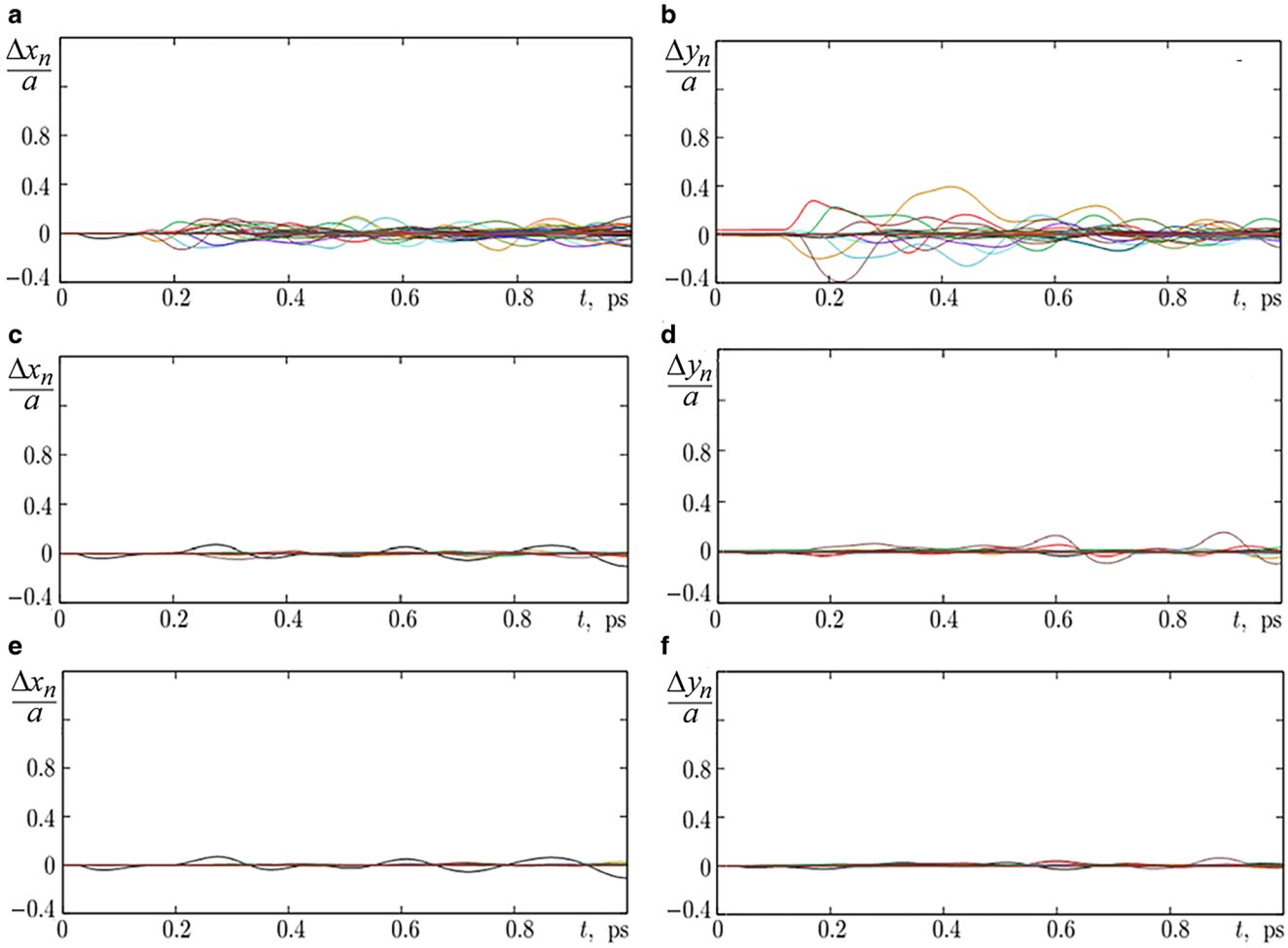

Fig. 3 Time dependences of atom displacement at excitation of supersonic 1-crowdion: **a**, **c**, **e** along *X*-axis, **b**, **d**, **f** along *Y*-axis. Initial pulse energy: 137 eV. Vacancy location: **a**, **b** 1st, **c**, **d** 2nd, **e**, **f** 3rd atomic row next to the motion path

