Stress-Induced Interaction of Pairs of Point Defects in bcc Solutions

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The theory of the stress-induced interaction[1] has been used to calculate the interaction energies of interstitials, vacancies as well as interstitials and vacancies, and host atom displacements around a vacancy and interstitial in four metals with the bcc lattice: αFe, V, Nb, and Ta. The cases of interstitial location both in octahedral and tetrahedral interstices are discussed. The elastic constants, cohesion energy (for vacancies), Born-Karman constant of the host lattice and coefficients of the concentration expansion of the solid solution lattice due to the interstitials are the numerical parameters of the theory. The computer calculation was carried out in the general form suitable for any interstitial in these four metals and specifically for the interstitial solutions H, O, N in V, Nb, Ta and C, and N in αFe. In the only case when the quantitative comparison of the calculated characteristics with the experimental one is possible (interaction of the vacancies with C in αFe), there is good agreement between calculated and observed values.

1. INTRODUCTION

AS is known, the interaction between point defects is a very important effect for understanding such phenomena as short-range and long-range order, diffusion, aging in irradiated materials, internal friction, and so on. This interaction is especially strong between interstitial atoms in a bcc host lattice since each interstitial atom produces a large crystal-lattice distortion resulting in the stress-induced interaction (the estimation of a typical pairwise stress-induced interaction energy in a bcc host lattice gives a value of the order of 1 eV).

The purpose of this paper is the calculation of stress-induced interaction energies of the interstitial-interstitial, and interstitial-host atom vacancy pairs (interstitials in octahedral as well as tetrahedral interstices). Consideration[1] of employed static crystal lattices takes into account the discrete atomic structure of a host lattice in the analysis of elastic atomic displacements and corresponding stress-induced energies, and therefore enables the calculation of pair-wise energies of pairs whose separation vector is commensurable with interatomic distances.

Computer calculations are carried out in the general form which enables obtaining the stress-induced energies for *any* kind of interstitial atoms (for example, H, O, N, C) in V, NC, Ta, αFe, and therefore are universal for these metals.

2. CALCULATION TECHNIQUE

The calculation technique employed in this paper is based on the lattice statics theory formulated in Ref. 1.

The real stress-induced pairwise interaction energies $W_{pq}(\mathbf{R})$ between p-type and q-type defects separated by the bcc lattice translation vector $\mathbf{R}$ is

calculated by means of the inverse Fourier-transformation:

$$W_{pq}(\mathbf{R}) = \frac{1}{N} \sum_{\mathbf{k}} V_{pq}(\mathbf{k}) \, e^{-i\mathbf{K}\mathbf{R}} \qquad [1]$$

where N is a total number of the host atoms, the summation is carried out over all N points of quasi-continuum inside the first Brillouin of the bcc lattice, allowed by the cyclic boundary condition, $V_{pq}(\mathbf{k})$ is the Fourier-transform of the interaction energies. According to Ref. 1 the function $V_{pq}(\mathbf{k})$ can be expressed through such material constants as coefficients of the concentration expansion of the host lattice and frequencies of crystal lattice vibrations. This function looks like the scalar product:

$$V_{pq}(\mathbf{k}) = - \mathbf{F}(p,\mathbf{k})\mathbf{V}^*(q,\mathbf{k}) \qquad [2]$$

where

$$\mathbf{F}(p,\mathbf{k}) = \sum_{\mathbf{R}} \mathbf{f}(p,\mathbf{R}) \, e^{i\mathbf{k}\mathbf{R}} \qquad [3]$$

is a Fourier transform of the coupling force acting on undisplaced host atom at the site $\mathbf{R}$ from a p-type defect at $\mathbf{R} = 0$ (the force $\mathbf{f}(p,\mathbf{R})$ as well as the vector $\mathbf{F}(p,\mathbf{k})$ are material constants),[†]

[†]The value $V_{pq}(\mathbf{k})$ in Eq. [2] is presented without the term QS_{pq} ($Q = \frac{1}{N} \sum_{\mathbf{k}} \mathbf{F}(p,\mathbf{k})\mathbf{V}^*(p,\mathbf{k})$, S_{pq} is the Kronecker symbol) since this term does not give any contribution in $W_{pq}(\mathbf{R})$ at $\mathbf{R} \neq 0$. It is also necessary to bear in mind that Eq. [2] is not valid for $\mathbf{k} = 0$.[1]

$$\mathbf{V}(p,\mathbf{k}) = \sum_{\mathbf{R}} \mathbf{U}(p,\mathbf{R}) \, e^{i\mathbf{k}\mathbf{R}} \qquad [4]$$

is a Fourier-transform of the host atom displacement $\mathbf{U}(p,\mathbf{R})$ at a site $\mathbf{R}$ produced by a p-type point defect in the unit cell at $\mathbf{R} = 0$.

The value $\mathbf{V}(p,\mathbf{k})$ can be found from the equation of lattice statics

$$D_{ij}(\mathbf{k})V_j(p,\mathbf{k}) = F_i(p,\mathbf{k}) \qquad [5]$$

where $i, j = 1, 2, 3$ are the Cartesian indicies, the tensor $D_{ij}(\mathbf{k})$ is a dynamical matrix which is the

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Fourier-transform of the Born-Karman constants of the host lattice. The eigenvalues of a dynamical matrix are squared crystal lattice vibrations frequencies multiplied by the host atom mass.*

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*There is the point of view that Born-Karman approximation for the dynamical problem may be not sufficiently accurate. However, the final purpose of calculations is not determining the Born-Karman constants, but the calculation of the dynamical matrix $D_{ij}(\mathbf{k})$ at any $\mathbf{k}$ vectors if we know $D_{ij}(\mathbf{k})$ at $\mathbf{k}$ vectors along symmetry direction ($D_{ij}(\mathbf{k})$ at symmetry direction is directly determined from nonelastic neutron scattering data). Eqs. [AI.1] and [AI.2] give the simplest and sufficiently accurate extrapolation of $D_{ij}(\mathbf{k})$ at $\mathbf{k}$ points between the symmetrical directions.

The representation of the dynamic matrix in terms of the Born-Karman constants is presented in Appendix I. The solution of Eq. [5] is

$$V_i(p,\mathbf{k}) = G_{ij}(\mathbf{k})\, F_j(p,\mathbf{k}) \qquad [6]$$

where $G_{ij}(\mathbf{k})$ is the Fourier-transform of the static Green function $i.e.$ the reciprocal tensor of the dynamical tensor $D_{ij}(\mathbf{k})$.

The real atomic displacements $\mathbf{U}(p,\mathbf{R})$ of a host atom at the site $\mathbf{R}$ associated with a defect p can be found from the inverse Fourier-transformation:

$$\mathbf{U}(p,\mathbf{R}) = \frac{1}{N}\sum_{\mathbf{k}}\mathbf{V}(p,\mathbf{k})\, e^{-i\mathbf{k}\mathbf{R}}. \qquad [7]$$

There are two types of interstices in the bcc lattice: octahedral and tetrahedral. Each unit cell of a bcc lattice has three types of octahedral sites with coordinates $(\frac{1}{2},0,0)$, $(0,\frac{1}{2},0)$, $(0,0,\frac{1}{2})$ (the origin coincides with the nearest host atom position). These interstitial positions are identified by indices $p = 1, 2, 3$ respectively. There are also six tetrahedral sites in each unit cell: $(\frac{1}{4},\frac{1}{4},0)$, $(\frac{1}{4},\frac{3}{4},0)$, $(0,\frac{1}{4},\frac{1}{4})$, $(0,\frac{3}{4},\frac{3}{4})$, $(\frac{1}{4},0,\frac{1}{4})$, and $(\frac{3}{4},0,\frac{1}{4})$ ($p = 1, \bar{1}, 2, \bar{2}, 3,$ and $\bar{3}$, respectively).

