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Simulation of diffusion under pressure in bcc metals

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Abstract

This work is devoted to simulation of atom configurations in bcc metals near the point defect using the molecular static method. The values of migration and formation volumes are very sensitive to the atomic structure in the vicinity of a defect, which makes it necessary to consider a large number of atoms in the computation cell and to take into account an elastic matrix around the cell. We have developed the new model taking into the consideration these factors. It allows to define "fine structure" of displacement atoms near the point defect. The atoms of third zone were embedded in an elastic continuum. The displacement of each atom embedded in an elastic continuum was defined as the first and the second terms in solution of elastic equation. In the framework of this model we calculated the formation and migration volumes of defect. Also we take into the consideration that the energy of system (in particular the system with defect) depends on the outer pressure. This dependence gives an addition to the values of migration and formation volumes.

Keywords: Diffusion, pressure, activation volume, point defect, vacancy

1. Introduction

Point defects (vacancies and interstitials) directly affect the kinetics and thermodynamics of metals and alloys and it is thus very important to develop a good understanding of their properties, i.e., their structure and mobility. One of the methods, which allow to get information on defects being involved in diffusion process and choosing the diffusion mechanism from several variants, is the study of the pressure influence on the diffusion coefficient. This influence is determined by the activation volume V^{act}, which consist of two items: the formation volume V^f and the migration volume V^m. The expression for the diffusion coefficient usually is written [1]:

$$D = D_0 \cdot exp(\frac{E^f + E^m + p \cdot V^f + p \cdot V^m}{k \cdot T}) . \quad (1)$$

Microscopic calculations of volumes associated with defect migration are difficult, as emphasized by Lazarus [1]. Calculations of migration volumes are few and they do not agree with each other and with the experimental results. In this paper the new model for simulation of the diffusion features of point defects is suggested. First variant of this model and some prior simulation results were presented at the conference DISO2005 and will be published in the conference proceedings [2]. We used a new approach that take into account the features of lattice discreteness more detailed and the displacements of atoms in an elastic matrix around the computation cell. Apart from it the contributions in activation volumes concerned with the pressure dependencies of the formation and migration energies are took into account. Earlier the evaluation of these contributions was performed in the rigid lattice approximation and a qualitative agreement with existent experimental data was obtained [3].

In Section 2 the formalism and the model for the calculation of the formation energies and volumes as well as pressure dependencies of the formation and migration energies are introduced. The model is developed in terms of the molecular static method. The main features of the atomic structure optimization are described. Section 3 is devoted to the description of the simulation results for the vacancy and interstitial atom in α-iron.

2. Model for simulation of the diffusion features of point defects

It is known that the displacements of atoms obtained by means of simulation are different with those calculated using the theory of elasticity. These differences decrease with increasing distance from the defect. The values of migration and formation volumes are very sensitive to the atomic structure in the vicinity of a defect, which makes it necessary to consider a large number of atoms in the computation cell and to take into account an elastic matrix around the cell. We have developed the new model taking into the consideration these factors.

The computation cell contains about 50000 atoms (zone I, II). The equilibrium positions of these atoms are simulated by usual Molecular Static Method. The atoms of a third zone (fig. 1) are embedded in an elastic continuum and their displacements are defined using the theory of elasticity.

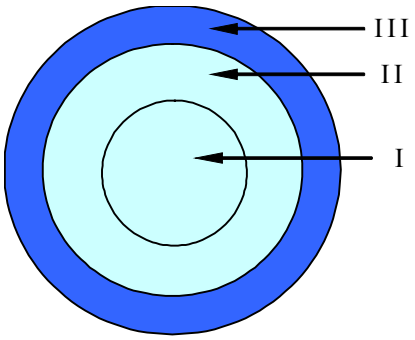

Fig. 1: Scheme of computation cell: I, II – directly computation cell, III – atoms of elastic continuum.

In the framework of Johnson's and Brown's model [4] the displacements of atoms of a third zone ($\boldsymbol{u}$) are defined as a first term in a solution of elastic equation because Johnson and Brown considered that activation energies are insensitive to all terms expect $\boldsymbol{u}_1$:

$$\boldsymbol{u}_1 = C_1 \boldsymbol{r}/r^3, \tag{2}$$

In our model in addition to this term we take into account a cubic symmetrical one as we found that total activation volume is susceptible to its influence on lattice distortion:

$$\boldsymbol{u}_2 = C_2 \nabla\left(\frac{1}{r^5}\left(\frac{x^4 + y^4 + z^4}{r^4} - \frac{3}{5}\right)\right), \tag{3}$$

where $r = \sqrt{x^2 + y^2 + z^2}$ is a distance from the defect, C_1,C_2 – constants.