Figure 4 shows time dependences of the atom displacement for the supersonic 2-crowdion. When the vacancy locates in the atomic row next to the row of the motion path, a significant atom displacement occurs perpendicular to the direction of motion. This displacement becomes noticeable already for eight atoms in the immediate vicinity of the point defect. Such a behavior is determined by the crowdion energy dissipation nearby the vacancy. When the crowdion moves through defects, its velocity vector begins to include its perpendicular components, that leads to a significant energy loss. This perpendicular displacement is especially noticeable in Fig. 3. One can see that atoms near the vacancy deviate from their equilibrium positions along the *Y*-axis, which disrupts the normal energy transfer.

The atom displacement gradually attenuate, as the crowdion moves away from the vacancy, which is explained by its self-focusing. After passing the vacancy, the crowdion restores its ability to efficiently transfer energy along the main direction of motion. The self-focusing effect allows the crowdion to compensate for temporal deviations and the energy loss caused by its interaction with the defect. As a result, the velocity vector of the crowdion is again directed strictly along its initial motion path, and the energy transfer becomes more efficient.

As can be seen from Fig. 4, the defect significantly affects the dynamics of the supersonic 2-crowdion, which is less sensitive to the presence of point defects compared to the supersonic 1-crowdion. Its interaction with the vacancy leads to the atom displacement, but due to the high velocity and self-focusing effect, the 2-crowdion rapidly recovers its energy and continues its motion.