In the case when coupling forces $\mathbf{f}(p,\mathbf{R})$ do not vanish for the nearest and next-nearest coordination shell around the interstitial at p-position only, the equation for $\mathbf{F}(p,\mathbf{k})$ has an especially simple form. They can be directly represented in the term of elastic constants of the host lattice c_{11}, c_{12}, c_{44} spacing of bcc lattice and coefficients of the bcc lattice concentration expansion.

If an interstitial atom is situated in the octahedral site with $p = 3$ (Ref. 2):

$$\mathbf{F}^{\text{oct}}(3,\mathbf{k}) = ia^2(\sigma_1 \sin\tfrac{1}{2}\,\mathbf{k}\mathbf{a}_1 \cos\tfrac{1}{2}\,\mathbf{k}\mathbf{a}_2,\ \sigma_1 \sin\tfrac{1}{2}\,\mathbf{k}\mathbf{a}_2$$

$$\times \cos\tfrac{1}{2}\,\mathbf{k}\mathbf{a}_1,\ \sigma_3 \sin\tfrac{1}{2}\,\mathbf{k}\mathbf{a}_3)\, e^{\frac{i\mathbf{k}\mathbf{a}_3}{2}} \qquad [8]$$

If an interstitial is situated in the tetrahedral interstices with $p = 3$ and $p = \bar{3}$ (Ref. 3):

$$\mathbf{F}^{\text{tetr}}(3,\mathbf{k}) = ia^2\, e^{i\,\mathbf{k}\mathbf{a}_1/2}\left\{ \sigma_1 \sin\frac{\mathbf{k}\mathbf{a}_1}{2},\ \sigma_1 \sin\frac{\mathbf{k}\mathbf{a}_2}{2}\, e^{i\,\mathbf{k}\mathbf{a}_3/2}, \right.$$

$$\left. -i\sigma_3\left(\cos\frac{\mathbf{k}\mathbf{a}_2}{2}\, e^{i\,\mathbf{k}\mathbf{a}_3/2} - \cos\frac{\mathbf{k}\mathbf{a}_1}{2}\right)\right\}$$

$$\mathbf{F}^{\text{tetr}}(\bar{3},\mathbf{k}) = ia^2\, e^{-i\,\mathbf{k}\mathbf{a}_1/2}\left\{ -\sigma_1 \sin\frac{\mathbf{k}\mathbf{a}_1}{2},\ -\sigma_1 \sin\frac{\mathbf{k}\mathbf{a}_2}{2}\, e^{-i\,\mathbf{k}\mathbf{a}_3/2}, \right.$$

$$\left. -i\sigma_3\left(\cos\frac{\mathbf{k}\mathbf{a}_2}{2}\, e^{-i\,\mathbf{k}\mathbf{a}_3/2} - \cos\frac{\mathbf{k}\mathbf{a}_1}{2}\right)\right\} \qquad [9]$$

where

$$\sigma_1 = (C_{11} + C_{12})U_{11} + C_{12}U_{33} = U_{33}[C_{12} + (C_{11} + C_{12})t]$$

$$\sigma_3 = C_{11}U_{33} + 2C_{12}U_{11} = U_{33}[C_{11} + 2C_{12}t] \qquad [9a]$$

$$t = U_{11}/U_{33}.$$

$\mathbf{a}_1$, $\mathbf{a}_2$, and $\mathbf{a}_3$ are translations of the bcc lattice along [100], [010] and [001] directions:

$$U_{11} = \frac{da_1}{a_1 dc}, \qquad U_{33} = \frac{da_3}{a_3 dc} \qquad [9b]$$

are the coefficients of the concentration expansion of bcc interstitial solution caused by interstitials situated in $p = 3$-type interstices only (C-concentration). These coefficients are elements of the concentration expansion tensor U_{ij} (Ref. 3) at $p = 3$:

$$U_{ij}(3) = \begin{pmatrix} U_{11} & 0 & 0 \\ 0 & U_{11} & 0 \\ 0 & 0 & U_{33} \end{pmatrix}. \qquad [10]$$

The numerical values of U_{11} and U_{33} are presented in Appendix II for the cases C and N in αFe as well as H, O, N in V, Nb, and Ta.

Equations [8] and [9] enable the values of the Fourier-transform $\mathbf{F}(p,\mathbf{k})$ of the coupling force to be obtained for any other positions p and $\bar{p}$ by means of both the cyclic permutation of the indices of the vectors $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$, and the vector component within the curly brackets.

The numerical values of the coefficients U_{11} and U_{33} displayed in Appendix II cannot be considered highly reliable and need to be determined more accurately in the future. That is why the energy values of the stress-induced interactions of interstitials in αFe, V, Nb, Ta, and host atom displacements were calculated in the form being suitable for arbitrary values of the coefficients U_{11} and U_{33}. The results of these calculations easily enable one to find the numerical values of interaction energies and displacements for any interstitials in αFe, V, Nb, and Ta without an additional computer calculation. To do that, it is sufficient to make use of the numerical values of U_{11} and U_{33} inherent for the relevent interstitial atom and the results of numerical computer calculations listed in the tables.

The calculation of displacements caused by vacancies and stress-induced interaction energies of interstitial atom-vacancy pairs is based on the pair-wise interaction potential between host atoms employed in Ref. 4:

$$E(R) = -\frac{A}{R^4} + \frac{B}{R^8}$$

where

$$A = \frac{9\,\epsilon a^4}{8 S_1},\ B = -\frac{81\,\epsilon a^8}{25\,6 S_2},\ S_1 = 22.638,\ S_2 = 10.355,\ \text{and}$$

ϵ is a cohesion energy.

The parameters A and B entering in the potential are chosen so that the cohesion energy and spacings calculated by means of the potential would be equal to the experimental observed ones. The vector $\mathbf{F}^{\text{vac}}(\mathbf{k})$ corresponding to such a potential is

Table I. Coefficients for Calculation of the Pairwise Stress-Induced Interaction Energies of Interstitials in Octahedral Interstices