The first term $\boldsymbol{u}_1$ has a spherical symmetry and gives rise to an expansion or contraction of the lattice. All other terms (including $\boldsymbol{u}_2$) used distort the shape of the lattice, and were adjusted where necessary by adding or subtracting some $\boldsymbol{u}_1$ so that they don't give rise to net volume change [4].

The consistent iterative procedure of the constants C_1 calculations and the atomic structure simulations in the crystal with a defect is realized. Using Eq.2 the constant C_1 is calculated on the basis of displacements of atoms in II zone (in the middle of distance between the vacancy and the bound of the computation cell), obtained with the help of simulation. The constant C_1 calculated on a previous step of the iterative procedure is used to define the displacement of atoms in a third zone.

As stated above we also take into account a second term in the solution of the elastic equation. On the first step the constant C_1 is calculated using the iterative procedure, described above. Then the constant C_2 is calculated using the difference between the displacements of atoms obtained by means of simulation and those calculated using Eq. 2. The atoms of third zone are displaced taking into account both the constant C_1 and the constant C_2. This procedure is repeated till constants converge to a certain value. On the last step the constant C_1 is calculated using the difference between the displacements of atoms obtained by means of simulation and the additions to displacements of atoms calculated with the help of Eq. 3.

We obtained that the constants C_1 and C_2 converge to a certain values in some iterations (fig. 2).

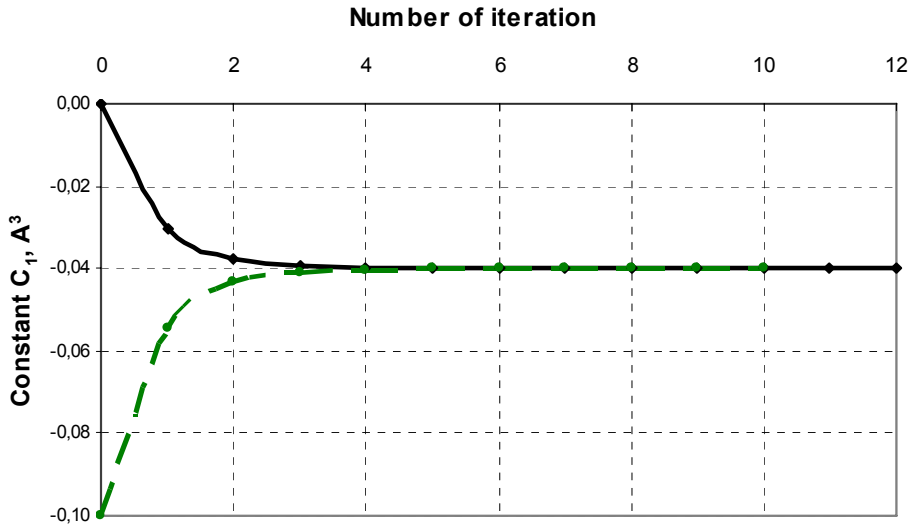

Fig. 2: The convergence of the constant C_1 to a certain value in some iterations.

The constant C_2 converges to a certain value more quickly.

We studied the dependence of the displacement atoms concerned with a cubic symmetrical term in a solution of elastic equation, i.e. with the constant C_2, on the distance from the defect. Results have showed that for the vacancy this term does not give noticeable contribution to the displacements of atoms if the computation cell has sufficiently large size. But this term gives appreciable contribution to the displacements of atoms if the computation cell has radius less then ten lattice parameters.

2.1. Calculation of formation volume for vacancy

The volume expansion associated with a lattice configuration is easily calculated and is known to be linear with constant C_1 [2].

$$\Delta V = \int\int u \cdot dS = 4\pi C_1 \tag{4}$$

$\Delta V'$ is seen to be dependent of the radius of the sphere only through the constant C_1. For a finite lattice, Eshelby [5] has shown that the boundary condition of zero stress at the surface of the lattice gives rise to an addition term in the volume expansion (the so-called "image force" correction). This correction may be written as an Eshelby factor:

$$\Delta V' = \Delta V(1 + \frac{4 \cdot (C_{11} - C_{12}) + 12 \cdot C_{44}}{15 \cdot K_0}), \tag{5}$$

where C_{11}, C_{12}, C_{44} – isotropic elastic constants, K_0 – bulk module.

