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Modes of motion of light atoms (hydrogen and helium) in diamond-like lattice

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The motion of a foreign atom (e.g. hydrogen or helium isotope) along the interstitials in a diamond-like silicon lattice is considered. The Lagrangian of the system „foreign atom + crystal" accounts for the influence of a foreign atom on the lattice atoms. The symmetries assumed by the Lagrange function allow the multidimensional system of equations describing the behavior of a foreign atom and lattice atoms to be reduced to a one-dimensional nonlinear equation. The solution to the equation is either the Frenkel–Kontorova soliton, which describes the translational behavior of a collective consisting of the foreign atom and the accompanying reversible displacements of the nearest lattice atoms, or the vibrational motion of a foreign atom, as a particle with the mass of an atom.

Keywords: Lagrange function, bilinear form, Frenkel–Kontorova soliton.

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1. Introduction

Motion of a foreign atom in a crystal lattice is usually considered as a 3D motion in a potential field generated by the lattice atoms. Methods of molecular dynamics are used most widely for this purpose [1–6]. In this case, the foreign atom is represented by a particle with the weight of this atom; sometimes quantum state of the atom is also taken into account [7].

At low temperatures the light atoms (hydrogen, helium) can also be described as particles with quantum properties, since de Broglie wavelength for these atoms is comparable with the lattice constant [8–11]. The mobility of these atoms, characterized by the diffusion coefficient, reveals abnormal properties. Thus, deuterium and tritium isotopes, which are twice and three times heavier than hydrogen atom, respectively, move on the surface of tungsten crystal with higher velocity than hydrogen [12,13], practically irrespective of temperature. The same anomaly was discovered in silicon crystal for deuterium and hydrogen: the diffusion coefficients at low temperatures indicate that deuterium actually moves faster than hydrogen [14].

Higher mobility of a heavier atom does not fit into the classical theory of atom motion in a crystal where the frequency of the foreign atom transitions between the neighboring positions in a crystal corresponds to $\nu \sim 1/\sqrt{m}$. Such an effect also could not be explained in terms of quantum mechanics, since de Broglie wavelength is inversely proportional to the weight of the foreign atom $\lambda \sim h/m$.

In all these cases the foreign atom is considered as a particle of non-zero mass moving in the potential field formed by the crystal lattice atoms, while the effect of the atom on this potential field is usually neglected [1–11]. The above effect, however, does take place; it is manifested as excitation of the lattice phonon sub-system. Under the action of a foreign atom the lattice atoms may perform two kinds of motion.

1. Oscillations near the equilibrium position. Collective nature of these oscillations is manifested as a phonon subsystem of the lattice [15,16].

2. Independent displacement of the lattice atom equilibrium position induced by interaction with the foreign atom. This type of displacement is generally neglected when considering the motion of the foreign atom in the crystal.

In this paper it is suggested to take into account the displacement of the lattice atoms induced by a foreign atom and to show that light atoms such as hydrogen and helium move through the crystal not like an isolated particle, but as a collective consisting of this atom and the accompanying reversible displacement of the nearest lattice atoms. The motion equations for such collective have a solution in the form of a discrete 1D Frenkel–Kontorova soliton. In other words, the translational motion of a foreign atom in the lattice field is only possible when accompanied by reversible displacements of the adjacent lattice atoms, while the motion of the foreign atom in the potential field is only possible in the oscillating mode.

The 1D form of the Frenkel–Kontorova soliton appears in many problems [17–19]. However, this unidimensionality occurs either due to the Frenkel–Kontorova model itself, or as a result of introducing the periodic potential [17,20,21].

In order to show the possibility to proceed from complex 3D translation motion to 1D one, we have selected two model objects:

1) Simple atoms of hydrogen and helium were selected as a foreign atom. Both of these elements have isotopes, which makes it possible to estimate the effect of atomic weight on the motion velocity.

2) Silicon crystal with a diamond-like lattice was selected as a medium. This type of lattice has a wide variety of interstices [22–28]. In particular, the volume of tetrahedral interstice can well accommodate either hydrogen or helium atom. The hydrogen atom in this position forms an unstable defect [22,23], and moves across the tetrahedral interstices mostly in the neutral state [22,24–28] and with a minimal activation energy.

2. Trial Lagrangian

To be specific, let us consider the hydrogen atom which, if introduced into the perfect silicon lattice, may only move through the tetrahedral interstices. The motion of the foreign atom can only be judged based on the difference between its kinetic and potential energy $(T - U)$. This difference makes a Lagrange function [29,30]. The principle of minimum action functional allows the motion equations for the foreign atom as well as for the lattice atoms to be found.

In general, we may introduce a trial Lagrange function for the hydrogen atom in the lattice

$$\mathscr{L} = \frac{1}{2} m\dot{\mathbf{\Gamma}}^2 - U(\mathbf{\Gamma}, \{\xi_n\}) + \sum_n \left[\frac{M_n \dot{\boldsymbol{\xi}}_n^2}{2} - \frac{1}{2} \sum_\beta \alpha_c (\boldsymbol{\xi}_n - \boldsymbol{\xi}_{n-1})_\beta (\boldsymbol{\xi}_{n+1} - \boldsymbol{\xi}_n)_\beta \right], \qquad (1)$$

where m — hydrogen atom weight; $\mathbf{\Gamma}$ — H atom displacement vector; $\boldsymbol{\xi}_n$ — displacement vector of n-th atom of the lattice in n-th position; M_n — weight of Si atom in n-th position; α_c — elastic interaction constant between the lattice atoms. Lower index β denotes a set of coordinates.

The upper line (1) describes the motion of a light atom in the potential field $U(\mathbf{\Gamma}, \{\xi_n\})$ of the neighboring atoms of the lattice, the second line describes the behavior of the silicon atoms. At that, potential energy $U(\mathbf{\Gamma},\{\xi_n\})$ of the foreign atom in the lattice field depends on both the position of the light atom Γ and positions of the lattice atoms $\{\xi_n\}$.

To find the equation for motion of the light atom in the silicon lattice, we need to find the potential energy $U(\mathbf{\Gamma},\{\xi_n\})$. For this, we need to know the local structure of the silicon lattice near the interstice hosting the light atom (hydrogen and helium).

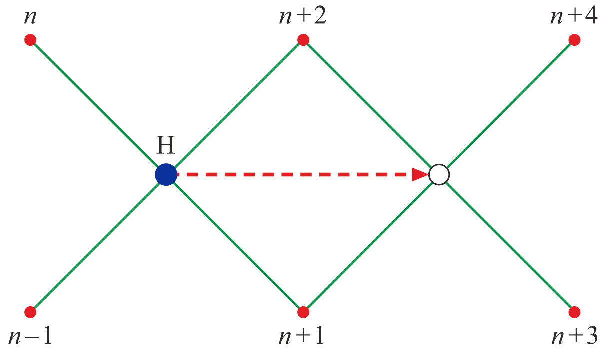

Figure 1. Diagram of the foreign atom (hydrogen) bonds with the lattice in the ordered medium and transitions of this atom between the neighboring interstices. The atoms of the neighboring lattice environment for convenience were numbered as follows: n — 1, n, $n + 1$, $n + 2$ and etc.

3. Approximation of the local chains of an ordered structure

Silicon lattice is a cubic face-centered diamond-like lattice, where each atom is surrounded by four other atoms [22,23]. The volume of silicon tetrahedral interstice is 0.00963 nm^3, while hydrogen atom volume (based on the atomic radius of 12 nm) equals to 0.00724 nm^3. Thus, a hydrogen (helium) atom can fit into this interstice.