(x, y, z)	V n	V b	V d	Nb n	Nb b	Nb d	Ta n	Ta b	Ta d	Fe n	Fe b	Fe d
(0, 1/2, 0)	-0.619	-2.892	-2.090	-1.020	-4.612	-3.407	-0.390	-1.689	-1.407	-0.162	-0.713	-0.546
(1/2, 0, 1/2)	-0.101	-0.671	-0.948	-0.160	-1.109	-1.531	-0.072	-0.424	-0.566	-0.038	-0.216	-0.277
(1/2, 1/2, 1/2)	-0.103	-0.199	-0.226	-0.192	-0.391	-0.419	-0.047	-0.110	-0.133	-0.032	-0.080	-0.089
(0, 0, 1)	+0.664	+1.121	+0.547	+0.868	+1.611	+0.880	+0.338	+0.656	+0.335	+0.122	+0.168	+0.022
(1, 0, 0)	+0.016	+0.032	-0.073	+0.017	-0.003	-0.252	-0.010	-0.028	-0.054	-0.018	-0.039	-0.045
(1, 1/2, 0)	+0.110	+0.561	+0.363	+0.519	+0.777	+0.165	+0.067	+0.318	+0.248	+0.013	+0.077	+0.042
(1/2, 1, 1/2)	-0.011	-0.004	+0.207	-0.037	-0.058	+0.251	+0.005	+0.054	+0.155	-0.005	-0.006	+0.048
(1, 1, 0)	+0.075	+0.352	+0.614	+0.139	+0.598	+0.981	+0.045	+0.227	+0.360	-0.002	+0.043	+0.131
(1, 0, 1)	-0.067	-0.126	-0.078	-0.092	-0.165	-0.077	-0.021	-0.052	-0.058	-0.003	-0.015	-0.021
(1, 1/2, 1)	-0.008	-0.138	-0.130	-0.007	-0.173	-0.192	+0.005	-0.031	-0.043	+0.009	+0.005	-0.011
(0, 3/2, 0)	-0.030	-0.088	-0.063	-0.068	-0.242	-0.200	-0.023	-0.087	-0.071	-0.007	-0.040	-0.022
(1/2, 0, 3/2)	-0.018	-0.043	-0.015	-0.039	-0.094	-0.046	-0.014	-0.036	-0.035	-0.006	-0.020	-0.026
(3/2, 1/2, 1/2)	-0.012	-0.045	-0.068	-0.001	-0.070	-0.145	-0.004	-0.033	-0.061	-0.006	-0.017	-0.015
(1/2, 1/2, 3/2)	+0.033	+0.015	-0.022	+0.036	+0.054	+0.050	+0.015	+0.005	+0.009	+0.012	+0.005	-0.011
(1, 1, 1)	-0.025	-0.025	-0.085	-0.017	-0.008	-0.100	-0.003	+0.020	+0.005	+0.005	+0.033	+0.020
(1, 3/2, 0)	+0.005	-0.008	-0.002	+0.004	-0.005	-0.022	0.000	-0.007	-0.010	-0.003	-0.012	-0.006
(3/2, 1, 1/2)	+0.008	+0.038	-0.009	+0.025	+0.082	+0.019	+0.003	+0.018	-0.001	+0.003	+0.016	+0.008
(2, 0, 0)	-0.020	-0.074	+0.006	-0.029	-0.070	+0.086	-0.004	-0.023	+0.005	-0.003	-0.008	-0.005
(0, 0, 2)	+0.049	-0.024	-0.057	+0.246	+0.263	+0.012	+0.014	-0.004	+0.002	+0.010	0.000	-0.010
(2, 1/2, 0)	-0.011	+0.007	-0.023	+0.001	+0.101	+0.044	-0.004	0.000	-0.006	-0.002	-0.002	-0.007
(1, 3/2, 1)	-0.015	-0.040	+0.022	-0.017	-0.032	+0.038	-0.007	-0.016	+0.010	+0.001	+0.007	+0.024
(1/2, 2, 1/2)	-0.004	-0.015	+0.021	-0.001	+0.028	+0.093	-0.001	-0.005	+0.003	-0.002	-0.009	-0.001
(3/2, 0, 3/2)	+0.010	+0.025	+0.025	+0.007	0.000	+0.023	+0.004	-0.002	-0.001	+0.002	0.000	-0.003
(3/2, 3/2, 1/2)	+0.009	+0.040	+0.084	+0.026	+0.098	+0.123	+0.002	+0.010	+0.033	0.000	+0.010	+0.029
(3/2, 1/2, 3/2)	-0.010	-0.012	-0.004	-0.029	-0.047	-0.020	-0.009	-0.017	-0.022	0.000	0.000	-0.004
(2, 1, 0)	-0.004	-0.008	+0.009	-0.011	-0.009	+0.058	0.000	-0.008	-0.020	-0.003	-0.007	+0.002
(0, 1, 2)	+0.023	+0.026	+0.001	-0.005	-0.038	-0.029	+0.011	+0.017	+0.016	+0.002	-0.003	-0.007
(2, 0, 1)	+0.006	+0.052	+0.056	+0.021	+0.079	+0.062	0.000	+0.011	+0.010	-0.002	-0.003	-0.003

$$\mathbf{F}^{vac}(\mathbf{k}) = \sum_{\mathbf{R}} -\frac{\partial E}{\partial \mathbf{R}} \, e^{i\,\mathbf{kR}} = i\,\frac{9\epsilon a^4}{2} \sum_{\mathbf{R}} \frac{\mathbf{R}}{R^6}$$

$$\times \left[\frac{1}{22.643} - \frac{9/16\,a^4}{10.355\,R^4} \right] e^{i\,\mathbf{kR}}. \qquad [11]$$

The inverse Fourier transformations Eqs. [1] and [7] have been carried out by means of the summation over 10,592 points in the first Brillouin zone of the bcc lattice. Increase in the density of these points has not resulted in significant change of $W_{pq}(\mathbf{R})$ and $U(p,\mathbf{R})$. All calculations were performed on the BESM-4 computer.

3. INTERACTION BETWEEN INTERSTITIALS OF THE SAME KIND

The stress-induced energies of the pairs of the same interstitial atoms separated by a vector $\mathbf{r} = x\mathbf{a}_1 + y\mathbf{a}_2 + z\mathbf{a}_3$ (x, y, z are the coordinates) were calculated vs the tetragonality factor $t = U_{11}/U_{33}$. Since $\mathbf{F}(p,\mathbf{k})$ is a linear function of t and $D_{ij}(\mathbf{k})$ is independent of t it follows from Eqs. [6] and [2] that the energies $W_{pq}(\mathbf{R}) = W(\mathbf{r})$ are a polynomial of the order of two with respect to the parameter t:

$$\frac{W(x,y,z)}{a^3 C_{44} U_{33}^2} = n(x,y,z) + b(x,y,z)t + d(x,y,z)t^2 \qquad [12]$$

where $n(x,y,z)$, $b(x,y,z)$ and $d(x,y,z)$ are universal coefficients which are valid for any interstitial solid solution based on the relevant host lattice. It is assumed that one interstitial whose position is taken to be zero occupies the octahedral position $(0,0,\frac{1}{2})$ ($p = 3$), the second occupies the arbitrary position

($q,\mathbf{R}$) separated by a vector $\mathbf{r} = (x,y,z)$ from the first one.

Table I gives the numerical values of coefficients n, b, and d for various distances $\mathbf{r}$ between interstitials in octahedral sites for αFe, V, Nb, and Ta. Table I can be directly employed to find the numerical values of the interaction energies by means of Eq. [12]. Table II demonstrates the numerical values of the interaction energies for specific of interstitials in octahedral sites.* These values were

*A negative interaction energy means attraction, a positive energy, repulsion.

calculated by means of the coefficients $n(\mathbf{r})$, $b(\mathbf{r})$ and $d(\mathbf{r})$ listed in Table I, numerical values of the parameters t and U_{33} taken from Appendix II and parameter $C_{44}a^3$ from Appendix III.

The interaction energies in Table II are large and range up to ≈ 1 eV. They are almost an order of magnitude higher than the values obtained from the internal friction data for the same solutions. This discrepancy can result from a number of causes.