For α – iron the Eshelby factor equal to 1.726.

The usual part of the formation volume may be written for the vacancy:

$$V^f = \Omega + \Delta V', \tag{6}$$

where Ω – atomic volume.

2.1. Peculiarity of formation volume calculation for interstitial

Analogous procedure realizes for definition of the interstitial atom formation volume. But in this case a central symmetry is broken as the interstitial atom and its neighbor form dumb-configuration. Configuration <110> split interstitial is the minimum energy configuration and is, therefore, stable. In real macroscopic crystals dumb-configurations are chaotically distributed. So cancellation of their influence on atomic displacements at a sufficiently large rage from the defects region takes place. Non-central constituent of displacements, including cylindrical symmetrical part, is lacking. We developed the model in which six <110> split interstitial are disposed in the system enough far from each other so as in primary case consider these effects (fig. 3). The constant C_1 is calculated on the basis of displacements of atoms at a sufficiently large distance from the defects region.

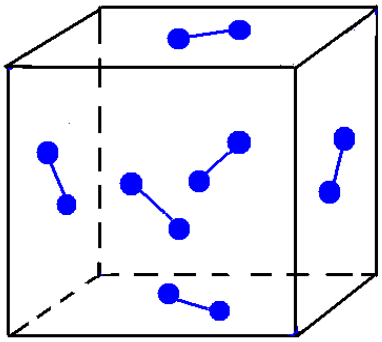

Fig. 3. Relative position of six <110> split interstitial in the computation cell.

The usual part of the formation volume may be written for the interstitial atom:

$$V^f = -\Omega + \Delta V', \tag{6a}$$

2.3. Calculation of migration volume for vacancy

To calculate the migration volume one of the atoms from the neighbors of the defect is moved in the direction of the defect by about some percent of the distance from the defect on the each step. When the atom pass by the centre of the triangle, which is made

by the neighbors of moving atom (fig. 4), the distance from the atoms is a minimum, the perturbation of the system become a maximum and, therefore, the change of the volume is a maximum.

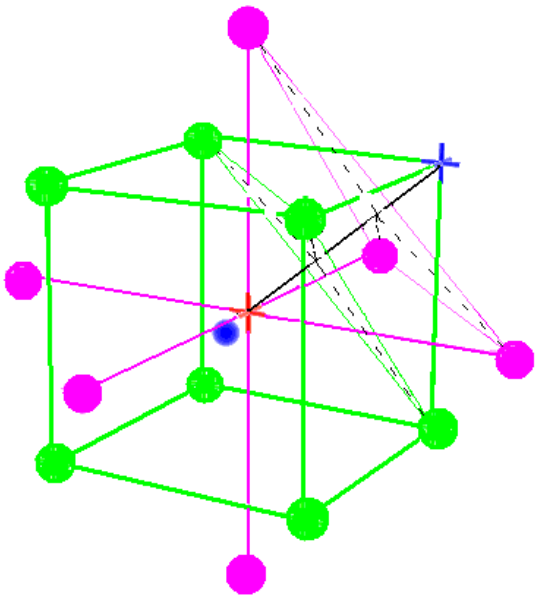

Fig. 4: The moving of the atom in the direction of the vacancy.

As a central symmetry is broken when the atom is moved, then we introduced two centers of dilatation for the calculation the constant C_1. One is concerned with the defect and second is concerned with the original position of the moving atom. Thus, the displacement field may be represented as a sum of two items. Each item is concerned with the respective dilatation center. The contribution of each dilatation center is determined by the weighting coefficient, which depends on the current position of moving atom.

On the each step the relaxation of the system is carried out and the constant C_1 is calculated using the iterative procedure, described above.

The migration volume is a difference between the volume of system, when the moving atom is in a saddle position, and the volume of system, when the moving atom is in an equilibrium position. The part of migration volume concerned with the alteration of the crystal volume as a whole is expressed through the respective constants C_1:

$$V^m = 4\pi(C_1' - C_1), \tag{7}$$

where C_1', C_1 are the constants corresponding to the system states, when the moving atom is in a saddle and in a equilibrium positions, respectively.

