Moving an atom by swapping places across a crystal lattice without vacancies

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Abstract. The mechanism of moving an atom through a crystal lattice without vacancies is considered. This situation can be observed when all sites of the lattice are occupied by atoms of the same type, or when some of them are occupied by isotopes of the same atoms. It is shown that in a three-dimensional crystal lattice constructed from identical atoms without vacancies, one-dimensional motion of the own atom along the lattice chain is possible. This movement is realized as a Frenkel-Kontorova soliton.

1. Introduction

One of the most common types of diffusion is self-diffusion. – A situation in which atoms of the same type (or substance) move along a lattice made up of (own) atoms of the same type (all sites are occupied by atoms). In addition, this situation is similar to that in which the sites of such a crystal can contain isotopes of atoms of the same type. When all the sites (nodes) are occupied, it is difficult for the atom to move. The realization of self-diffusion is facilitated if Frenkel’s defects are included (when the atom passes into the interstitial) or Schottky defects (when a vacancy occurs and it moves sequentially to the interface) [1]. On the other hand in the literature [1-3] models are proposed that allow us to take into account the possibility of moving an atom to a nearby occupied place by exchanging the places of the nearest atoms. This can be taken into account through the probability that the atom will move to a neighboring position, provided that the neighboring atom has left its place in the opposite direction. At the same time, the elementary mechanism of such a transition remains unclear. And, in addition, in the listed variants of self-diffusion implementation, it is not taken into account that the atom, moving along the lattice, participates in a collective movement, involving the entire environment in the act of its movement. Here we propose an approach for describing the motion of an own atom along a lattice without vacancies, taking into account the elementary mechanism of the exchange of places of the nearest atoms and taking into account the collective mechanism of such movement.

2. Model

Each atom in the lattice experiences deviations from its equilibrium position, thereby involving neighboring atoms in its displacements. We write down the Lagrangian for this behavior of atoms. To do this, select the two nearest atoms (Fig. 1).
\[ \mathcal{L} = \frac{m_1 \ddot{\mathbf{r}}^2}{2} + \frac{m_2 \ddot{\mathbf{d}}^2}{2} - A_1(1 - \cos(\mathbf{r} \cdot \mathbf{n})) - A_2(1 - \cos(\mathbf{d} \cdot \mathbf{n})) - \alpha_{jm}(\mathbf{r} - \mathbf{d})^2/2 - (\frac{1}{2}) \sum_j \mathcal{U}(\mathbf{r} - \mathbf{d}, \varepsilon_j) + \]

\[ + \left( \frac{m}{2} \right) \sum_j \varepsilon_j^2 - \left( \frac{\alpha}{2} \right) \sum_j (\varepsilon_j - \varepsilon_{j+1})^2 \]  

(1)

Here, \( \mathbf{r} \) and \( \mathbf{d} \) are the displacement vectors of the first and second separated atoms (Fig. 1). The first line in (1) expresses the Lagrangian for atoms with mass \( m_1 \) and \( m_2 \) as independently moving in the periodic field of the lattice for each with amplitude \( A_1 \) and \( A_2 \). In this case, each displacement of the selected atom will experience an "elastic" interaction with its neighbor and with the rest of the lattice atoms. The second line of the Lagrangian corresponds to this situation. The third line expresses the behavior of the lattice in the harmonic approximation. \( m \) is the mass of the atoms in the lattice; \( \varepsilon_j \) is the displacement vector of the \( j \)-th atom of the rest of the lattice; vector \( \mathbf{n} \) is the direction of motion.

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![Fig. 1. Diagram of the nearest neighbor offsets "1" and "2" in the lattice.](image)

The atom "1" has shifted to the position given by the vector \( \mathbf{r} \). The atom "2" has shifted to the position set by the vector \( \mathbf{d} \). This formulation of the problem turns out to be similar to the problem describing the movement of a nitrogen molecule along the core of a helical dislocation [4]. The local chain approximation [4] allows us to decompose the potential energy of the interaction of the selected atoms into the sum of the products of the differences between the deviations of the displacement of the selected atom and the displacements of the nearest neighbors in each local chain. The resulting equations of motion for the selected pair of atoms from (1) look like this:

\[ m_1 \frac{d^2 \mathbf{r}}{dt^2} = \alpha_{jm}(\mathbf{r} - \mathbf{d}) + \alpha_2(\mathbf{r} - \mathbf{\varepsilon}) + A_1\left(\frac{2\pi}{a}\right)\sin(\mathbf{r} \cdot \mathbf{n}) \]  

(2)

and

\[ m_2 \frac{d^2 \mathbf{d}}{dt^2} = \alpha_{jm}(\mathbf{d} - \mathbf{r}) + \alpha_2(\mathbf{d} - \mathbf{\varepsilon}) + A_2\left(\frac{2\pi}{a}\right)\sin(\mathbf{d} \cdot \mathbf{n}) \]  

(3)

Adding up these two equations and going to the center of mass

\[ R = \frac{(m_1 \mathbf{r} + m_2 \mathbf{d})}{(m_1 + m_2)} \]
and taking into account the relative position \( d = I - D \) of the isolated atoms, (provided that all the masses in the crystal are equal to each other \( m_1 = m_2 = m \) and are also equal to each other \( \alpha_1 = \alpha_2 = \alpha_{jm} = \alpha \)) we obtain:

\[
m\frac{d^2 R}{dt^2} = Z\alpha \left( \frac{d^2 R}{dt^2} \right) \cdot \tau^2 + A(2\pi/a) \cos(n \cdot \frac{d}{2}) \sin(n \cdot R)
\]

(4)

here \( Z \) is the number of nearest neighbors in the lattice, \( \tau \) – parameter (time) during which the neighboring deviations do not have time to change [4]. Equation (4) can be rewritten to take into account the effective mass \( m^* = m - Z\alpha \cdot \tau^2 \) and \( A(2\pi/a) \cos(n \cdot \frac{d}{2}) = \mathcal{A}(\theta) \) in a more compact form:

\[
m^* \frac{d^2 R}{dt^2} = \mathcal{A}(\theta) \sin(n \cdot R)
\]

(5)

here \( \theta \) is the angle between the direction \( n \) and \( \frac{d}{2} \) lies either in the plane \( oxz \) or \( oyz \). The solution to this equation is the Frenkel-Kontorova soliton:

\[
R_{n,z} = (\frac{2a}{n}) \arctg \left[ \pm 2\pi \left( -\frac{\mathcal{A}(\theta)}{m^*} \right)^{1/2} \frac{t}{a} \right]
\]

(6)

In this case, the Lagrangian is transformed to the form:

\[
\mathcal{L} = m^* \frac{R^2}{2} - \alpha(R_n - R_{n-1})^2/2 - \mathcal{A}(\theta)(1 - \cos(R_n \cdot n))
\]

(7)

here \( \mathcal{A}(\theta) \) from (6) describes the rotation of the selected pair of atoms relative to the center of mass. This means that the movement of its own atom along the lattice without vacancies will be carried out from site to site by mutual "rolling" of the atom located in position \( n - 1 \) and the atom moving towards it from position \( n \) relative to the center of mass of this pair. The very center of mass of such a "rolling" formation moves like a Frenkel-Kontorova soliton.

Conclusion

It is shown that the movement of an atom along a one-dimensional chain without vacancies, constructed from the same atoms, is realized as the movement of a pair of atoms, the center of mass of which moves like a Frenkel-Kontorova soliton, and its "core" is a pair of atoms rolling over each other. Such a one-dimensional situation is possible if the possible connections with the nearest neighbors in the three-dimensional crystal are taken into account.

References

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