To our mind, the main reason is that the internal friction data cannot be associated with interstitial pairs whose binding energy is of the order of 1 eV. In fact, the reorientation of such pairs during the relaxation process should result in the destruction of a pair with one orientation (this process is accompanied by an increase of the energy by the value of the order of 1 eV) and its restoration but with different orientation (the energy takes on its previous magnitude). This increase contributes to activation energy that results in a substantial shift of the internal friction peak, $i.e.$, the relaxation peak corresponding to these pairs cannot be observed at relevant temperature range. According to the experimental procedure,[5] the

Table II. The Stress-Induced Pairwise Interaction Energies W(x, y, z) (eV) of Specific Interstitials Located in Octahedral Interstices

(x, y, z)	V-O	V-N	Nb-O	Nb-N	Ta-O	Ta-N	Fe-C	Fe-N	V-O-N	Nb-O-N	Ta-O-N	Fe-C-N
(0, 1/2, 0)	-0.73	-0.41	-0.82	-1.52	-1.05	-1.44	-1.18	-1.27	-0.57	-1.12	-1.23	-1.23
(1/2, 0, 1/2)	-0.07	-0.01	-0.08	-0.18	-0.16	-0.22	-0.23	-0.26	-0.04	-0.12	-0.19	-0.25
(1/2, 1/2, 1/2)	-0.25	-0.25	-0.24	-0.37	-0.17	-0.22	-0.31	-0.31	-0.25	-0.30	-0.18	-0.31
(0, 0, 1)	+1.60	+1.59	+1.11	+1.71	+1.19	+1.62	+1.33	+1.38	+1.60	+1.37	+1.39	+1.33
(1, 0, 0)	+0.03	+0.02	+0.02	+0.04	-0.04	-0.05	-0.18	-0.18	+0.03	+0.03	-0.04	-0.18
(1, 1/2, 0)	+0.11	+0.04	+0.12	+0.24	+0.17	+0.23	+0.07	+0.08	+0.07	+0.17	+0.20	+0.08
(1/2, 1, 1/2)	-0.02	-0.01	-0.04	-0.07	0.00	+0.01	-0.05	-0.05	-0.01	-0.06	0.00	-0.05
(1, 1, 0)	+0.11	+0.10	+0.13	+0.22	+0.11	+0.16	-0.06	-0.06	+0.10	+0.17	+0.13	-0.06
(1, 0, 1)	-0.16	-0.15	-0.12	-0.18	-0.07	-0.10	-0.02	-0.02	-0.16	-0.15	-0.08	-0.02
(1, 1/2, 1)	+0.03	+0.05	+0.02	+0.01	+0.03	+0.04	+0.11	+0.10	+0.04	+0.02	+0.04	+0.10
(0, 3/2, 0)	-0.06	-0.05	-0.07	-0.11	-0.07	-0.09	-0.04	-0.05	-0.06	-0.09	-0.08	-0.04
(1/2, 0, 3/2)	-0.04	-0.03	-0.04	-0.07	-0.05	-0.06	-0.05	-0.05	-0.04	-0.06	-0.05	-0.05
(3/2, 1/2, 1/2)	-0.02	-0.02	+0.01	+0.01	-0.01	-0.01	-0.06	-0.06	-0.02	+0.01	-0.01	-0.06
(1/2, 1/2, 3/2)	+0.10	+0.10	+0.05	+0.07	+0.06	+0.08	+0.14	+0.14	+0.10	+0.06	+0.07	+0.14
(1, 1, 1)	-0.07	-0.08	-0.03	-0.04	-0.02	-0.03	+0.02	+0.03	-0.07	-0.03	-0.02	+0.03
(1, 3/2, 0)	+0.02	+0.02	+0.01	+0.01	0.00	0.00	-0.02	-0.02	+0.02	+0.01	+0.01	-0.02
(3/2, 1, 1/2)	+0.01	0.00	+0.03	+0.04	+0.01	+0.01	+0.02	+0.02	0.00	+0.03	+0.01	+0.02
(2, 0, 0)	-0.03	-0.02	-0.03	-0.05	-0.01	-0.01	-0.03	-0.03	-0.02	-0.04	-0.01	-0.03
(0, 0, 2)	+0.16	+0.18	+0.35	+0.52	+0.06	+0.08	+0.13	+0.12	+0.17	+0.42	+0.07	+0.12
(2, 1/2, 0)	-0.04	-0.05	-0.02	-0.02	-0.02	-0.03	-0.02	-0.02	-0.04	-0.02	-0.02	-0.02
(1, 3/2, 1)	-0.03	-0.02	-0.02	-0.03	-0.02	-0.03	+0.01	+0.01	-0.02	-0.03	-0.03	+0.01
(1/2, 2, 1/2)	0.00	0.00	0.00	-0.01	0.00	-0.01	-0.01	-0.02	0.00	-0.01	-0.01	-0.01
(3/2, 0, 3/2)	0.00	+0.02	+0.01	+0.02	+0.02	+0.03	+0.03	+0.02	+0.02	+0.01	+0.02	+0.02
(3/2, 3/2, 1/2)	+0.02	+0.01	+0.03	+0.04	0.00	0.00	-0.01	-0.01	+0.01	+0.03	0.00	-0.01
(3/2, 1/2, 3/2)	-0.02	-0.03	-0.04	-0.06	-0.03	-0.05	0.00	0.00	-0.02	-0.05	-0.04	0.00
(2, 1, 0)	-0.01	-0.01	-0.01	-0.02	0.00	0.00	-0.03	-0.03	-0.01	-0.02	0.00	-0.03
(0, 1, 2)	+0.01	+0.01	0.00	0.00	+0.04	+0.05	+0.03	+0.03	+0.06	-0.01	+0.05	+0.03
(2, 0, 1)	0.00	0.00	+0.02	+0.04	0.00	-0.01	-0.02	-0.02	0.00	+0.03	0.00	-0.02

Table III. Coefficients for Calculations of the Stress-Induced Pair-Wise Interaction Energies of Interstitials in Tetrahedral Interstices

(x, y, z)	V			Nb			Ta		
	n	b	d	n	b	d	n	b	d
(0, 1̄/4, 1̄/4)	-1.042	-4.817	-5.098	-1.745	- 7.341	- 7.114	-0.671	-2.933	-2.906
(0, 0, 1/2)	-1.074	-1.701	+2.607	-1.932	-10.236	+14.996	-0.435	-1.336	+2.406
(1̄/4, 1/2, 1̄/4)	-0.641	-2.793	-1.844	-1.070	- 4.096	- 1.306	-0.406	-1.608	-1.030
(0, 1̄/4, 3/4)	+0.040	-0.024	+0.166	+0.071	+ 0.108	+ 0.485	+0.009	-0.022	+0.060
(3/4, 1/2, 1̄/4)	+0.234	+1.097	+0.681	+0.391	+ 1.582	+ 0.441	+0.151	+0.623	+0.381
(1, 0, 0)	-0.413	+0.470	+0.485	-0.668	- 0.043	+ 2.508	-0.215	-0.069	+0.647
(0, 0, 1)	-0.079	-0.256	+0.102	-0.380	- 0.660	+ 0.690	+0.026	-0.028	+0.026
(1̄, 0, 1/2)	-0.495	-0.274	+1.023	-0.835	- 0.378	+ 2.737	-0.233	-0.084	+0.724
(3/4, 1/2, 3/4)	+0.011	-0.408	-0.454	-0.009	- 0.800	- 0.981	+0.008	-0.142	-0.193
(0, 0, 3/2)	-0.045	-0.124	-0.106	-0.057	- 0.168	- 0.122	+0.010	+0.007	-0.012
(1, 1, 1/2)	+0.215	+0.403	+0.125	+0.467	+ 0.800	- 0.256	+0.094	+0.222	+0.091
(1̄/4, 3/2, 1̄/4)	+0.006	-0.097	-0.087	-0.006	- 0.234	- 0.254	-0.008	-0.087	-0.079
(1, 1, 0)	+0.185	+0.173	-0.092	+0.436	+ 0.483	- 0.577	+0.054	+0.038	-0.045