The hydrogen atom residing in the tetrahedral interstice interacts with the neighboring silicon atoms. Using the approximation of a pair interaction, as in [31,32], we can distinguish the following pair interactions of the hydrogen atom with the neighboring lattice atoms (Figure 1):

$$\mathrm{Si}_{n-1}\mathrm{H} \text{ and } \mathrm{HSi}_n \quad \mathrm{Si}_n\mathrm{H} \text{ and } \mathrm{HSi}_{n+1}; \quad \mathrm{Si}_{n+1}\mathrm{H} \text{ and } \mathrm{HSi}_{n+2};$$
$$\mathrm{Si}_n\mathrm{H} \text{ and } \mathrm{HSi}_{n+2}; \; \mathrm{Si}_{n+2}\mathrm{H} \text{ and } \mathrm{HSi}_{n-1}; \; \mathrm{Si}_{n-1}\mathrm{H} \text{ and } \mathrm{HSi}_{n+1}. \qquad (2)$$

Such pairs can be written as the following combinations: $\mathrm{Si}_{j-1}\mathrm{HSi}_j$:

$$\mathrm{Si}_{n-1}\mathrm{HSi}_n, \quad \mathrm{Si}_n\mathrm{HSi}_{n+1}, \quad \mathrm{Si}_{n+1}\mathrm{HSi}_{n+2},$$
$$\mathrm{Si}_n\mathrm{HSi}_{n+2}, \quad \mathrm{Si}_{n+2}\mathrm{HSi}_{n-1}, \quad \mathrm{Si}_{n-1}\mathrm{HSi}_{n+1},$$

which are part of the local chains (see below (3)).

Any local chain should contain a foreign atom and the neighboring lattice environment atoms (as illustrated in Figure 2):

$$\ldots \mathrm{Si}_{n-4}\mathrm{Si}_{n-2}\mathrm{Si}_n\mathrm{HSi}_{n+2}\mathrm{Si}_{n+4} \ldots;$$
$$\ldots \mathrm{Si}_{n-4}\mathrm{Si}_{n-2}\mathrm{Si}_n\mathrm{HSi}_{n+1}\mathrm{Si}_{n+3}\mathrm{Si}_{n+5} \ldots;$$
$$\ldots \mathrm{Si}_{n-4}\mathrm{Si}_{n-2}\mathrm{Si}_n\mathrm{HSi}_{n-1}\mathrm{Si}_{n-3}\mathrm{Si}_{n-5} \ldots;$$
$$\ldots \mathrm{Si}_{n-7}\mathrm{Si}_{n-5}\mathrm{Si}_{n-3}\mathrm{Si}_{n-1}\mathrm{HSi}_{n+1}\mathrm{Si}_{n+3} \ldots;$$
$$\ldots \mathrm{Si}_{n-7}\mathrm{Si}_{n-5}\mathrm{Si}_{n-3}\mathrm{Si}_{n-1}\mathrm{HSi}_{n+2}\mathrm{Si}_{n+4} \ldots;$$
$$\ldots \mathrm{Si}_{n-6}\mathrm{Si}_{n-4}\mathrm{Si}_{n-2}\mathrm{Si}_n\mathrm{Si}_{n+2}\mathrm{HSi}_{n+1}\mathrm{Si}_{n+3}\mathrm{Si}_{n+5} \ldots. \qquad (3)$$

These chains are considered as independent.

Thus, for the tetrahedral position of the interstice accommodating the hydrogen atom, the number of local chains is 6 (while the number of silicon atoms neighboring to the hydrogen atom is 4). The elastic interaction of the hydrogen atom with the neighboring lattice atoms that is now expressed through the chains (3), can be equivalent to potential U_2.

On the other hand, the hydrogen atom experience translational motion from the initial position to the neighboring one, Figure 2. This is equivalent to transition $n \to n+2$.

For example,

$$\ldots \mathrm{Si}_{n-4}\mathrm{Si}_{n-2}\mathrm{Si}_{n}\mathrm{H}\mathrm{Si}_{n+2}\mathrm{Si}_{n+4}\ldots \to$$

$$\ldots \mathrm{Si}_{-4}\mathrm{Si}_{n-2}\mathrm{Si}_{n}\mathrm{Si}_{n+2}\mathrm{H}\mathrm{Si}_{n+4}\mathrm{Si}_{n+6}\ldots . \qquad (3a)$$

This transition, ($3a$), implies the presence of a translational potential, U_1, dragging the hydrogen atom to the neighboring position, Figure 1. Thus, motion of the foreign atom occurs under the action of two different fields: elastic field, U_2 of the chains (3), induced by the nearest neighbors of the atom, and U_1 field causing the translational movement of this atom to the neighboring position.

$$U(\mathbf{\Gamma}, \{\xi_n\}) = U_1 + U_2. \qquad (4)$$

To find the potential (4), we need to make use of the specifics of local chains approach (3), namely, occurrence of a new multi-dimensional space where hydrogen atom can move in some way.

4. Construction of a 6-D space in the approximation of local chains

Each local chain (3) can be associated with vector γ_j, ($j = 1, 2, 3, 4, 5, 6$); any chain contains a foreign atom. Each vector indicates a possible exit of the hydrogen atom from the corresponding chain (3). For convenience, when moving to the neighboring position we'll consider only silicon atoms neighboring to this hydrogen atom.

$$\begin{cases} \mathrm{Si}_n\mathrm{H}\mathrm{Si}_{n+2} \sim \gamma_1, \\ \mathrm{Si}_n\mathrm{H}\mathrm{Si}_{n+1} \sim \gamma_2, \\ \mathrm{Si}_n\mathrm{H}\mathrm{Si}_{n-1} \sim \gamma_3 \\ \mathrm{Si}_{n-1}\mathrm{H}\mathrm{Si}_{n+1} \sim \gamma_4 \\ \mathrm{Si}_{n-1}\mathrm{H}\mathrm{Si}_{n+2} \sim \gamma_5 \\ \mathrm{Si}_{n+2}\mathrm{H}\mathrm{Si}_{n+1} \sim \gamma_6 \end{cases} \qquad (5)$$

Since the chains are independent the vectors

$$\gamma_1, \gamma_2, \gamma_3, \gamma_4, \gamma_5, \gamma_6. \qquad (5a)$$

are also linearly independent. This means that they are orthogonal

$$\gamma_{k,k-1} \cdot \gamma_{k,k+1} = 0 \qquad (6)$$

and each of them is a 6 × 1-D column.

$$\gamma_1 = \begin{pmatrix} \gamma_{1,x_1} \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}; \ldots; \quad \gamma_6 = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ \gamma_{6,x_6} \end{pmatrix}. \qquad (6a)$$

Moreover, the neighboring site is not connected with the previous one

$$\gamma_{k,k+1} \cdot \gamma_{k+m,k-1} = 0. \qquad (6b)$$

In this case, the full displacement vector $\mathbf{\Gamma}$ of H atom may be decomposed into these independent vectors without the need for normalization

$$\mathbf{\Gamma} = \sum_{k=1}^{n} \gamma_{k,k-1}, \qquad (6c)$$

where n — number of local chains.

(NB: construction of linearly independent vectors ($5a$) implies the selection of their directions in such a way that only one of them could be directed towards the neighboring position. Such vectors arrangement ($5a$) simplifies the motion equation sufficiently.

5. Conversion of potential U_2

Let us represent the potential U_2 as a bilinear form since the atom displacement in each of the local chains (3) is regarded independently

$$U_2 = \frac{1}{2}\sum_{k=1}^{k=n}\sum_{\beta} U_{k-1,k;\beta\beta}(\gamma_{k-1,k} - \xi_{k-1})_\beta(\xi_{\mathbf{k}} - \gamma_{k-1,k})_\beta. \qquad (7)$$

$U_{k-1,k,\beta\beta}$ is the interaction constant (i.e. amount of energy per one bond) between H-atom in the corresponding chain with the nearest silicon atoms in positions $k-1$ and k; $\beta = x_1, x_2, x_3, x_4, x_5, x_6$. Under the summation symbol there is a scalar product of difference in displacement vectors in every local chain $\mathrm{Si}_{k-1}\mathrm{H}\mathrm{Si}_k(\gamma_{k-1,k} - \xi_{k-1}) \cdot (\xi_k - \gamma_{k-1,k})$, where ξ_k — displacement vector of k-th atom of silicon; $\gamma_{k,k-1}$ — displacement vector of the hydrogen atom enclosed in k-th local chain (3) and (5).