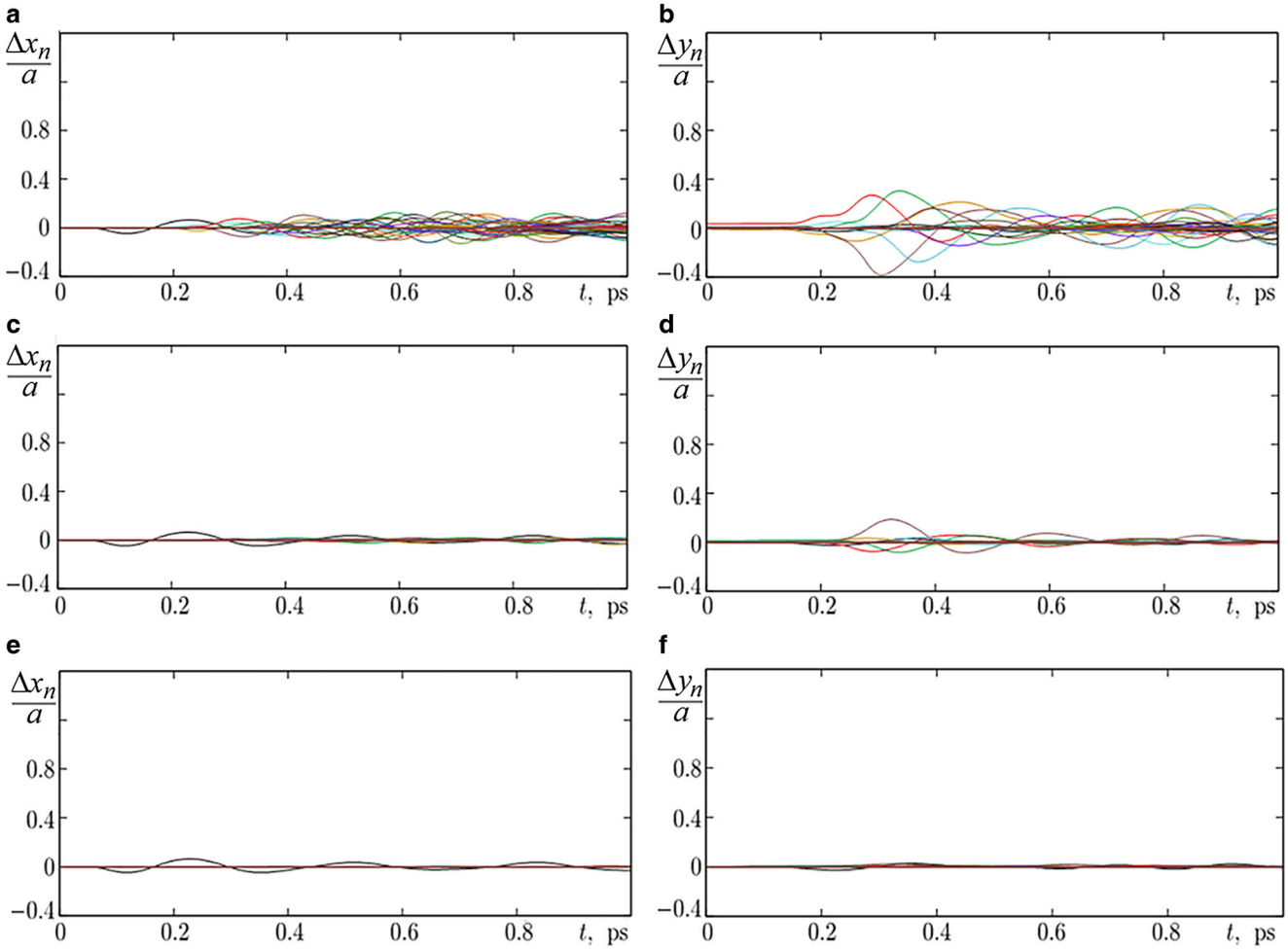

Fig. 4 Time dependences of atom displacement at excitation of supersonic 2-crowdion: **a**, **c**, **e** along *X*-axis, **b**, **d**, **f** along *Y*-axis. Initial pulse energy: 137 eV. Vacancy location: **a**, **b** 1st, **c**, **d** 2nd, **e**, **f** 3rd atomic row next to the motion path

Let us consider the lattice containing a divacancy for a more detailed study of its influence on the crowdion propagation. The atom displacement in the row with the 1-crowdion propagation along *X*- and *Y*-axes, is shown in Fig. 5. In this case, there is a discernible atom displacement along both axes. This displacement is clearly observed in a subset of atoms, which is smaller than in the case with the atomic vacancy. However, the atom displacement is more pronounced. In the previous case, the maximum displacement is not over 0.4 Å, whereas in the present case, it exceeds 0.75 Å. Additionally, a notable displacement of a single atom is observed along the *Y*-axis at the divacancy localization across two atomic rows. When the divacancy passes through three atomic rows, no significant changes are observed in the dynamics of the 1-crowdion unlike its dynamics in ideal lattice.

The atom displacement along *X*- and *Y*-axes at the excitation of the 2-crowdion, is presented in Fig. 6. Along the *X*-axis, the atom displacement is the lowest, with the maximum at 0.15 Å. Along the *Y*-axis, the atom displacement is much more pronounced. One of the atoms displaces by over 0.8 Å, while the displacement of remaining seven atoms ranges between 0.2 and 0.1 Å. In the case of the divacancy localization in two atomic rows, the atom displacement along the *Y*-axis is significantly lower and does not exceed 0.15 Å. This is a significant decrease in the atom displacement as compared to that at the excitation of the 1-crowdion.