Table IV. The Stress-Induced Pairwise Interaction Energies W(x, y, z) (eV) of Specific Interstitials Located in Tetrahedral Interstices

(x, y, z)	Nb-H	Ta-H	V-H
(0, 1̄/4, 1̄/4)	-0.058	-0.193	-0.118
(0, 0, 1/2)	-0.018	-0.009	-0.054
(1̄/4, 1/2, 1̄/4)	-0.026	-0.094	-0.065
(0, 1̄/4, 3/4)	+0.002	+0.001	+0.002
(3/4, 1/2, 1̄/4)	+0.010	+0.036	+0.025
(1, 0, 0)	+0.001	+0.002	-0.009
(0, 0, 1)	-0.003	+0.001	-0.006
(1̄, 0, 1/2)	-0.001	+0.003	-0.019
(3/4, 1/2, 3/4)	-0.006	-0.009	-0.006
(0, 0, 3/2)	-0.001	0.000	-0.004
(1, 1, 1/2)	+0.006	+0.014	+0.014
(1̄/4, 3/2, 1̄/4)	-0.001	-0.005	-0.001
(1, 1, 0)	-0.003	+0.003	+0.009

temperature range employed provides the reorientation of pairs whose binding energy is of the order of 0.1 eV.

The second reason may be associated with a screening of direct stress-induced interaction of a pair which is caused by other interstitials (a similar phenomenon—the Debye screening Coulomb interaction—occurs at a set of charges).

Equation [12] is also valid in the case when interstitial atoms occupy tetrahedral sites. The corresponding numerical calculations give the coefficients $n(x,y,z)$, $b(x,y,z)$, $d(x,y,z)$ which, naturally, differ from ones in the case of the octahedral site occupation. These coefficients are listed in Table III.* Table IV

*It is assumed that one interstitial whose position is taken to be zero occupies the tetrahedral position (½,0,¼) (p = 3).

displays the stress-induced energies of H-H pairs in V, Nb, and Ta when H-atoms occupy tetrahedral sites (neutron diffraction studies[6] demonstrate that H-atoms in Nb, Ta and V are distributed along tetrahedral and octahedral sites, preferentially occupying tetrahedral sites).

4. INTERACTION OF DIFFERENT KINDS OF INTERSTITIALS IN OCTAHEDRAL INTERSTICES

One can easily see from Eq. [6] that in the case of interaction of different kinds of interstitial atoms (α and β kinds of interstitials) their interaction energy $W(\alpha,\beta; x,y,z)$ is

$$\frac{W_{\alpha\beta}(x,y,z)}{a^3 C_{44} U_{33}^\alpha U_{33}^\beta} = n(x,y,z) + b(x,y,z)\frac{t_\alpha + t_\beta}{2} + d(x,y,z)t_\alpha t_\beta$$

[13]

where $t_\alpha = U_{11}^\alpha/U_{33}^\alpha$, $t_\beta = U_{11}^\beta/U_{33}^\beta$ are the parameters related to the α- and β-kind interstitials, respectively; n, b and d are the same coefficients which enter in Eq. [12] and are presented in Table I (different kind atoms occupy octahedral sites) and in Table III (different kind atoms occupy tetrahedral sites).

It follows from Eq. [13] that

$$W_{\alpha\alpha}(x,y,z) < W_{\alpha\beta}(x,y,z) < W_{\beta\beta}(x,y,z)$$

if $W_{\alpha\alpha}(x,y,z) < W_{\beta\beta}(x,y,z)$. It means that the strongest interaction in an interstitial solution containing two solute elements in the host lattice is observed between pairs of the same atoms. The energies of a number of such solutions are presented in Table II.

5. METAL ATOM DISPLACEMENTS CAUSED BY AN INTERSTITIAL ATOM

It follows from Eqs. [5] and [7] that host atom displacement function $U(p,R) = U(R)$ is a linear function of the factor $t = U_{11}/U_{33}$.

$$\frac{U(R)}{aU_{33}} = h(R) + g(R)t$$

[14]

where R is a distance between the coordinate origin and displaced host atom. We assume that an interstitial atom in the octahedral site occupies the position $(0,0,\frac{1}{2})$ ($p = 3$), in the tetrahedral one $-(\frac{1}{2},0,\frac{1}{4})$ ($p = 3$). The vector $h(R)$ and $g(R)$ in Eq. [14] are material constants of the relevant host atom crystal. For the case of occupation of octahedral sites, these constants are presented in Table V; for the case of occupation of tetrahedral sites, in Table VI. The components of vector $U(R)$ for the specific solid solutions are presented in Tables VII and VIII.

Taking into account the calculated displacements of the nearest host atoms, one can see that the ef-

Table V. Coefficients for Calculation of Host Atom Displacement with Respect to the Interstitial in Octahedral Interstice (0, 0, 1/2)

R		V		Nb		Ta		Fe	
		h	g	h	g	h	g	h	g
(0, 0, 0)	U_1/a	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
	U_2/a	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
	U_3/a	−0.307	−0.184	−0.305	−0.216	−0.225	−0.265	−0.187	−0.134
(1/2, 1/2, 1/2)	U_1/a	+0.038	+0.218	+0.049	+0.333	+0.042	+0.188	+0.023	+0.128
	U_2/a	+0.038	+0.218	+0.049	+0.333	+0.042	+0.188	+0.023	+0.128
	U_3/a	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
(1, 0, 0)	U_1/a	−0.008	−0.010	−0.016	−0.013	−0.009	−0.001	−0.004	+0.012
	U_2/a	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
	U_3/a	+0.003	+0.012	+0.004	+0.025	−0.003	+0.004	−0.008	0.000
(1, 1, 1)	U_1/a	+0.006	+0.043	+0.014	+0.083	+0.006	+0.035	+0.006	+0.035
	U_2/a	+0.006	+0.043	+0.014	+0.083	+0.006	+0.035	+0.006	+0.035
	U_3/a	−0.004	+0.010	−0.008	0.000	−0.001	+0.014	+0.006	+0.021

Table VI. Coefficients for Calculation of Host Atom Displacement with Respect to the Interstitial in Tetrahedral Interstice (1/2, 0, 1/4)

R		V		Nb		Ta	
		h	g	h	g	h	g
(0, 0, 0)	U_1/a	−0.107	−0.424	−0.115	−0.458	−0.112	−0.392
	U_2/a	0.000	0.000	0.000	0.000	0.000	0.000
	U_3/a	−0.284	−0.216	−0.295	−0.088	−0.235	−0.176
(1/2, 1/2, 1/2)	U_1/a	0.000	0.000	0.000	0.000	0.000	0.000
	U_2/a	+0.107	+0.424	+0.115	+0.458	+0.112	+0.392
	U_3/a	+0.284	+0.216	+0.295	+0.088	+0.235	+0.176
(0, 1, 0)	U_1/a	+0.016	−0.004	+0.018	−0.013	+0.011	−0.018
	U_2/a	−0.019	+0.021	−0.022	+0.038	−0.015	+0.018
	U_3/a	+0.040	+0.021	+0.062	+0.017	+0.022	+0.002
(0, 0, 1)	U_1/a	−0.011	+0.044	−0.002	+0.065	−0.008	+0.038
	U_2/a	0.000	0.000	0.000	0.000	0.000	0.000
	U_3/a	+0.021	−0.055	+0.006	−0.100	+0.028	−0.047
(0, 1, 1)	U_1/a	−0.017	−0.023	−0.019	−0.010	−0.018	−0.027
	U_2/a	+0.031	+0.073	+0.040	+0.092	+0.025	+0.063
	U_3/a	+0.042	+0.046	+0.063	+0.040	+0.034	+0.039