5.1. Properties of bilinear form

First property. The rank of characteristic matrix $(U_{k-1,k;\beta} - \lambda E)$ for (7) is equal to zero (E — unit matrix), since the bilinear form (7) is reduced one. In this case, all eigenvalues are equal to each other, i.e. $\lambda_1 = \lambda_2 = \ldots = \lambda$. Hence, all $U_{k-1,k;\beta}$ elements of bilinear form are equal to each other.

$$U_{k-1,k;\beta} = \alpha_\gamma. \qquad (8)$$

The bilinear form (7), with account for (8) has the form

$$U_2 = \frac{1}{2}\alpha_\gamma \sum_{k=1}^{k=n}\sum_{\beta}(\gamma_{k-1,k} - \xi_{k-1})_\beta)(\xi_k - \gamma_{k-1,k})_\beta. \tag{9}$$

Thus, U_2 is characterized by the same interaction constant α_γ of the foreign atom with the surrounding environment for all local chains (if the crystalline lattice has also other atoms, e. g., germanium atoms (in system Si−Ge), the interaction will be characterized by two interaction constants α_γ).

Second property. The number of terms in the bilinear form corresponds to the number of local chains binding the hydrogen atom with its neighbors. E. g., number of terms (9) is equal to six for the number of bonds $Z = 6$. This allows the defects in silicon lattice to be taken into account.

Third property is manifested only after partial transformation of equations of hydrogen motion in the lattice and taking into account the specific nature of defects in this lattice. The sum of displacements differences for the hydrogen (helium) atom and any two nearest silicon atoms in any local chain, belonging to the given defect cavity, does not depend on the position of j or k in this cavity (see below (14) and (15)).

5.2. Motion equations

Equations for the foreign atom motion along direction $\mathbf{j}$ are

$$\frac{d}{dt}\left(\frac{\partial \mathscr{L}}{\partial \dot{\gamma}_{j,\beta}}\right) - \frac{\partial \mathscr{L}}{\partial \gamma_{j,\beta}} = 0.$$

The motion equations for some k of (9) comprise six sets, six equations in each set. By summing up the left parts of the first (second and etc.) motion equations and taking into account the properties (6a), we obtain

$$\frac{d^2}{dt^2}(\gamma_{j,x_j}) = \frac{d^2}{dt^2}\Gamma_{xj}. \tag{10}$$

where $j = 1, 2, 3, 4, 5, 6$.

Thus, the full displacement vector, $\mathbf{\Gamma}$, of (6c) can be written as:

$$\mathbf{\Gamma} = (\gamma_{1,x_1}; \gamma_{2,x_2}; \gamma_{3,x_3}; \gamma_{4,x_4}; \gamma_{5,x_5}; \gamma_{6,x_6}). \tag{11}$$

Or in the final form:

$$\mathbf{\Gamma} = (\Gamma_{1,x_1}; \Gamma_{2,x_2}; \Gamma_{3,x_3}; \Gamma_{4,x_4}; \Gamma_{5,x_5}; \Gamma_{6,x_6}). \tag{11a}$$

To finish the transformation of potential U_2 the influence of defects should be taken into account.

5.3. Defects

The most important among the lattice defects in this case are the vacancies and Frenkel defects occurring near the foreign light atom residing in the interstice (Figure 2). The defects significantly change the potential energy $U(\mathbf{\Gamma}, \{\xi_n\})$ of interaction between light foreign atom and the nearest environment (4), however, the number of lattice atoms + hydrogen atom remains the same.

As illustrated in Figure 2 the local chains for Frenkel defects have the following form:

$$\ldots \mathrm{Si}_{n-4}\mathrm{Si}_{n-3}\mathrm{Si}_{n-2}\mathrm{Si}_{n-1}\mathrm{H}\,\mathrm{Si}_{n}\mathrm{Si}_{n+2}\mathrm{Si}_{n+3}\ldots;$$

$$\ldots \mathrm{Si}_{n-4}\mathrm{Si}_{n-3}\mathrm{Si}_{n-2}\mathrm{Si}_{n-1}\mathrm{Si}_{n}\mathrm{H}\,\mathrm{Si}_{n+1}\mathrm{Si}_{n+2}\ldots;$$

$$\ldots \mathrm{Si}_{n-4}\mathrm{Si}_{n-3}\mathrm{Si}_{n-2}\mathrm{Si}_{n}\mathrm{H}\,\mathrm{Si}_{n+2}\mathrm{Si}_{n+3}\ldots;$$

$$\ldots \mathrm{Si}_{n-4}\mathrm{Si}_{n-3}\mathrm{Si}_{n-2}\mathrm{Si}_{n-1}\mathrm{Si}_{n}\mathrm{H}\,\mathrm{Si}_{n+3}\mathrm{Si}_{n+4}\ldots;$$

$$\ldots \mathrm{Si}_{n-4}\mathrm{Si}_{n-3}\mathrm{Si}_{n-2}\mathrm{Si}_{n-1}\mathrm{H}\,\mathrm{Si}_{n+3}\mathrm{Si}_{n+4}\ldots;$$

$$\ldots \mathrm{Si}_{n-4}\mathrm{Si}_{n-3}\mathrm{Si}_{n-2}\mathrm{Si}_{n-1}\mathrm{H}\,\mathrm{Si}_{n+1}\mathrm{Si}_{n+2}\ldots;$$

$$\ldots \mathrm{Si}_{n-4}\mathrm{Si}_{n-3}\mathrm{Si}_{n-2}\mathrm{Si}_{n-1}\mathrm{Si}_{n+1}\mathrm{H}\,\mathrm{Si}_{n+2}\mathrm{Si}_{n+3}\ldots;$$

$$\ldots \mathrm{Si}_{n-4}\mathrm{Si}_{n-3}\mathrm{Si}_{n-2}\mathrm{Si}_{n-1}\mathrm{Si}_{n+2}\mathrm{H}\,\mathrm{Si}_{n+3}\mathrm{Si}_{n+4}\ldots;$$

$$\ldots \mathrm{Si}_{n-4}\mathrm{Si}_{n-3}\mathrm{Si}_{n-2}\mathrm{Si}_{n-1}\mathrm{H}\,\mathrm{Si}_{n+2}\mathrm{Si}_{n+3}\mathrm{Si}_{n+4}\ldots;$$

$$\ldots \mathrm{Si}_{n-4}\mathrm{Si}_{n-3}\mathrm{Si}_{n-2}\mathrm{Si}_{n-1}\mathrm{Si}_{n+1}\mathrm{H}\,\mathrm{Si}_{n+3}\mathrm{Si}_{n+4}\ldots. \tag{12}$$

10 local chains were obtained in total.

Following the logic of constructing linear spaces (3), (5)−(6b), in case of Frenkel defect we would obtain the dimension 10, and in case of vacancy — 15. Such an approach would entangle the problem completely. However, there is another way of solving this problem, that allows to fully use the initial properties of an undisturbed lattice. For convenience of further analysis of potential U_2 we only consider Frenkel defect (where the number of chains is less than for the vacancy, and all operations are the same).

5.4. Conversion of potential U_2

Note, that, in accordance with the second property of a bilinear form, U_2 is proportional to the number of local chains (9). Then, potential U_2 for the imperfect structure (structure with defects) can be represented as a sum of regular $U_2(Z)$ and disturbed $U_2(\varsigma)$ potentials

$$U_2 = U_2(Z) + U_2(\xi). \tag{13}$$

The number of terms in $U_2(Z)$ corresponds to the number of local chains (of the nearest hydrogen environment in the undisturbed structure), and the number of terms in $U_2(\xi)$ is equal to ξ. In the considered problem the number of local chains Z is 6, and the number ξ of local chains in case of Frenkel defect is 4.