2.4. Additions to the values of the activation volumes concerned with dependence the energy of the system on the outer pressure

We take into consideration that the energy of the system (in particular the system with the defect) depends on the outer pressure [6, 7]. This dependence gives an addition to the values of migration and formation volumes.

In concordance with a well-known thermodynamic relation [8], the formation volume associated with a defect is defined as

$$V^f = \frac{\partial(G^v - G^0)}{\partial p}\Big|_{T=Const} = \frac{\partial\left\{(E^v - E^0) + p(V^v - V^0) - S_v T\right\}}{\partial p}\Big|_{T=Const} \qquad (8)$$

where G^v, E^v, V^v and G^0, E^0,V^0 are the thermodynamic potential, the energy and the volume related to the defect crystal and to the perfect crystal, respectively. Taking into account that the vibrational entropy S_v practically does not depend on the pressure equation (8) gives the addition to the value of the formation volume concerned with dependence the energy of the system on the outer pressure:

$$V^f_E = \frac{\partial \Delta E}{\partial p}\Big|_{T=Const} \qquad (9)$$

$\Delta E = E^v - E^0$, is the difference between the potential energies of systems with and without vacancy. The total vacancy formation volume:

$$V^f_\Sigma = \Omega + \Delta V + V^f_E \qquad (10)$$

If the potential energy of an atom s can be put under the form $E_s = E(\mathbf{r}_k - \mathbf{r}_s)$, $k=\{1,n\}$ the stress field alters it to $E_s = E(\mathbf{r}_k + \mathbf{u}_k - \mathbf{r}_s - \mathbf{u}_s)$, $k=\{1,n\}$, where $\mathbf{u}_k \equiv \mathbf{u}(\mathbf{r}_k)$ is the displacement of atom k, which is a function of its location $\mathbf{r}_k$. The change of the potential energy of the system ΔE, when the vacancy formed, can be represented by a Taylor's expansion with respect to the relative displacements of each atom and its surroundings:

$$\Delta E = \frac{1}{2}\sum_s \left[\frac{\partial E^v{}_s}{\partial\left(\left|\mathbf{r}_k - \mathbf{r}_s\right|\right)}\left(\left|\mathbf{u}_k - \mathbf{u}_s\right|\right) - \frac{\partial E^0{}_s}{\partial\left(\left|\mathbf{r}_k - \mathbf{r}_s\right|\right)}\left(\left|\mathbf{u}_k - \mathbf{u}_s\right|\right) + \ldots \right] \qquad (11)$$

The summation in Eq. 10 through s is taken over all atoms inside a computation cell.

In most actual cases, the differences in the displacements for the neighboring atoms are small, and only first order terms are kept. Using the fact that $\mathbf{u}$ varies little at distances of the order of the interatomic spacing [9], we represent all the $\mathbf{u}_k$ by:

$$u_k^x = u_s^x + \frac{\partial u_s^x}{\partial x} r_{sk}^x + \frac{\partial u_s^x}{\partial y} r_{sk}^y + \ldots \tag{12}$$

with $\boldsymbol{u}_s \equiv \boldsymbol{u}(\boldsymbol{r}_s)$, $\boldsymbol{r}_s$ is the location of the atom s, and $\boldsymbol{r}_{sk} = \boldsymbol{r}_s - \boldsymbol{r}_k$.

If we can use the first order expansion in Eq. 11, then after transformation we obtain:

$$\Delta E = \frac{1}{2}\sum_s \frac{1}{R_{sk}} \frac{\partial E_s^v}{\partial R}\bigg|_{R_{sk}^v} \left(x_{sk}^2 \varepsilon_{11} + y_{sk}^2 \varepsilon_{22} + z_{sk}^2 \varepsilon_{33} + 2x_{sk} y_{sk} \varepsilon_{12} + 2x_{sk} z_{sk} \varepsilon_{13} + 2y_{sk} z_{sk} \varepsilon_{12} \right) - \\ -\frac{1}{2}\sum_s \frac{1}{R_{sk}} \frac{\partial E_s^0}{\partial R}\bigg|_{R_{sk}^0} \left(x_{sk}^2 \varepsilon_{11} + y_{sk}^2 \varepsilon_{22} + z_{sk}^2 \varepsilon_{33} + 2x_{sk} y_{sk} \varepsilon_{12} + 2x_{sk} z_{sk} \varepsilon_{13} + 2y_{sk} z_{sk} \varepsilon_{12} \right) \tag{13}$$

where $\varepsilon_{sk} = (1/2)\left(\partial u_k / \partial x_s + \partial u_s / \partial x_k \right)$, and $R_{sk} \equiv \left| r_k - r_s \right| = \sqrt{x_{sk}^2 + y_{sk}^2 + z_{sk}^2}$ for all atoms s and k.