Table VII. Atom Displacements with Respect to the Specific Interstitials in Octahedral Interstices (0,0,½)

R		V-O	V-N	Nb-O	Nb-N	Ta-O	Ta-N	Fe-C	Fe-N
(0,0,0)	U_1/a	0	0	0	0	0	0	0	0
	U_2/a	0	0	0	0	0	0	0	0
	U_3/a	-0.184	-0.185	-0.142	-0.175	-0.117	-0.137	-0.149	-0.146
(½,½,½)	U_1/a	0.003	-0.005	0.006	0.013	0.012	0.014	0.008	0.010
	U_2/a	0.003	-0.005	0.006	0.013	0.012	0.014	0.008	0.010
	U_3/a	0	0	0	0	0	0	0	0
(1,0,0)	U_1/a	-0.006	-0.007	-0.007	-0.009	-0.004	-0.005	-0.005	-0.004
	U_2/a	0	0	0	0	0	0	0	0
	U_3/a	0.001	0.000	0.001	-0.001	-0.002	-0.002	-0.007	-0.007
(1,1,1)	U_1/a	0	-0.002	0.002	0.004	0.001	0.001	0.002	0.002
	U_2/a	0	-0.002	0.002	0.004	0.001	0.001	0.002	0.002
	U_3/a	-0.004	-0.004	-0.004	-0.005	-0.001	-0.001	0.003	0.003

Table VIII. Atom Displacements Caused by Specific Interstitials in Tetrahedral Interstices (½,0,¼)

R		V-H	Ta-H	Nb-H
(0,0,0)	U_1/a	-0.017	-0.019	-0.012
	U_2/a	0	0	0
	U_3/a	-0.026	-0.018	-0.011
(½,½,½)	U_1/a	0	0	0
	U_2/a	+0.017	+0.019	+0.012
	U_3/a	+0.026	+0.018	+0.011
(0,1,0)	U_1/a	0.001	0	0
	U_2/a	0.001	0	0
	U_3/a	0.003	+0.001	+0.002
(0,0,1)	U_1/a	0	+0.001	0
	U_2/a	0	0	0
	U_3/a	0.001	0	0
(0,1,1)	U_1/a	-0.002	-0.002	-0.001
	U_2/a	+0.004	+0.003	+0.003
	U_3/a	+0.004	+0.003	+0.003

Table IX. Calculations of the Vacancy and Bivacancy Characteristics

Metal	Nearest Atom Displacement, U/a	Ratio of the Vacancy Volume to the Atom Volume	Interaction Energy of Two Vacancies (in eV)	
			First coordination Shell	Second coordination Shell
V	0.038	0.87	-0.029	-0.109
Nb	0.037	0.88	-0.030	-0.169
Ta	0.033	0.89	-0.036	-0.155
Fe	0.024	0.92	-0.028	-0.068

It is interesting to note the fact that the attraction between the vacancy and a next-nearest vacancy is stronger than that between the vacancy and a nearest vacancy. The interaction of vacancy pairs increases in the sequence αFe → V → NC → Ta, which corresponds to the increase in the cohesion energy.

The calculated displacements caused by a vacancy are in good agreement with the values which can be obtained by other methods: displacement of the nearest atom for αFe is $0.024a$ in comparison to $0.019a$ in Ref. 8, for V is $0.046a$ in comparison to $0.038a$ in Ref. 8.

fective radius of an oxygen interstitial atom (which is equal to the radius of the octahedral interstice after penetration of an interstitial atom) is 0.76Å for V, 0.69Å for Nb, and 0.61Å for Ta. The radius of an N-atom is 0.76Å for V, 0.80Å for Nb, 0.68Å for Ta, and 0.61Å for αFe. The radius of a C-atom in αFe is 0.64Å. The values of a radius differ from the usual accepted atomic radii of free atoms: oxygen at 0.66Å, nitrogen at 0.71Å, and carbon at 0.77Å.[7] It means that interstitial atoms cannot be considered as a rigid sphere inserted into octahedral interstice and displacing the nearest host atoms.

6. INTERACTION OF VACANCIES

Host Atom Displacements

The Fourier-transforms of atomic displacements around a vacancy and of the stress-induced interaction of vacancies are determined by Eqs. [2] and [5] where $\mathbf{F}^{vac}(\mathbf{k})$ is determined by Eq. [11]. The inverse Fourier-transformation gives the numerical values for displacements and stress-induced energies of pairs of vacancies. These values are presented in Table IX. The volume of a vacancy depending on the atomic displacements of the nearest atoms is also included in this table.

7. INTERACTION BETWEEN A VACANCY AND INTERSTITIAL ATOM IN OCTAHEDRAL INTERSTICES

According to Eqs. [2] and [6], the Fourier-transform of stress-induced energies between a vacancy and interstitial atom is

$$V^{vac}(p,\mathbf{k}) = -\mathbf{F}^{vac}(\mathbf{k})V^*(p,\mathbf{k}) = -F_i^{vac}(\mathbf{k})G_{ij}(\mathbf{k})$$

$$\times F_j^{oct}(p,\mathbf{k}) \qquad [15]$$

where $\mathbf{F}^{vac}(\mathbf{k})$ and $\mathbf{F}^{oct}(p,\mathbf{k})$ are determined by Eqs. [11] and [8].

Since $F^{oct}(p,k)$ is a linear function of t, the interaction energy $W(vac,p; x,y,z)$ between a vacancy and interstitial atom is also a linear function of t:

$$\frac{W(vac; x,y,z)}{U_{33}} = l(x,y,z) + m(x,y,z)t. \qquad [16]$$

The coefficients $l(x,y,z)$ and $m(x,y,z)$ in Eq. [16] are the material constants for each metal and do not depend on the kind of the interstitial. The calculated values of these constants are presented in Table X

and the specific values of interaction energies calculated by means of the Table X data for a number of solid solutions are shown in Table XI.

One can easily see from Table XI that there is a great attractive interaction between a vacancy and the nearest interstitial, and as in the case of the interaction between two vacancies, the strongest interaction is proved to be with the next-nearest interstitial.

The calculated data agree qualitatively with the experimental data for V-O and Nb-O (Refs. 9,10) solutions in which the relaxation methods reveal a significant quantity of vacancy-oxygen pairs.

αFe-C is the only case for which there are reliable experimental data on the vacancy-interstitial binding energy. It is the case of αFe-C solution that was studied in Ref. 11. According to Ref. 11, the binding energy of a vacancy-carbon pair in irradiated αFe is 0.41 eV. The calculated value presented in Table XI is 0.37 eV. These quantities are in good agreement with each other.