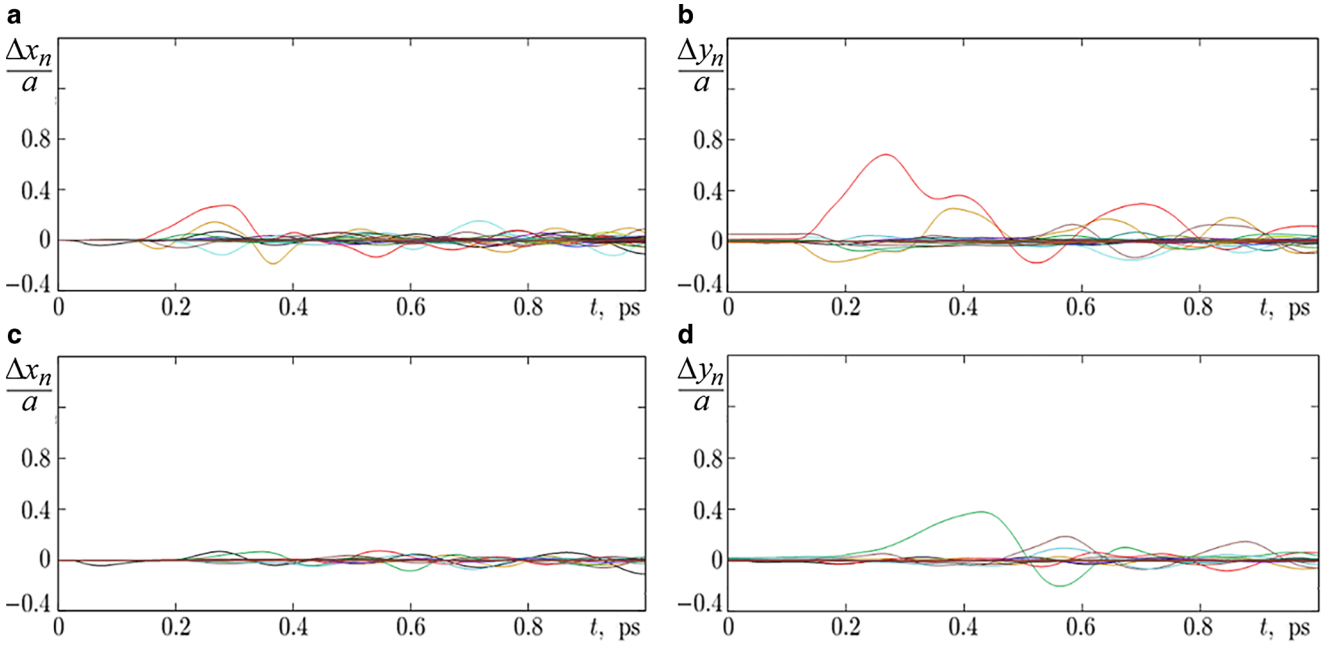

Fig. 5 Time dependences of atom displacement at excitation of supersonic 1-crowdion: **a**, **c** along *X*-axis, **b**, **d** along *Y*-axis. Initial pulse energy: 137 eV. Divacancy location: **a**, **b** 1st, **c**, **d** 2nd atomic row next to the motion path