In the case of an hydrostatic pressure, with $Sp\varepsilon = \varepsilon_{11} + \varepsilon_{22} + \varepsilon_{33} = -P/K_0$:

$$\varepsilon_{ii} = -P/3K_0; \quad \varepsilon_{ii} = 0; \quad i \neq j,$$

where P is the pressure. If we express the potential energy of an atom in Eq. 13 as a sum of the pair potentials Φ, then we obtain the expression for the ΔE. If we substitute ΔE in Eq. 9 then we shall obtain the expression for the addition to the value of the formation volume concerned with dependence the energy of the system on the outer pressure:

$$V_E^f = -\frac{1}{6K_0} \sum_s \sum_k \left(R_{sk}^v \frac{\partial \Phi}{\partial r}\bigg|_{R_{sk}^v} - R_{sk}^0 \frac{\partial \Phi}{\partial r}\bigg|_{R_{sk}^0} \right), \tag{14}$$

where K_0 – bulk module, R_{sk}^v – distance between atom s and atom k for the system with vacancy, R_{sk}^0 - distance between atom s and atom k for the perfect system (without vacancy). The summation through k is taken over all atoms inside a sphere of radius R centered on the atom s. The magnitude of R is governed by the atomic interaction range.

Similarly, the addition to the migration volume:

$$V_E^m = -\frac{1}{6K_0} \sum_s \sum_k \left(R_{sk}^w \frac{\partial \Phi}{\partial r}\bigg|_{R_{sk}^w} - R_{sk}^v \frac{\partial \Phi}{\partial r}\bigg|_{R_{sk}^v} \right), \tag{15}$$

Where R_{sk}^{w} – distance between atom s and atom k for the system with vacancy, when the moving atom is in saddle position, R_{sk}^{v} - distance between atom s and atom k for the system with vacancy, when the moving atom is in equilibrium position.

3. Results and discussions

3.1. Calculation results for vacancy in α -iron

For α -iron the interaction between neighbor atoms i and j in the computation cell was assumed to be a Johnson's pair potential [4]. With the help of this new model "fine structure" of displacement atoms near the point defect is defined. As mentioned above the displacements of atoms calculated using the theory of elasticity are different with those obtained by means of simulation (fig. 5).

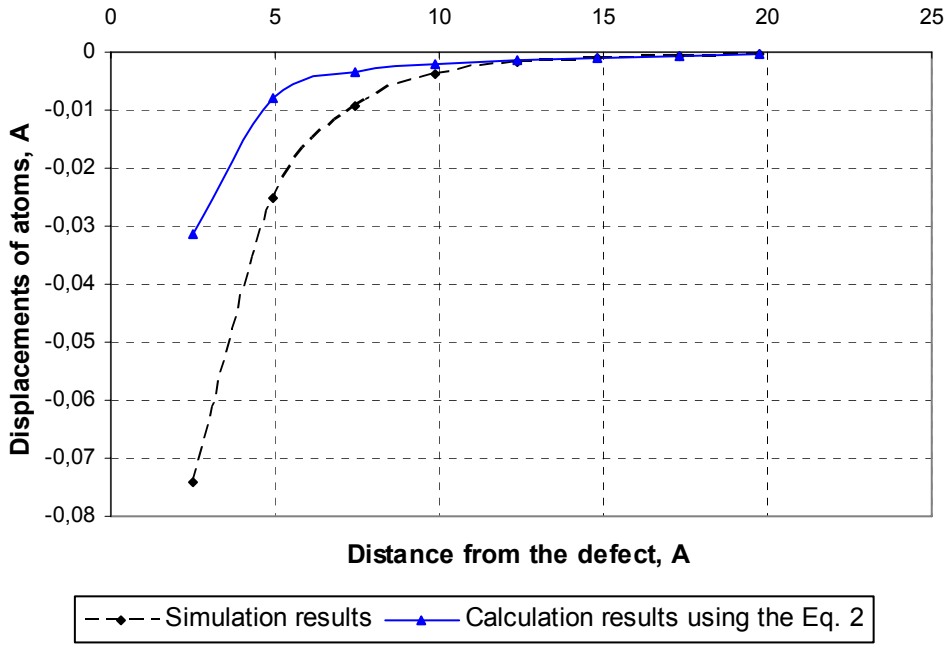

Fig. 5: Displacement of atoms in the vicinity of a defect (for <111> crystallographic direction).

