Interaction of supersonic 2-crowdions in fcc platinum

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Abstract. In metals subjected to ion implantation or irradiation, mass transfer by supersonic crowdion clusters takes place. The interaction between supersonic 2-crowdions moving in parallel close-packed atomic rows has been studied only in 2D Morse lattice and here it is analysed with the use of molecular dynamics simulations in fcc platinum.

1. Introduction

It is widely accepted that point defect play an important role in the diffusion in crystal lattices thus contributing to the structure evolution upon the external impacts [1]. Among different types of zero-dimension defects present in the material, one can distinguish vacancies [2] or voidions [3] and interstitials in the form of atoms embedded in an octahedral or tetrahedral pore [4] or crowdions [5–9]. Crowdions are much more mobile than conventional interstitial defects, however having higher formation enthalpy. These facts allow to conclude that crowdions play an important role in mass transfer in crystals during extreme impacts. Recently a phenomenon of supersonic crowdion has been extended to supersonic N-crowdion where several (N) atoms move at a high speed simultaneously in a close packed row and this type of motion was found to be much more effective than the single crowdion propagation [10].

Features of supersonic crowdion motion have been described in different types of crystals [5,6,11-13]. However the scenarios of crowdion interaction remain uncovered at the moment. The aim of the present work is to analyze peculiarities of interaction of supersonic 2-crowdions in fcc platinum crystal by means of molecular dynamics simulations.

2. Simulation details

Since crowdion motion is studied at the atomic scale, molecular dynamics is an effective tool for this study. Previously this approach, based in the solving of Newtonian equations of motion, has recommended itself as a powerful method allowing to analyze nonlinear dynamics of crystal lattices.
[14–20], phase transformations [21], evolution of atomic structure and mechanical properties upon external loading [22–25] and many other features.

At the initial stage, the fcc lattice of Pt was simulated with the lattice parameter $a = 3.920 \, \text{Å}$ and the interatomic distance $d = a/\sqrt{2} = 2.772 \, \text{Å}$. The $x$ and $y$ axes of the Cartesian coordinate system are oriented along the close-packed directions $\{110\}$ and $\{\overline{1}10\}$, and the $z$ axis is oriented along the $\{001\}$ direction (see Fig. 1). The computational cell includes 30, 8 and 8 cubic translational cells in the $x$, $y$ and $z$ direction, respectively, and each cell contains 4 atoms. The total number of atoms is 15360. Periodic boundary conditions are used. Integration time step is 0.2 fs.

We have studied interaction between three supersonic 2-crowdions. Single 2-crowdion is excited by giving same initial velocity to two neighbouring atoms in a close packed row along this row (along the $x$-axis). The initial velocities of all other atoms and the initial displacements of all atoms in the computational cell are equal to zero. Thermal vibrations were not introduced, i.e. the simulation was carried out at a temperature of 0 K. Thus, the total energy of the system is equal to the kinetic energy of excited atoms at $t=0$. The atomic mass of Pt is 195.084 amu. The simulation was carried out using the LAMMPS software package and the many-body interatomic potential [26].

The following configurations of three 2-crowdions were investigated: (i) vertical parallel to the $xz$ plane, (ii) horizontal parallel to the $xy$ plane, and (iii) diagonal (see figure 2).

![Figure 1.](image1.png)

**Figure 1.**Atoms of the fcc Pt crystal projected onto the $xy$ plane, where the axes of the Cartesian coordinate system $x$, $y$ and $z$ are directed along the crystallographic directions $<110>$, $<-110>$ and $<001>$, respectively.

![Figure 2.](image2.png)

**Figure 2.** In (a), the atoms located on the front plane are highlighted in blue, while red atoms are on the second plane. Three investigated configurations of clusters of supersonic 2-crowdions: (b) horizontal, (c) diagonal and (d) vertical.

3. **Simulation results**

In the course of molecular dynamics modeling of three supersonic 2-crowdions with an initial velocity of 60 Å/ps, it was revealed that the vertical configuration shows itself to be the most stable in comparison with the horizontal and diagonal configurations (see figure 3). The degree of instability depends on the distance between close-packed rows, where 2-crowdions are launched. In the case of the horizontal and diagonal configuration, the distance $S_d = S_b = d = 2.772 \, \text{Å}$ is less than in the case of
the vertical configuration $S_v = a = 3.92 \, \text{Å}$. Therefore, in horizontal and diagonal configurations the interaction of adjacent 2-crowdions is expected to be greater than in the vertical one. The diagonal configuration has a violation of symmetry, which is an additional factor affecting the dynamics of this cluster of 2-crowdions.

It should be noted that, with a diagonal configuration, the appearance of an additional crowdion is observed at a 450 time step, which is explained by the recombination of atoms in the cone-shaped tail of 2-crowdion clusters.

Figure 4 demonstrates atomic displacements as the functions of time for the atoms in the central close-packed row. The displacements satisfy the self-focusing condition [10] in all three cases. At the same time, it can be observed that the displacements in the horizontal and diagonal configurations intersect. This indicates a tendency to the formation of an additional vacancy, which also indicates an unstable dynamics of the three supersonic 2-crowdion in horizontal and diagonal configurations.

![Figure 3](image1.png)

![Figure 4](image2.png)

**Figure 3.** Dynamics of the studied configurations of clusters of supersonic 2-crowdions: (a) horizontal, (b) vertical and (c) diagonal configuration.

**Figure 4.** Displacement of atoms as a function of time in the central close-packed row for (a) vertical, (b) horizontal and (c) diagonal configuration.

## 4. Conclusions

Molecular dynamics modeling was carried out for three supersonic 2-crowdions moving in parallel close-packed rows in the crystal lattice of platinum, using a many-body interatomic potential. A stable vertical configuration was found, in which the three 2-crowdions propagate with minimal disturbances. In this case, the dynamics of the 2-crowdions practically does not differ from how they move without interacting with each other. In the case of a horizontal configuration, there is a stronger interaction of the compound 2-crowdions with each other and a difference in the dynamics of movement. The movement is unstable, however, the three 2-crowdions still propagate along the close packed directions. When three 2-crowdions are launched in a diagonal configuration, the two outer 2-crowdions are converted into 1-crowdions, at which an additional 1-crowdion appears in the central close-packed direction. Obtained results contribute to the fundamental understanding of mass transfer mechanisms in crystals in non-equilibrium conditions.
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