With the increase of excess silicon atoms (number of defects is p) in the hydrogen atom environment with Frenkel defect the potential energy is increasing (13). Number of atoms in the system „crystal + foreign atom" remains the

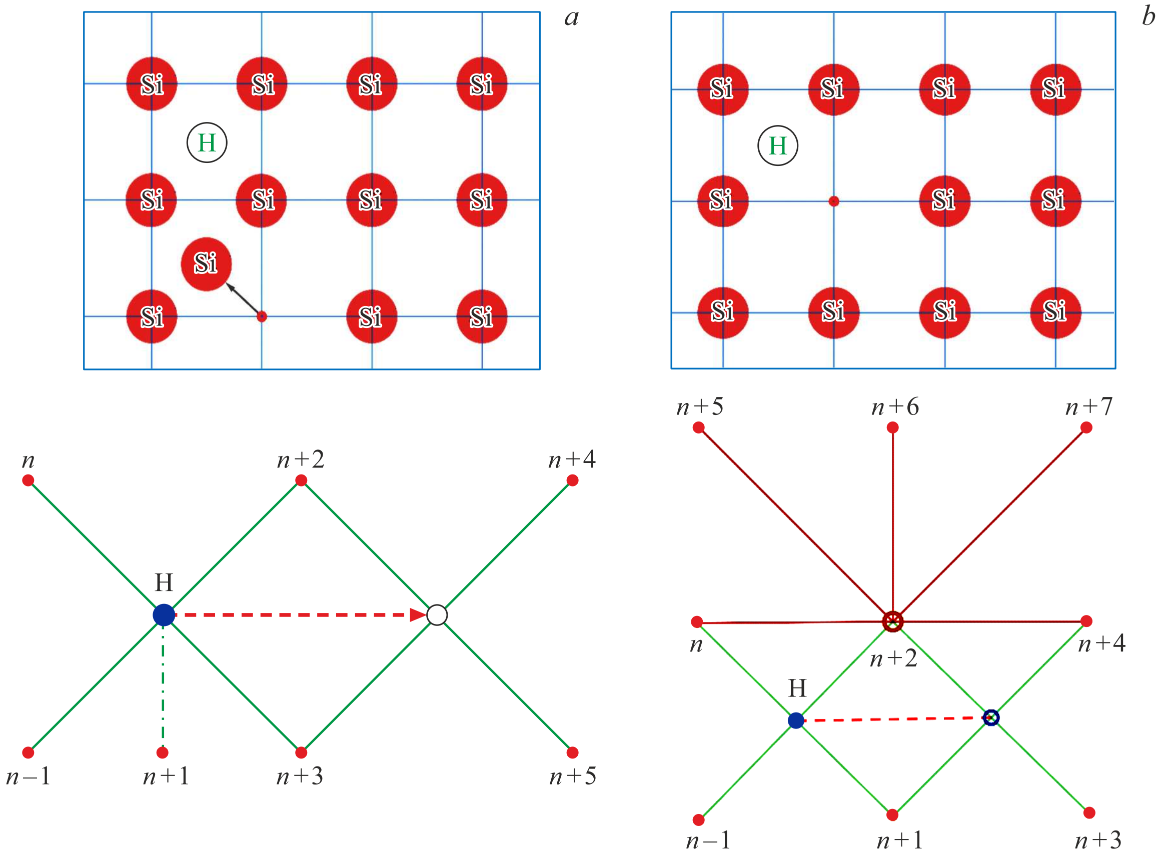

Figure 2. Top: Frenkel defect (a) and a vacancy (b). Bottom: diagrams of the hydrogen local chains in silicon lattice with defects (a) in $n+1$ position and (b) in $n+2$ position. For convenient account for bonds the neighboring atoms were numbered (see Figure 1).

same. If now we compare the number of additional local chains for a vacancy, η, and Frenkel defect, σ, respectively, it turns out that the square of excess silicon atoms (p^2) is less than a dependence of η, σ from p (Figure 3). (p^2) is considered for a reason, because each fragment of the bilinear form corresponds in size to the area spanned by vectors

$$(\gamma_{j,j-1} - \xi_{j-1}) \text{ and } (\xi_j - \gamma_{j,j-1}),$$

and this means that, to describe a motion system it is better to replace the excessive local bonds by an area, formed by excessive silicon atoms, i. e. by p^2. Especially since the potential energy of hydrogen atom with such area reduces U_2.

Thus, an excessive Si atom in the vicinity of H atom creates „surface“ or „cavity“ with an area of p^2.

Hence, the perturbed potential $U_2(\xi)$ can be written in one of the given forms below

$$\begin{aligned} U_2(\xi) &\sim \sum_k \sum_\beta (\gamma_{k,k-1} - \xi_{k-1})_\beta (\xi_k - \gamma_{k,k-1})_{\beta'} \\ &\sim \xi \sum_\beta (\gamma_{j,j-1} - \xi_{j-1})_\beta (\xi_j - \gamma_{j,j-1})_{\beta'} \\ &\sim p^2 \sum_\beta (\gamma_{j,j-1} - \xi_{j-1})_\beta (\xi_j - \gamma_{j,j-1})_\beta. \qquad (14) \end{aligned}$$

At that, the summation in (14) in two lower lines is performed only by coordinates.

6. Transfer to 1D motion

An important property of the equations (13) and (14) is that the sum in Eq. (14) may host any two silicon atoms from the vicinity of the hydrogen atom in the generated cavity with randomly arranged indices

$$j-1,\ j; \quad j-1,\ j+1; \quad j-1,\ j+2 \quad \text{etc.} \qquad (15)$$

including also the indices of a pair of atoms providing the direction of entering into the defect. Such random atom arrangement in the environment for a light atom allows the potential energy of the defect to be expressed through potential energy of regular lattice. It implies that the direction of exit from the defect coincides with the direction of entrance into this defect. Thus, we can assume that the defect influence does not change the direction of motion. Consequently, we may select the most convenient direction corresponding to the problem that would make the motion equation most simple and clear. Fir this purpose we may convert the system of vectors (5) or ($6a$), ($11a$) so as to choose the most convenient direction. We also

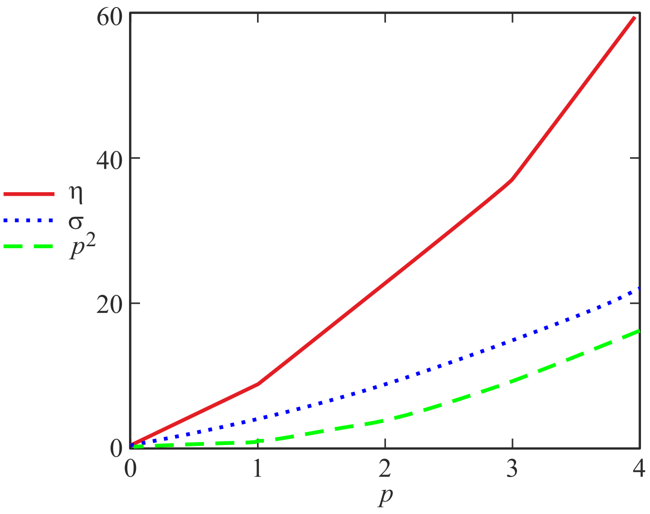

Figure 3. Dependence of excess local chains on the number of defects p for various types of defects: for vacancy η and for Frenkel defect σ; p^2 — square of excess silicon atoms that emerged in the new positions p.

may use a more simple approach by selecting for (11), (11a) some arbitrary direction, e.g., the direction towards the neighboring interstice. For this, without the loss of generality, let us select the direction for the vector $\mathbf{\Gamma}$ (11a) allowing for the note to (6c) corresponding to

$$\mathbf{\Gamma}_{1,x_1} = (\Gamma_{1,x_1}; 0; 0; 0; 0; 0). \tag{16}$$

To save the direction of motion in potential energy U_2, we rewrite the expression (9) in an equivalent bilinear form for the Frenkel defect (12). The bilinear form (9) for 10 local chains may be divided into a part responsible for the regular order $U_2(Z)$, that include six sums over coordinates and a part arisen from defect occurrence $U_2(\xi)$ that consist of the four such sums. Given that the condition (15) is fulfilled in these last sums we may express $U_2(\xi)$ as (14), second line. Since 4 identical defect lines can be represented as part of the sum of initial local chains, this sum can be written as 4/6 of the total number of identical local chains. Then, the expression U_2 allowing for defect influence, $U_2(\xi)$

$$U_2(\xi) = \frac{2}{3}\,p^2 U_2(Z),$$

can be written as

$$U_2 = \left(1 + \frac{2}{3}\,p^2\right) U_2(Z). \tag{17}$$

It follows from this equation, that the defect $\left(\frac{2}{3}\,p^2\right)$ from (17) does not distort the direction (16) along which hydrogen atom can move.