Therefore, we carry out calculation for a large number of atoms in the computation cell.

Moreover, the displacements of atoms are different for various crystallographic directions (Table 1). Absolute value of constant C_1 is maximum for crystallographic directions <111> and minimum for directions <100>. So it is necessary to average constant C_1 over some spherical layer which is sufficiently distant both from the defect and from the boundary of the computation cell.

Table 1. The displacement of atoms in the vicinity of a vacancy depending on crystallographic directions

Distance from the defect	Crystallo-graphic direction	(100) displacement, $a \cdot 10^{-4}$	(010) displacement, $a \cdot 10^{-4}$	(001) displacement, $a \cdot 10^{-4}$	Total displace-ment, $a \cdot 10^{-4}$
~ 4.3 a (a – lattice parameter)	(100)	0.258	0.000	0.000	0.258
	(110)	-1.524	-1.524	0.000	-2.155
	(111)	-3.177	-3.177	-3.177	-5.503
	(112)	-0.163	-0.163	-0.422	-0.478

Taking into account the calculated atomic structure and the interaction in the system the formation and the migration volumes have been calculated for the vacancy in α -iron including the additions concerned with the dependence of the energy of the system on the outer pressure. As written above to calculate the migration volume we take into account two centers of dilatation. The results (Tables 2, 3) show that the addition of the term, concerned with the dependence of energy of the system on the outer pressure, in the formation volume is congruent to the usual one and this addition in the migration volume exceeds the usual term. The value of formation volume makes agree with results obtained by other researchers (table 4).

Table 2. The relaxation and the formation volumes for vacancy calculated for various numbers of atoms in the computational cell for α –iron.

Number of atoms in computation cell	$\Delta V/\Omega$	V^f_E/Ω	V^f_Σ/Ω	$\Delta V'/\Omega$	V^f_Σ'/Ω
without taking constant C_2 into consideration					
4285	-0.043	-0.031	0.926	-0.074	0.895
8393	-0.042	-0.030	0.928	-0.072	0.898
23049	-0.043	-0.029	0.928	-0.074	0.897
41151	-0.042	-0.029	0.929	-0.072	0.899
taking constant C_2 into account					
4285	-0.036	-0.027	0.937	-0.062	0.911
8393	-0.036	-0.025	0.939	-0.062	0.913
23049	-0.038	-0.024	0.938	-0.067	0.909
41151	-0.038	-0.025	0.937	-0.067	0.908

ΔV – relaxation volume, V^f_E - addition to the value of the formation volume concerned with dependence the energy of the system on the outer pressure, V^f_Σ - total formation volume, $\Delta V'$, V^f_Σ' - diffusion features taking into account the Eshelby factor; Ω - atomic volume.

Table 3. The migration and activation volumes for vacancy calculated for various numbers of atoms in the computational cell for α –iron.

Number of atoms in computation cell	V^m/Ω	$V^m{}_E/\Omega$	$V^m{}_\Sigma/\Omega$	V^{act}/Ω
4285	-0.004	-0.025	-0.029	0.897
8393	-0.020	-0.021	-0.041	0.887
14361	-0.026	-0.020	-0.046	0.882
23049	-0.025	-0.020	-0.045	0.884

V^m – part of the migration volume concerned with the alteration of the crystal volume as a whole, $V^m{}_E$ - addition to the value of the migration volume concerned with dependence the energy of the system on the outer pressure, $V^m{}_\Sigma$ - total migration volume, $V^{act} = V^f{}_\Sigma + V^m{}_\Sigma$ – activation volume; Ω - atomic volume.

Moreover, the taking constant C_2 into account gives the noticeable addition to the obtained features of the vacancy, when the numbers of the atoms in the computation cell a lot more then Johnson and Brown thought. For the vacancy the part of the displacement atoms concerned with a cubic symmetrical term gives noticeable contribution to the displacement atoms if the computation cell has radius less then ten lattice parameters (fig. 6).