8. CONCLUSION

The numerical calculations of the stress-induced interaction energies of interstitials, vacancies, interstitials and vacancies in bcc metals αFe, V, Nb, and Ta, as well as displacements of host atoms caused by these defects have been performed. The cases of occupation of octahedral and tetrahedral interstices are discussed. The numerical coefficients b, n, d, l, m, h, and g, which are the material constants of αFe, V, Nb, and Ta have been calculated by means of a computer. These coefficients enable directly calculating stress-induced pairwise interaction energies between any interstitials, between interstitials and vacancies, as well as being able to calculate host atom displacements if the coefficients of the concen-

tration expansion of the host bcc lattice (concerning the relevant interstitial) are known.

Such formulation seems useful since the available experimental data for U_{11} and U_{33} can hardly be considered as final and should be more accurate. The microscopic theory employed in this paper allows taking into account an atomic structure of a solid solution; the Born-Karman constants being the only parameters made use of in the computer calculations. These constants for αFe, Nb, and Ta were found by the inelastic neutron scattering method, and V- was found by the X-ray diffuse scattering method.

The stress-induced interaction energies and host atom displacements for concrete solid solutions have been evaluated proceeding from the calculated numerical coefficients b, n, d, l, m, h, g, and available experimental data on U_{11} and U_{33} (far from being completely accurate).

The large stress-induced interaction of the interstitials in all four discussed metals reveals that these solid solutions cannot be considered as ideal because of the extremely small content of interstitial atoms and the possibility of short-range or long-range order or decomposition which should be taken into account.

APPENDIX I

Equation for the calculation of $D_{ij}(\mathbf{k})$ (interaction in eight coordination shells):

$$D_{11}(\mathbf{k}) = 8\alpha_1 \left[1 - \cos \frac{ka_1}{2} \cos \frac{ka_2}{2} \cos \frac{ka_3}{2} \right]$$
$$+ \left[4\alpha_2 \sin^2 \frac{ka_1}{2} + 4\beta_2 \left(\sin^2 \frac{ka_2}{2} + \sin^2 \frac{ka_3}{2} \right) \right]$$
$$+ \left[4\alpha_3 (2 - \cos ka_1 \cos ka_2 - \cos ka_1 \cos ka_3) \right]$$

Table X. Coefficients (in eV) for Calculations of the Stress-Induced Interaction Energies of a Vacancy Located in the Coordinate Origin and Interstitial Located in Octahedral Site with the Coordinates (x,y,z)

(x,y,z)	V l	V m	Nb l	Nb m	Ta l	Ta m	Fe l	Fe m
(0,0,½)	−0.881	−2.776	−1.290	−3.892	−1.329	−3.624	−0.537	−1.463
(½,½,0)	−0.861	−0.908	−1.155	−1.168	−1.191	−1.448	−0.497	−0.590
(1,0,½)	−0.049	−0.021	−0.068	−0.013	−0.070	−0.082	−0.058	−0.084
(½,½,1)	0.322	0.174	0.404	0.294	0.489	0.442	0.159	0.075
(1,1,½)	0.102	0.454	0.132	0.575	0.021	0.706	0.046	0.243
(1,1,³⁄₂)	0.020	−0.070	0.031	−0.034	0.036	−0.036	0.044	0.017
(½,³⁄₂,2)	0.013	0.034	0	0.070	0.016	0.006	0.010	0.001
(2,1,½)	−0.001	−0.009	0.015	0.075	−0.005	−0.030	−0.007	−0.004

Table XI. Interaction Energies (in eV) of a Vacancy Located in the Coordinate Origin with the Specific Interstitial Located in Octahedral Interstice with the Coordinate (x,y,z)

(x,y,z)	V-O	V-N	Nb-O	Nb-N	Ta-O	Ta-N	Fe-C	Fe-N
(0,0,½)	−0.299	−0.221	−0.398	−0.560	−0.479	−0.563	−0.330	−0.344
(½,½,0)	−0.479	−0.469	−0.518	−0.645	−0.501	−0.589	−0.374	−0.371
(1,0,½)	−0.034	−0.033	−0.037	−0.048	−0.030	−0.035	−0.042	−0.042
(½,½,1)	0.194	0.196	0.187	0.230	0.212	0.249	0.130	0.127
(1,1,½)	0.020	0.006	0.035	0.055	0.055	0.068	0.018	0.021
(1,1,³⁄₂)	0.020	0.023	0.017	0.019	0.018	0.021	0.036	0.035
(½,³⁄₂,2)	0.005	0.005	−0.006	−0.007	0.007	0.008	0.009	0.008
(2,1,½)	0	0.001	0.005	0.006	−0.001	−0.002	−0.006	−0.006

$+ 4\beta_3(1 - \cos\mathbf{ka}_2 \cos\mathbf{ka}_3)] + [8\alpha_4 (1 - \cos\frac{3\mathbf{ka}_1}{2}$

$\times \cos\frac{\mathbf{ka}_2}{2} \cos\frac{\mathbf{ka}_3}{2}) + 8\beta_4 (2 - \cos\frac{3\mathbf{ka}_2}{2}$

$\times \cos\frac{\mathbf{ka}_1}{2} \cos\frac{\mathbf{ka}_3}{2} - \cos\frac{3\mathbf{ka}_3}{2} \cos\frac{\mathbf{ka}_1}{2} \cos\frac{\mathbf{ka}_2}{2})]$

$+ 8\alpha_5 (1 - \cos\mathbf{ka}_1 \cos\mathbf{ka}_2 \cos\mathbf{ka}_3) + [4\alpha_6 \sin^2\mathbf{ka}_1$

$+ 4\beta_6 (\sin^2\mathbf{ka}_2 + \sin^2\mathbf{ka}_3)] + [8\beta_7 (1 - \cos\frac{\mathbf{ka}_1}{2}$

$\times \cos\frac{3\mathbf{ka}_2}{2} \cos\frac{3\mathbf{ka}_3}{2}) + 8\alpha_7 (2 - \cos\frac{\mathbf{ka}_2}{2}$

$\times \cos\frac{3\mathbf{ka}_1}{2} \cos\frac{3\mathbf{ka}_3}{2} - \cos\frac{\mathbf{ka}_3}{2} \cos\frac{3\mathbf{ka}_1}{2}$

$\times \cos\frac{3\mathbf{ka}_2}{2})] + [4\alpha_8(2 - \cos2\mathbf{ka}_1 \cos\mathbf{ka}_2$

$- \cos2\mathbf{ka}_1 \cos\mathbf{ka}_3) + 4\beta_8(2 - \cos\mathbf{ka}_1 \cos2\mathbf{ka}_2$

$- \cos\mathbf{ka}_1 \cos2\mathbf{ka}_3) + 4\gamma_8 (2 - \cos2\mathbf{ka}_2 \cos\mathbf{ka}_3$

$- \cos\mathbf{ka}_2 \cos2\mathbf{ka}_3)];$ [AI.1]

$D_{12}(\mathbf{k}) = 8\beta_1 \sin\frac{\mathbf{ka}_1}{2} \sin\frac{\mathbf{ka}_2}{2} \cos\frac{\mathbf{ka}_3}{2} + 4\gamma_3 \sin\mathbf{ka}_1 \sin\mathbf{ka}_2$

$+ [8\delta_4 (\sin\frac{3\mathbf{ka}_1}{2} \sin\frac{\mathbf{ka}_2}{2} + \sin\frac{3\mathbf{ka}_2}{2} \sin\frac{\mathbf{ka}_1}{2})$

$\times \cos\frac{\mathbf{ka}_3}{2} + 8\gamma_4 \sin\frac{\mathbf{ka}_1}{2} \sin\frac{\mathbf{ka}_2}{2} \cos\frac{3\mathbf{ka}_3}{2}]$