Moreover, the relation (17) indicates that potential energy of interaction of hydrogen atom with its environment doesn't depend on the location of the defect. It means that potential energy of hydrogen atom interaction with the defect is delocalized.

In case of a vacancy the potential energy U_2, after similar transformations, differ from (17) only in terms of the type of the defect form

$$U_2 = \left(1 + \frac{3}{2}\,p^2\right) U_2(Z). \tag{18}$$

Thus, in the problem of calculating the potential energy it is enough to consider only transition along the direction (16).

The motion equation for the system „crystal with defect + foreign atom“ may now be written as:

$$\begin{cases} m\,\dfrac{d^2\gamma_\beta}{dt^2} = -\dfrac{\partial U_1}{\partial \gamma_\beta} - \dfrac{\partial U_2}{\partial \gamma_\beta}, \\ M\,\dfrac{d^2\xi_{n,\beta}}{dt^2} = +\alpha_c \cdot \big[(\xi_{n+1,\beta} + \xi_{n-1,\beta} - 2\gamma_{n,\beta}) \\ + (\xi_{n+2,\beta} + \xi_{n-1,\beta} - 2\gamma_{n,\beta}) + (\xi_{n+3,\beta} + \xi_{n-1,\beta} - 2\gamma_{n,\beta}) \\ + (\xi_{n+2,\beta} + \xi_{n+1,\beta} - 2\gamma_{n,\beta}) + (\xi_{n+2,\beta} + \xi_{n+1,\beta} - 2\gamma_{n,\beta}) \\ + (\xi_{n+3,\beta} + \xi_{n+2,\beta} - 2\gamma_{n,\beta})\big] \\ + \alpha_\gamma \cdot \dfrac{2}{3}\,bp^2 \cdot \big[(\xi_{n+1,\beta} + \xi_{n-1,\beta} - 2\gamma_{n,\beta}) \\ + (\xi_{n+2,\beta} + \xi_{n-1,\beta} - 2\gamma_{n,\beta}) + (\xi_{n+3,\beta} + \xi_{n-1,\beta} - 2\gamma_{n,\beta}) \\ + (\xi_{n+2\beta} + \xi_{n+1,\beta} - 2\gamma_{n,\beta}) + (\xi_{n+2,\beta} + \xi_{n+1,\beta} - 2\gamma_{n,\beta}) \\ + (\xi_{n+3,\beta} + \xi_{n+2,\beta} - 2\gamma_{n,\beta})\big], \end{cases} \tag{19}$$

where $\beta = x_1, x_2, x_3, x_4, x_5, x_6$.

The new system of motion equations represents a system of interlocking differential equations linking the foreign atom displacement with the atomic displacements of the nearest lattice.

For simplicity we use the adiabatic approximation which states that atomic displacement of lattice $\xi_{n,\beta}(t)$ cannot exceed displacement of the foreign atom γ_β [31,32]:

$$\xi_{n,\beta}(t) \le \gamma_\beta(t). \tag{20}$$

Then, the hydrogen atom displacement between the two lattice sites is added [31,32]

$$\xi_{n+1,\beta} + \xi_{n-1,\beta} - 2\xi_{n,\beta} = \tau^2 \cdot \frac{d^2\xi_{n,\beta}}{dt^2} \tag{21}$$

to the difference of displacements between the neighboring lattice sites [21,32]:

$$\xi_{n+1,\beta} + \xi_{n-1,\beta} - 2\gamma_\beta \approx \tau^2 \cdot \frac{d^2\gamma_\beta}{dt^2}, \tag{22}$$

where $\beta = x_1, x_2, x_3, x_4, x_5, x_6$.

6.1. Simplified motion equations

Now we may replace the parentheses for the mutual atomic displacements in the lattice and mutual displacement of the light atom and lattice atoms in the system of equations (19) with (21) and (22), and, allowing for (6a), (11) and (11a), we obtain the system of equations.

Having selected the vector direction $\mathbf{\Gamma}$, (16) we simplify the motion equations written in (19). Now we obtain the system (23) that indicates that motion of the foreign atom is unidimensional and rectilinear.

$$\begin{cases} m^{\#}\dfrac{d^2\Gamma_{x_1}}{dt^2} = -\dfrac{\partial U_1}{\partial \Gamma_{x_1}} \\ m^{\#}\dfrac{d^2\Gamma_{x_2}}{dt^2} = 0, \\ m^{\#}\dfrac{d^2\Gamma_{x_3}}{dt^2} = 0, \\ m^{\#}\dfrac{d^2\Gamma_{x_4}}{dt^2} = 0, \\ m^{\#}\dfrac{d^2\Gamma_{x_5}}{dt^2} = 0, \\ m^{\#}\dfrac{d^2\Gamma_{x_6}}{dt^2} = 0, \\ M\dfrac{d^2\xi_{n,x_1}}{dt^2} = +\alpha_\gamma\tau^2\left(1+\dfrac{2bp^2}{3}\right)\dfrac{d^2\Gamma_{x_1}}{dt^2}, \\ M^{\#}\dfrac{d^2\xi_{n,x_2}}{dt^2} = 0, \\ M^{\#}\dfrac{d^2\xi_{n,x_3}}{dt^2} = 0, \\ M^{\#}\dfrac{d^2\xi_{n,x_4}}{dt^2} = 0, \\ M^{\#}\dfrac{d^2\xi_{n,x_5}}{dt^2} = 0, \\ M^{\#}\dfrac{d^2\xi_{n,x_6}}{dt^2} = 0, \end{cases} \tag{23}$$

where $m^{\#}$ is effective mass of the foreign atom,

$$m^{\#} = m - \alpha_\gamma\tau^2. \tag{23a}$$

$M^{\#}$ — effective mass of lattice atom from the nearest environment of the foreign atom

$$M^{\#} = M - \alpha_c\tau^2. \tag{23b}$$

α_γ — Interaction constant of the foreign atom with the nearest environment atoms, α_c — mutual interaction constant of the lattice atoms.

The system (23) consists actually of the non-related equations which facilitates their further investigation.

6.2. Discreteness of foreign atom motion, momentum conservation law

The seventh line of the system of equations (23) can be expressed in another way

$$\frac{d^2}{dt^2}\left(M_n^{\#}\xi_{n,j} + \frac{2bp^2}{3}\cdot\alpha_\gamma\tau^2\Gamma_{x_1}\right) = 0. \tag{24}$$

This indicates the following two facts:

1) Locally, the momentum of sub-system „Si$_n$ + H“ is preserved (n-th atom of the silicon lattice and foreign atom):

$$\frac{d}{dt}\left(M_n^{\#}\xi_{n,z} + \frac{2bp^2}{3}\alpha_\gamma\tau^2\Gamma_\beta\right) = \text{const}. \tag{25}$$

The equation (25) is defined with an accuracy up to the momentum imparted to the lattice.