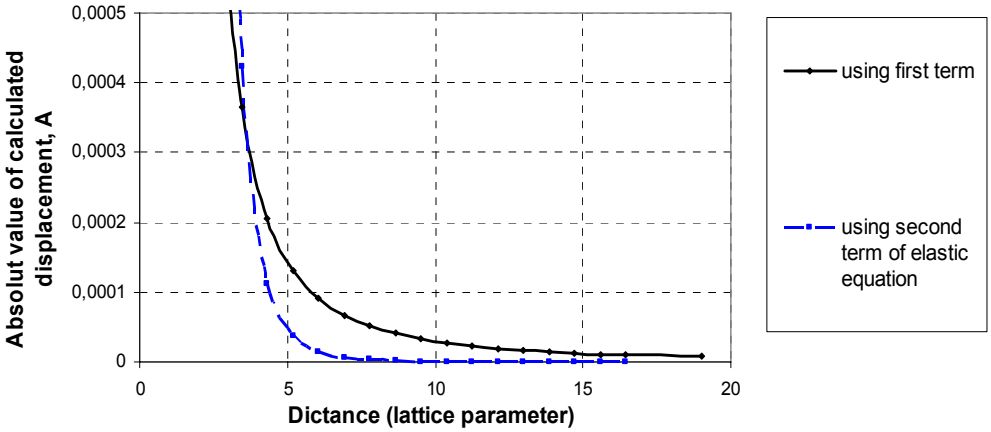

Fig. 6: Displacement of atoms calculated using various terms of the theory of elasticity (for <111> crystallographic direction).

The values of the formation and the migration energies amount to 2.90 eV and 0.68 eV respectively that in agreement with results obtained by Johnson and other researchers [1, 4].

Table 4. Diffusion features of the vacancy in α-iron obtained by various researchers.

	E_v^f, eV	E_v^m, eV	$\Delta V/\Omega$
Simulation results			
Johnson *et al.* (1962)		0.68	
Ackland *et al.* (1997)	1.70	0.82	-0.22
Osetsky *et al.* (1995)	2.05	0.71	-0.47
Calder and Bacon (1993)	1.83	0.79	
Harder and Bacon (1986)	1.81	0.85	-0.09
Experimental results			
Schaefer *et al.* (1977); Furderer *et al.* (1987)	1.6 – 1.7	0.9 – 1.3	
Ehrhart *et al.* (1979); De Schepper *et al.* (1987)	~2.0	~0.6	

3.1. Calculation results for interstitial in α -iron

We calculated the formation energy and volume for the interstitial atom in α –iron using the model described above. The results (table 5) show that the relaxation volume when the interstitial atom is formed larger then 1. It means that the total volume of system increases. Moreover, results obtained for system with six <110> split interstitial differ from results obtained for system with single dumb-configuration of interstitial atom.

Table 5. The relaxation and the formation volumes and the formation energies for interstitial atom calculated for various numbers of atoms in the computational cell for α –iron.

Number of atoms in computation cell	$\Delta V/\Omega$	V^f_E/Ω	V^f_Σ/Ω	$\Delta V'/\Omega$	V^f_Σ'/Ω	E^f, eV
for system with single <110> dumb-configuration						
4286	1.336	0.799	1.136	2.306	2.105	3.043
8394	1.340	0.792	1.132	2.313	2.105	3.037
23050	1.370	0.763	1.133	2.365	2.128	3.059
for system with six <110> split interstitial						
8399	1.590	0.778	1.368	2.744	2.522	3.092
34339	1.612	0.768	1.380	2.782	2.550	3.069
66959	1.611	0.754	1.365	2.781	2.536	3.069

ΔV – relaxation volume, V^f_E - addition to the value of the formation volume concerned with dependence the energy of the system on the outer pressure, V^f_Σ - total formation volume, $\Delta V'$, V^f_Σ' - diffusion features taking into account the Eshelby factor; Ω - atomic volume.

The displacements of atoms for system with single <110> dumb-configuration are different not only for various crystallographic directions but also within the same

crystallographic direction (table 6). The displacements of atoms for system with six <110> split interstitial have a greater symmetry within the crystallographic direction (table 7) that allows to define average constant C_1 more precise.