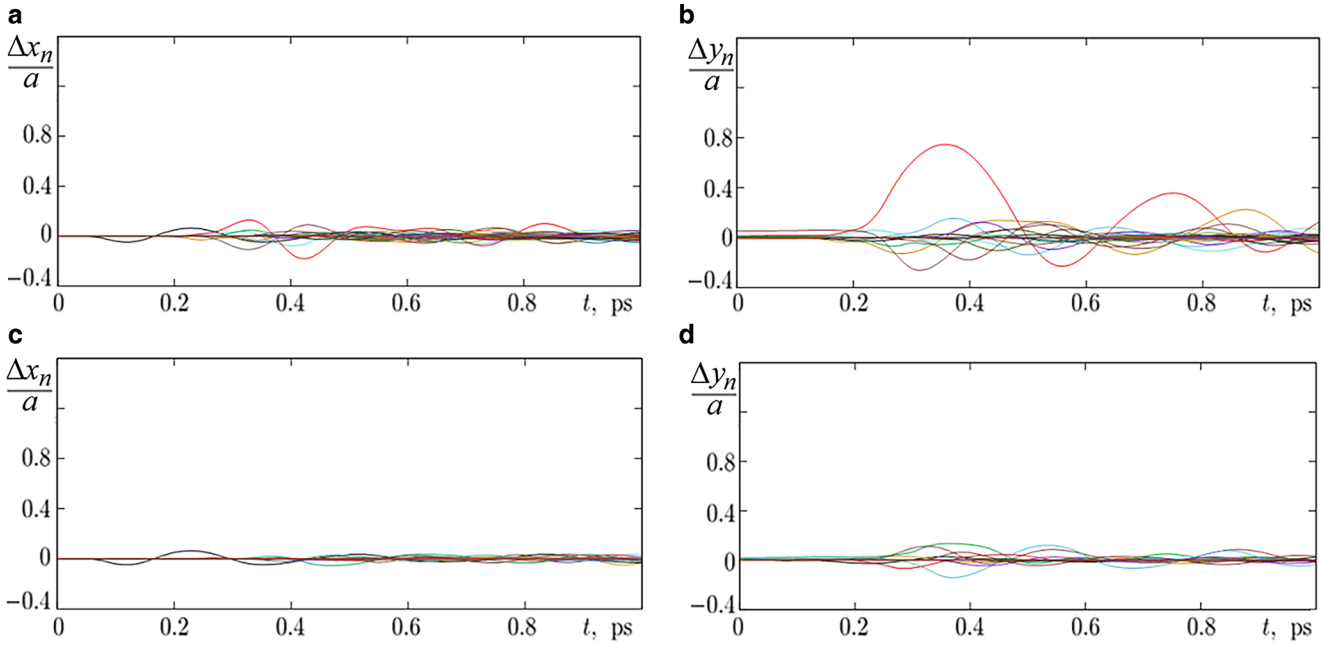

Fig. 6 Time dependences of atom displacement at excitation of supersonic 2-crowdion: **a**, **c** along *X*-axis, **b**, **d** along *Y*-axis. Initial pulse energy: 137 eV. Divacancy location: **a**, **b** 1st, **c**, **d** 2nd atomic row next to the motion path

Conclusions

This work investigated the crowdion interaction with vacancies and divacancies in BCC tungsten with supersonic 1- and 2-crowdions. It was shown that the strongest influence on the dynamics of supersonic crowdions was exerted by defects located in the row nearest to the crowdion moving path. Moreover, the 2-crowdion was found

to be less sensitive to this type of defects than the 1-crowdion, making it a more efficient means of mass and energy transfer.

This work demonstrated that when the point defect located two or more rows away from the row along which the crowdion moved, its effect on the motion was negligible and the crowdion dynamics remained almost unchanged. This was in agreement with our research [12, 13] into the behavior of supersonic crowdions in FCC crystal strcutures.

It was proven that the supersonic 2-crowdion was more preferable for the efficient mass and energy transfer in materials with point defects. This discovery can be used to control the mass and energy transfer where appropriate.

Our future work will consider the influence of other defect types on the dynamics of supersonic crowdions in BCC crystal structures. An investigation of the interaction between crowdions and different defects such as dislocations and interstitials, will provide a more complete understanding of the mass and energy transfer in materials subjected to the influence of such external factors as mechanical or high-temperature treatment. Our research findings will assist in the development of new materials with improved properties for applications in thermodynamic devices (compressors, turbines, diffusers) capable of the heat and mass transfer.

Funding This work was financially supported by Grant No. 075-03-2024-123/1 from the Ministry of Science and Higher Education of the Russian Federation and Grant No. 24-11-00139 from the Russian Science Foundation.

Conflicts of interest The authors declare no conflict of interest.

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Authors and Affiliations

Yu. R. Sharapova[1] · A. M. Kazakov[1] · R. I. Babicheva[1,2] · A. A. Isosimov[3] · E. A. Korznikova[1]

✉ Yu. R. Sharapova
ulya_usinsk@mail.ru

A. M. Kazakov
ezabfarm@mail.ru

R. I. Babicheva
ri.babicheva@gmail.com

A. A. Isosimov
Artem-is-ufa@rambler.ru

E. A. Korznikova
elena.a.korznikova@gmail.com

[1] Ufa University of Science and Technology, Ufa, Russian Federation

[2] Institute of Molecule and Crystal Physics of the Ufa Federal Research Center, Russian Academy of Sciences, Ufa, Russian Federation

[3] Ufa, Russian Federation