2) Since the displacements of $\xi_{n,j}$ n-th atoms of the silicon lattice are discrete, (i. e. ξ_n each is attributed to its n-th node), they only take on discrete values $\Gamma_{\beta,n}$. Moreover, this leads to the discreteness of the hydrogen atomic displacement vector itself.

$$\mathbf{\Gamma} = \mathbf{\Gamma}_n. \tag{26}$$

Displacements of the foreign atom appear to be discrete and controlled through the interaction with the nearest Si$_n$ — atoms.

Given the (26), the first equation of the system (23) provides a possibility of being re-written as

$$m^{\#}\frac{d^2\Gamma_n}{dt^2} = -\frac{\partial U_1}{\partial \Gamma_n}. \tag{27}$$

7. Expansion of potential U_1

Motion of the foreign atom in a disordered structure is well defined by the regular portion of the potential (17) and (18). When the foreign atom in the regular lattice is moving from one position to another, the environment of this atom remains unchanged and, consequently, the potential energy of this interaction remains the same. Therefore there should be a transition operator $\hat{T}$, acting as follows:

$$\hat{T}(\mathbf{a}_n)U_1(\mathbf{\Gamma}) = U_1(\mathbf{\Gamma} + \mathbf{a}_n),$$

where $\mathbf{a}_n$ — minimal displacement vector of H-atom in direction towards n-th position,

$$\mathbf{\Gamma} = n\mathbf{a}_n.$$

Let’s expand $U_1(\mathbf{\Gamma} + \mathbf{a}_n)$ in a series in a point defined by the end of the vector $\mathbf{\Gamma}$:

$$\begin{aligned} U_1(\mathbf{\Gamma} + \mathbf{a}_n) &= \sum_{m=0}^{\infty}\frac{1}{m!}\frac{\partial^m}{\partial \mathbf{\Gamma}^m}U_1(\mathbf{\Gamma})a_n^m \\ &= \left(\sum_{m=0}^{\infty}\frac{1}{m!}\frac{\partial^m}{\partial \mathbf{\Gamma}^m}a_n^m\right)U_1(\mathbf{\Gamma}) = \hat{T}(\mathbf{a}_n)U_1(\mathbf{\Gamma}). \end{aligned} \tag{28}$$

The forward motion of the light atom along its possible positions is equivalent to backward motion, because the direction was not specified in the first place. Therefore, the operator of transition from one position into the neighboring one does not depend on the direction of this transition. In this case, the nearest member of series (28), which in the disordered system is irrespective of the transition direction, and only depends on distance, is a second order operator with the squared distance (a_n^2).

$$\frac{1}{2!}\cdot\frac{\partial^2 U_1(\mathbf{\Gamma})}{\partial \mathbf{\Gamma}^2}(\mathbf{a}_n^2) = \hat{T}(\mathbf{a}_n^2)U_1(\mathbf{\Gamma}).$$

As follows from (28), operator $\hat{T}(\mathbf{a}_n)$ commutes with operator $\partial^2/\partial\mathbf{\Gamma}^2$, and they have same eigenfunctions. Here, the eigenfunction is $U_1(\mathbf{\Gamma})$, which represents the potential field dragging the foreign atom from one position to another. In this case the behavior of functions $U_1(\mathbf{\Gamma})$, as a value preserved in transition from position $\mathbf{\Gamma}_n$ to $\mathbf{\Gamma}_{n+1} = \mathbf{\Gamma}_n + \mathbf{a}_n$ may be represented as a Sturm–Liouville eigenvalue problem

$$\partial^2 U_1/\partial\mathbf{\Gamma}^2 = -\Lambda U_1,$$

here Λ — eigenvalue. Thus, the eigenfunctions have a form of a space-periodic function:

$$U_1(\mathbf{\Gamma}_k) \sim \exp[\pm j2\pi\Gamma_k/a_n].$$

It means that preservation of the short-range order during random transitions between the nearest spatial tetrahedral positions will lead to a space-periodic function of potential $U_1(\mathbf{\Gamma}_k)$. Let us choose the cosine type for such potential [21,33]:

$$U_1 = A[1-\cos(2\pi\Gamma_n/a_n)]. \tag{29}$$

Hence, the first equation of system (23) with potential (29) results in Frenkel–Kontorova equation

$$m^{\#}\frac{d^2\Gamma_n}{dt^2} = -\frac{2\pi}{a_n}\cdot A\cdot\sin\frac{2\pi\Gamma_n}{a_n}, \tag{30}$$

where $m^{\#}$ is effective mass defined by the ratio (23a), A is amplitude of periodic potential defined by the property and configuration of the crystal short-range order [31]. Equation (30) is called Frenkel–Kontorova equation. This equation in our problem defines the displacement of n-th node of the virtual chain of possible light atom locations.

Thus, having reviewed potential energies from the Lagrangian (1) and having significantly transformed the motion equations we obtained the Frenkel–Kontorova equation. By solving this equation we may describe the „kink" (inflection) translational motion [21,31,32]:

$$\Gamma_n = \left(\frac{2a_n}{\pi}\right)\operatorname{arctg} C_0\exp\left(\pm\frac{2\pi}{a_n}\sqrt{-A/m^{\#}}\cdot(t-n\tau)\right). \tag{31}$$

The following Lagrangian corresponds to the equation (30):

$$\mathscr{L} = \sum_n\left[\frac{m}{2}\left(\frac{d\Gamma_n}{dt}\right)^2 - \frac{1}{2}\alpha_\gamma\left(1+\frac{2}{3}\cdot bp^2\right)(\Gamma_n-\Gamma_{n-1})^2 - A(1-\cos(2\pi\Gamma_n/a_n))\right]$$

This Lagrangian describes 1D Γ_n kink motion and contains data about the defects of the 3D lattice.

8. Soliton structure and forms of foreign atom motion

The magnitude A is an amplitude of periodic field (31) defined by the ratio [31]:

$$A = Ga_n^3/4\pi^2, \tag{32}$$

where G is silicon shear modulus, $79.9\cdot 10^{10}$ din/cm^2; a_n is distance between the neighboring tetrahedral interstices.

Effective mass

$$m^{\#} = m - \alpha_\gamma\left(1+\frac{2bp^2}{3}\right)\tau^2. \tag{33}$$

Here τ is decomposition time, $\tau < 10^{-13}$ s, which now serves as a parameter of equation. From (32) it follows that the soliton moves if it has negative effective mass [31,32]: $m^{\#} < 0$. In order to calculate $m^{\#}$ we need to know α_γ. The magnitude α_γ is defined by the atom polarizability $\beta(n)$:

$$\alpha_\gamma = \frac{e^2}{\beta^{(n)}},$$

where e is electron charge equal to $4.8\cdot 10^{-10}\,\mathrm{g}^{1/2}\cdot\mathrm{cm}^{3/2}/\mathrm{s}$.

The value of the inter-crystalline field in the covalent crystals reaches the values of $\varepsilon \approx 10^7 \div 10^8$ V/cm. The intensity of this field is enough to polarize the selected atoms [34–36]. This field distorts the n-th energy level E_n of the foreign atom by value ΔE_n and is a squared value in terms of field ε [36,37]

$$\Delta E_n = -\frac{1}{2}\beta^{(n)}\varepsilon^2.$$

Hence, the polarizability $\beta^{(n)}$ depends on the quantum state of the light atom, thus, if there's no conductivity electrons in the covalent crystal, then the atom in n-th quantum state placed in the crystal, would remain in the same state. Thus, the behavior of effective mass defined by (24a) shows how the atom weight m and quantum state expressed through polarizability $\beta^{(n)}$ affect the behavior of soliton Γ_n.