Table 6. The displacement of atoms in the vicinity of a single <110> split interstitial depending on crystallographic directions

Distance from the defect	Crystallographic direction	(100) displacement, $a \cdot 10^{-4}$	(010) displacement, $a \cdot 10^{-4}$	(001) displacement, $a \cdot 10^{-4}$
~ 4-5 a (a – lattice parameter)	(100), $(\bar{1}00)$	1.041	0.000	14.106
	(010), $(0\bar{1}0)$	0.000	15.335	0.000
	(001), $(00\bar{1})$	14.106	0.000	1.041
	(101), $(\bar{1}0\bar{1})$	33.160	0.000	33.160
	$(10\bar{1})$, $(\bar{1}01)$	-3.250	0.000	-3.250
	The rest of (011)	1.893	29.761	25.428

Table 7. The displacement of atoms in the system with six <110> split interstitial depending on crystallographic directions

Distance from the defects region	Crystallographic direction	(100) displacement, $a \cdot 10^{-4}$	(010) displacement, $a \cdot 10^{-4}$	(001) displacement, $a \cdot 10^{-4}$
~ 4-5 a (a – lattice parameter)	(100)	33.233	0.000	0.000
	(110)	0.997	24.763	24.763
	$(\bar{1}\bar{1}\bar{1})$, $(11\bar{1})$, $(1\bar{1}1)$, $(\bar{1}11)$	37.407	37.407	37.407
	$(1\bar{1}\bar{1})$, $(\bar{1}1\bar{1})$, $(\bar{1}\bar{1}1)$, (111)	13.629	13.629	13.629

For the single <110> split interstitial the part of the displacement atoms concerned with a cubic symmetrical term gives noticeable contribution to the displacement atoms when the computation cell has radius less then 7 (fig. 7). So in the case of interstitial this contribution is less then in the case of vacancy.

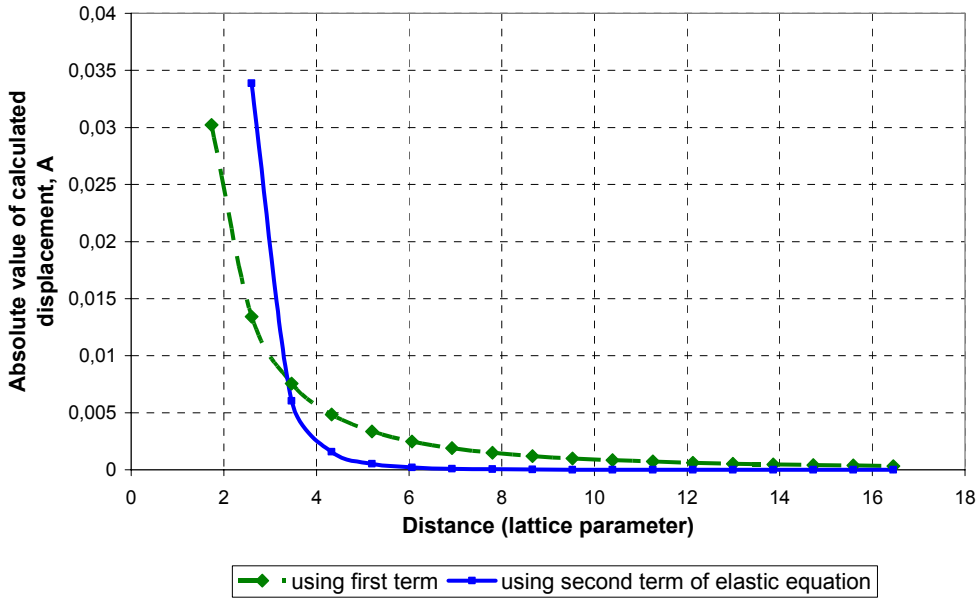

Fig. 7: Displacement of atoms calculated using various terms of the theory of elasticity (for <111> crystallographic direction).

The relaxation volume for interstitial atom obtained by Johnson [4] is equal 1.7 atomic volumes. Comparing our results with results received by Johnson for interstitial in α-iron one can see that Johnson's results similar with those obtained for system with six <110> split interstitial.

4. Conclusion

The new model for simulation of the diffusion features of point defects is suggested. This model bases on a molecular static method and takes into account the displacements of atoms in an elastic matrix around the computation cell. The convergence of the iterative procedure for simulation atomic structure and calculation of the constants C_1, C_2, which stabilizes the atomic structure in the vicinity of a defect, is obtained. With the help of this new model the formation and the migration volumes have been calculated including the additions concerned with the dependence of the energy of the system on the outer pressure.

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