$+ 8\beta_5 \sin\mathbf{ka}_1 \sin\mathbf{ka}_2 \cos\mathbf{ka}_3 + [8\delta_7 (\sin\frac{\mathbf{ka}_1}{2}$

$\times \sin\frac{3\mathbf{ka}_2}{2} + \sin\frac{\mathbf{ka}_2}{2} \sin\frac{3\mathbf{ka}_1}{2}) \cos\frac{3\mathbf{ka}_3}{2}$

$+ 8\gamma_7 \sin\frac{3\mathbf{ka}_1}{2} \sin\frac{3\mathbf{ka}_2}{2} \cos\frac{\mathbf{ka}_3}{2}] + 4\delta_8 (\sin2\mathbf{ka}_1$

$\times \sin\mathbf{ka}_2 + \sin\mathbf{ka}_1 \sin2\mathbf{ka}_2);$ [AI.2]

where α, β, γ, and δ are the Born-Karman constants in notations according to Woods.[12,13] The remaining components of the matrix $D_{ij}(\mathbf{k})$ are obtained by cyclic permutation of the subscripts.

APPENDIX II. DETERMINATION OF U_{11} AND U_{33}

The coefficients U_{11}, U_{33}, and $t = U_{11}/U_{33}$ of the concentration expansion of bcc solid solution were determined by two various methods.

1) For αFe-C and αFe-N which form an ordered supersaturated interstitial solution (carbon and nitrogen martensite) as well as for V-H, Nb-H, and Ta-H, ordered β phase determination has been performed over crystal lattice parameter data (Eq. [9b]).

2) For the interstitial solutions of oxygen and nitrogen in V, Nb, and Ta, the coefficients U_{11} and U_{33} were found proceeding from the concentration dependence of the crystal lattice parameter of a disordered solid solution and from Snoek relaxation caused by interstitials[14,15] by means of the following equations:

$$U_{33} + 2U_{11} = 3 \frac{da}{adC}$$

$$U_{33} - U_{11} = \left(\frac{3\,kT_n}{a^3 G\Gamma} \frac{dQ_{max}^{-1}}{dC} \right)^{1/2}$$ [AII.1]

where C is the fraction of interstitial atoms related to the total number of host atoms; Q_{max}^{-1} is the height of the Snoek-peak; T_n is the absolute temperature of the peak; and Γ is the effective crystal orientation factor ($\Gamma \approx 0.2$ for polycrystal without a texture):

$$G = \frac{1}{S_{44}' + 2\Gamma(2S_{11}' - 2S_{12}' - S_{44}')}$$ [AII.2]

the rigidity modulus; S_{11}', S_{12}', and S_{44}' are the compliance coefficients of a cubic crystal in usual notations. The values which were made use of for calculation are shown in Table XII and Appendix III.

It is necessary to note that the value $2U_{11} + U_{33}$ for V-H disordered solution at low H-atom content[16] is distinct from that for ordered β phase. This can be understandable if one remembers that H-atoms

Table XII. Experimental Data for Determination of U_{11} and U_{33}

Alloy	$\frac{1}{a}\frac{da}{dc} \times 10^1$	$\frac{dQ_{max}^{-1}}{dc}$	T_n°, K^*	ΔC	Δa_1, Å	Δa_3, Å	Employed Values U_{11}	U_{33}	t
Fe-C							-0.09	+0.86	-0.10 (Ref. 20)
Fe-N							-0.07	+0.83	-0.08 (Ref. 21)
V-O	1.5 (Ref. 22)	8 (Refs. 30, 31)	453				-0.10	+0.66	-0.15
V-N	1.38 (Ref. 25)	8 (Refs. 31, 32)	540				-0.14	+0.69	-0.2
Nb-O	1.26 (Ref. 23)	4.9 (Refs. 5, 33, 34)	413				-0.06	+0.50	-0.12
Nb-N	1.67 (Refs. 28, 26)	4.8 (Refs. 34, 35)	550				-0.05	+0.60	-0.08
Ta-O	1.33 (Refs. 24, 27)	7.4 (Ref. 36)	413				-0.04	+0.47	-0.08
Ta-N	1.5 (Refs. 27–29)	7.3 (Ref. 37)	610				-0.05	+0.56	-0.09
V-H				0.43 to 0.73 / 0.5 to 0.75	2.98 to 3.00 / 3.01 to 3.03	3.27 to 3.32 (Ref. 38) / 3.31 to 3.39 (Ref. 39)	+0.025	+0.074	+0.3
Nb-H				0.7 to 0.97	3.405 to 3.420† / 3.435 to 3.455	3.42 to 3.45 (Ref. 40)	+0.019	+0.032	+0.6
Ta-H				0.45 to 0.75	3.363 to 3.397	3.397 to 3.445 (Ref. 41)	+0.034	+0.051	+0.7

*Peak temperatures are presented at those frequencies ($\sim$1 Hz) at which heights of Snoek peak were determined.

†a_1 and a_2 differ slightly in this solid solution, and U_{11} is taken as an average of the values determined from a_1 and a_2.

in V occupy simultaneous tetrahedral interstices as well as octahedral ones and their distribution along both of them depends on the composition and ordering.

Appendix III. The Magnitude of Constants Used in Calculations

	a, Å	$a^3 C_{44}$, eV	ϵ, eV Ref. 4	$\times 10^{-11}$ (units dyn/cm²)[17]			$\times 10^{12}$ (units cm²/dyn)[17]		
				C_{11}	C_{12}	C_{44}	S'_{11}	$-S'_{12}$	S'_{44}
V	3.026	7.35	-5.30	24.6	13.4	2.87	0.760	0.287	0.892
Nb	3.300	6.45	-7.46	22.8	11.9	4.26	0.660	0.233	3.48
Ta	3.303	18.5	-8.05	26.7	16.1	8.25	0.686	0.258	1.212
Fe	2.87	17.2	-4.29	24.2	14.65	11.2	0.683	0.234	2.348

Born-Karman Force Constants ($\times 10^{-3}$ units dyn/cm)

	a_1	β_1	a_2	β_2	a_3	β_3	γ_3	a_4	β_4	γ_4	δ_4	a_5	β_5	a_6	β_6	a_7	β_7	γ_7
Fe (Ref. 18)	17.86	14.91	14.92	0.36	1.24	-1.09	0.3	-0.6	-0.06	0.28	0.1	-0.23	-0.24					
V (Ref. 19)	10.87	7.24	6.49	-2.15	-4.69	2.99	0.57	1.44	0.29	-1.15	1.22	0.01	-0.12	-1.39	0.34	-0.36	-0.14	0.09
Nb (Ref. 12)	14.14	8.84	14.16	-3.64	2.27	-6.38	0.76	3.61	-0.75	-0.95	1.26	-1.16	-1.33	-7.08	1.32	-0.03	-0.1	0.37
Ta (Ref. 13)	16.98	11.2	11.82	1.42	3.55	-5.43	1.94	3.58	-0.72	-1.73	0.98	-0.49	0.81	-3.70	0.13	0.56	-0.24	0.11

V (Ref. 19): δ_7 = -0.43

Nb (Ref. 12): δ_7 = -0.17, a_8 = 0.51, β_8 = -0.27, γ_8 = 0.81, δ_8 = -0.06

Ta (Ref. 13): δ_7 = -0.68

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