Table 1. Effective masses of hydrogen isotopes at $\beta = 0.667 \cdot 10^{-3}$ (nm^3)

Atom	Weight, m, (g) $\times 10^{-24}$	Effective mass m^*, (g) $\times 10^{-26}$
^{1}H	1.67	-2.5059
^{2}H	$2 \cdot 1.67$	-5.0118
^{3}H	$3 \cdot 1.67$	-7.5176

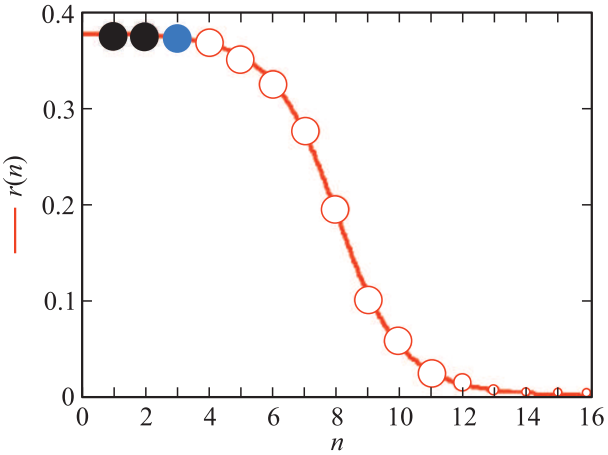

Figure 4. Formation of soliton in the virtual chain of possible locations of the hydrogen atom. Y-axis shows the displacements in n-th site of the virtual chain (nm). X-axis shows n — number of sites of the virtual chain.

Effective soliton mass is negative for all hydrogen isotopes (Table 1). All these isotopes may move in crystal only as a collective consisting of the foreign isotope and the accompanying reversible atomic displacements.

Transition of hydrogen atom from one position to another (as illustrated in Figure 4) allows to monitor the number of lattice atoms participating in the formation of the soliton. According to the local momentum conservation law (25) each virtual location of the hydrogen atom in the virtual chain is directly related to the silicon atoms. This circumstance allows us to trace how many atoms of the lattice take part in the soliton formation. Thus, the soliton in Figure 4, involves 10 atoms (although there are only 4 neighboring atoms), starting from the atom marked in blue color and other atoms marked in white. The soliton shown is moving from the left to the right. Black color denotes the steady states that the soliton has already passed. Blue color designates the state where the atom is located at the present moment. White color shows unsteady states where the atom is yet to come.

8.1. Parameter impact on the soliton structure formation

Formation of soliton can be traced by selecting different scale τ in (31). Since the interaction constant is defined by polarizability of the foreign atom, the ultimate minimal time of soliton tracing can be limited, e.g. by the value $\tau \sim 10^{-17}$, which is comparable with the „period of the electron circulation in Bohr hydrogen atom“ or by comparing the reverse frequency of electronic density oscillations [38] (Figure 5).

8.2. Impact of atom mass and polarizability on the form of soliton

To form a „step“ for hydrogen: we need 8 atoms for H, 9 atoms for ^{2}H, and 11 atoms for ^{3}H (Figure 6, *a*). Heavier tritium starts moving earlier than light atoms (hydrogen and deuterium) and continues longer.

The situation is somewhat different for helium (Table 2). Each helium isotope, irrespective of its mass, has three different types of polarization [34,35]. At $\beta = 0,0203\,\mathrm{nm}^3$ the effective mass is less than zero which provides the translational motion. The heaviest ^{4}He has the lowest effective mass, and, vice versa, the lightest ^{2}He has the highest effective mass. Two other polarizability types can only ensure oscillatory motion of helium isotopes, since their effective masses would be positive. To form the soliton of helium isotopes a very large number of silicon atoms is required (Figure 6, *b*).

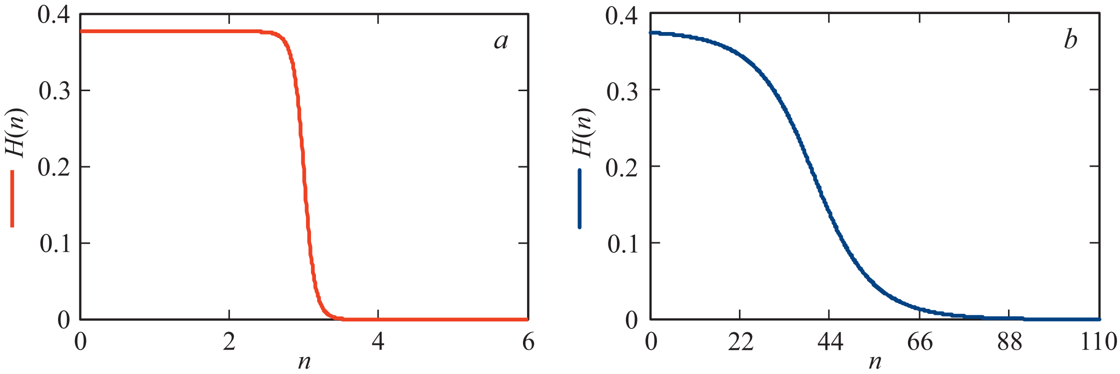

Figure 5. Form of soliton at $\tau = 10^{-14}$s (*a*) and $\tau = 10^{-16}$s (*b*). Y-axis shows the displacements in n-th site of the virtual chain (nm). X-axis shows n — number of sites of the virtual chain.

Table 2. Effective mass of helium isotopes in three ground states

Condition	Atom	Polarizability β, (nm^3)	Weight, m, $\times10^{-24}$ g	Effective mass, $m^{\#}$, $\times10^{-24}$ g
1^1S_0	^{2}He ^{3}He ^{4}He	0.0203	$2\cdot1.67$ $3\cdot1.67$ $4\cdot1.67$	-2.73098 -4.09647 -5.46195
2^1S_0	He ^{3}He ^{4}He	11.8	$3\cdot1.67$ $3\cdot1.67$ $4\cdot1.67$	3.4691 5.0203 6.938
2^3S_1	^{2}He ^{3}He ^{4}He	4.67	$2\cdot1.67$ $3\cdot1.67$ $4\cdot1.67$	3.695 5.542 7.389

8.3. Impact of defects

Frenkel defects and vacancies significantly influence the form of the soliton and the number of atoms in its environment, (Figure 7).

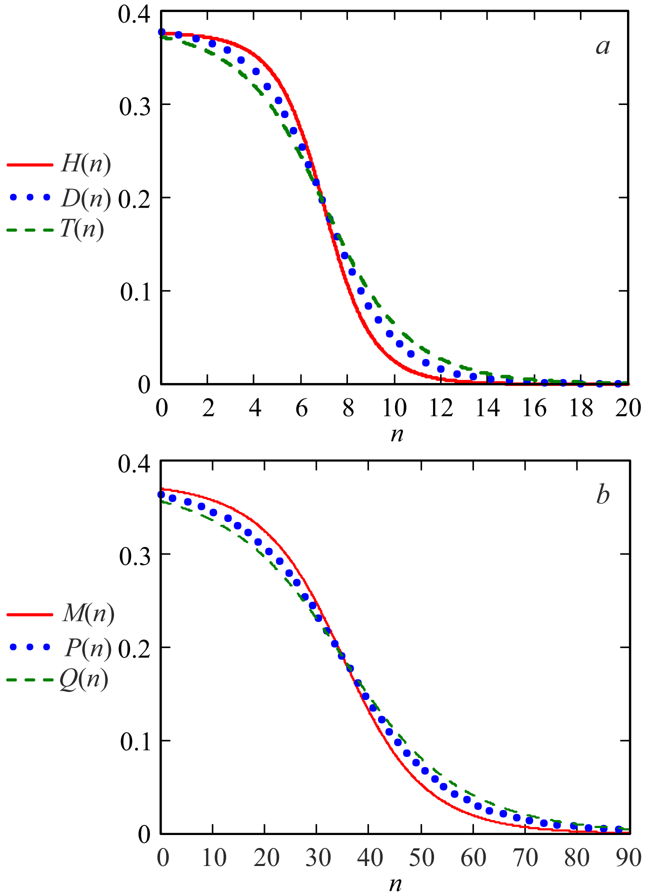

Figure 6. Comparison of transitions to the neighboring position for hydrogen (*a*) and helium (*b*) isotopes. (*a*) T(n) — tritium, D(n) — deuterium, H(n) — hydrogen. (*b*) Q(n), P(n), M(n) — helium isotopes ^{4}He, ^{3}He, ^{2}He, respectively (short-lived radioactive isotope ^{2}He was added to indicate the systematic nature of dependence). Y-axis indicates the displacements in n-th site of the virtual chain (nm). X-axis shows n — number of sites of the virtual chain.

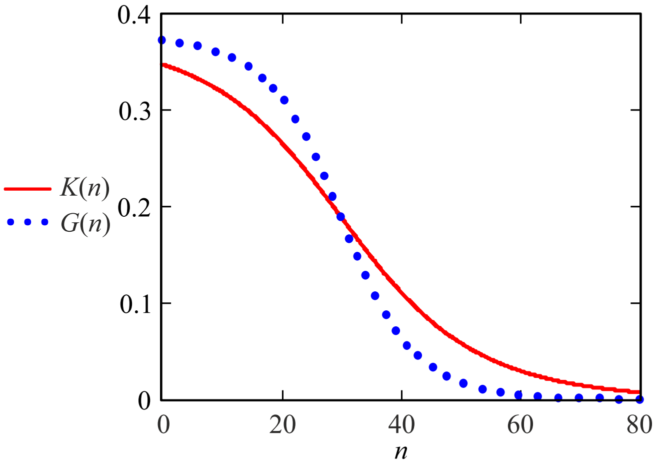

Figure 7. Displacement of soliton of helium isotope ^{4}He in its ground state in a regular structure corresponds to the function $K(n)$, kink displacement in the lattice with a defect corresponds to $G(n)$. Y-axis shows the displacements in n-th site of the virtual chain (nm). X-axis shows — the number of nodes in the virtual chain.

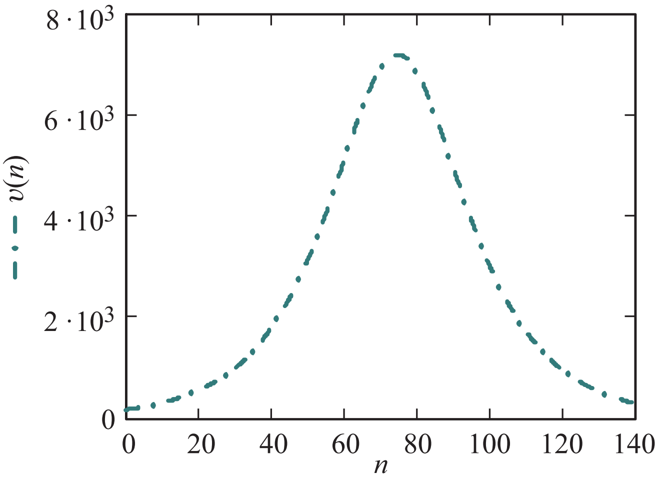

Figure 8. Velocity distribution in a soliton formed by helium atom for various virtual positions.

Table 3. Oscillation frequencies of helium isotopes

Polarizability	2^1S_0	Effective mass	Angular frequency ω, $\times 10^{14}$
$11.8\,\text{nm}^3$	^{2}He	$3.3528 \cdot 10^{-24}$ g	0.0940143
	^{3}He	$5.0292 \cdot 10^{-24}$ g	0.0781504
	^{4}He	$6.70564 \cdot 10^{-24}$ g	0.0664782

Finally, let us consider the velocity distribution in the soliton (Figure 8). Soliton velocity is hard to determine since its formation involves about 140 lattice atomic displacements (see Figure 8). Velocity of the foreign atom within the soliton would be different at every lattice node (virtual path). Maximal velocity in this distribution would be the sound speed in silicon crystal [39]. Such velocity maximum corresponds to the most unstable state, e. g., position corresponding to the inflection point (Figure 7).

9. Influence of soliton motion on the lattice

From the last equation of set (23) with account for (31) it follows that the displacements of lattice atoms are fully defined by the soliton behavior. Maximal displacement of this soliton $\xi_{n,j} \approx 0.02$ nm is an order of magnitude less than maximal soliton displacement for the foreign atom at the node (which is equal to the distance between the neighboring tetrahedral interstices) and corresponds to $\Gamma_n \approx 0.4$ nm (Figure 9).

10. Oscillatory motion of the foreign atom

It follows from the ratio (31) that, provided the effective mass is positive, the value

$$\frac{2\pi}{a_n}\sqrt{-\frac{A}{m^{\#}}}$$

is imaginary and equal to the angular frequency of the foreign atom in the interstice $j\omega = \sqrt{-A/m^{\#}}$. Table 3 lists the oscillation frequencies of helium isotopes in the interstice with such a polarizability when the effective mass is positive (Table 2). It is evident from the table that frequency decreases with the increase of mass.

Soliton motion ceases and the foreign atom turns to the oscillation mode.

11. Conclusion

This paper considers the problem of light foreign atom (hydrogen, helium) motion through a crystal lattice. It was taken into account that the foreign atom exerts influence upon the adjacent lattice atoms.

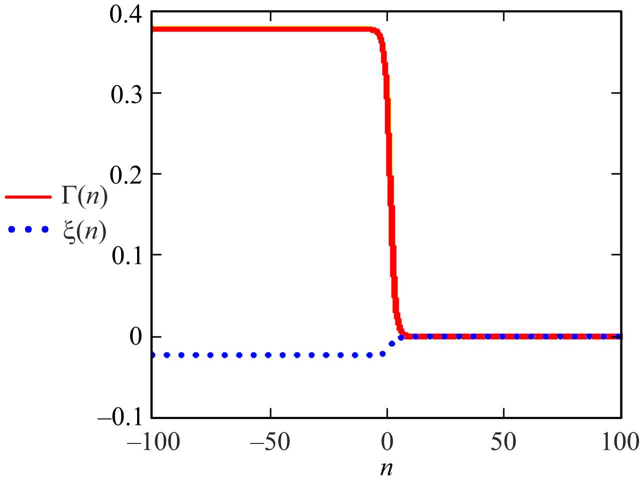

Figure 9. Influence of foreign atom soliton on the reversible lattice atoms displacements. Red color indicates the kink for the foreign atom moving to the right. Blue color shows the kink for the reversible displacements of lattice atoms.

The silicon crystal was chosen because of its diamond-like lattice and a set of interstices capable of hosting the foreign atoms chosen. Only tetrahedral interstices were taken into account.

The number of possible interactions (bonds) of the foreign atom with its environment — lattice atoms, is provided due to a local structure of the crystal interstices. This number of local bonds (chains) allowed to introduce a linear multi-dimensional space where the foreign atom is moving.

The use of Lagrangian for such system enabled us to find a motion equation describing the motion of both the foreign atom and the lattice atoms in a multidimensional space. The symmetries assumed by the initial (trial) Lagrangian resulted in appearance of a 1D Lagrangian which helped us discover various options of the foreign atom motion and account for the defects in the lattice.

1. The foreign atom may move across the crystal only as a part of the collective, accompanied by reversible displacements of the nearest lattice atoms. Effective mass of such soliton is negative. This collective can be described by the Frenkel–Kontorova equation (soliton) obtained from from the 1D Lagrangian.

2. The foreign atom is only manifested in the lattice as an individual particle when in the oscillations mode. The effective mass of such atom is positive. Oscillation frequency of this atom is $\sim 1/\sqrt{m}$.

Since selected foreign atoms have a set of isotopes and, independently, possible quantum states that could be manifested through the polarizability of hydrogen and helium atoms, the new situations have come about.

3. It turned out that solitons for heavier isotopes move faster across the lattice compared to the solitons for lighter isotopes.

4. Effective mass of soliton depends on the actual mass of the foreign atom and its polarizability. Therefore, because of the ratio of the real mass and polarizability the chosen foreign atoms (isotopes) can manifest themselves either during motion through the crystal as a Frenkel–Kontorova soliton, a collective comprising the foreign atom and the accompanying reversible displacements of the lattice atoms, or as an individual atom in the oscillation mode.

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Conflict of interest

The authors declare that they have no conflict of interest.

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