Herrn Dr. B. HILLENBRAND und Herrn B. SAUVAGEOT danken wir für die zahlreichen I_c- und T_c-Messungen, Frau A. URSTADT und Herrn Y. UZEL für Untersuchungen an der Röntgen-Mikrosonde bzw. am Elektronenmikroskop und den Herren W. LIEBISCH und G. STENGEL für ihre Mithilfe bei der Präparation der Leiter. — Die diesem Bericht zugrunde liegenden Arbeiten werden mit Mitteln des BMBW im Rahmen des Technologieprogramms gefördert.

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Calculation of the Correlation Factor for Diffusion in the Diamond Structure Including Electrostatic Impurity-Vacancy Interaction

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(Z. Naturforsch. **27 a**, 1467—1472 [1972]; received 7 April 1972)

An expression for the correlation factor of impurity diffusion in the diamond structure as a function of five distinct atom-vacancy exchange rates is derived.

Furthermore, the effect on the correlation factor of electrostatic vacancy-impurity interaction is included in the calculation. Differences with results obtained by other authors are discussed.

Introduction

Substitutional atomic migration in solids often occurs via unoccupied lattice sites. When such a vacancy mechanism is responsible for the diffusion of marked atoms (e. g. radioactive tracers) the effect of *correlation* between successive tracer jumps must be included in random-walk calculations. Then it turns out that the mean square displacement of an atom is somewhat smaller than to be expected on the basis of the atomic jump frequency Γ. This can be understood by taking into consideration that after a tracer jump not all possible next tracer jumps have equal probability of occurrence, because there will be a tendency for the tracer to jump back into the vacancy (so into its initial position). Thus only a fraction f of tracer jumps are "effective" ($0 \leqq f \leqq 1$) and we get for the diffusion-coefficient [1]

$$D = \tfrac{1}{6} f \Gamma r^2, \qquad (1)$$

r being the jump distance.

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The correlationfactor f is essential for the interpretation of diffusion coefficient measurements. Moreover, it can be determined directly by measuring the so-called isotope effect [2–4].

In order to calculate correlationfactors for impurity diffusion in pure matrices one usually assumes the atom-vacancy exchange rates to be disturbed in the neighbourhood of the impurity, whereas at larger distances from the impurity the vacancy migrates as in the pure material.

Up to now there are three computations on the correlation factor for impurity tracer diffusion by means of vacancies in the diamond structure. MANNING [5, 6] took into account four different disturbed vacancy jump frequencies to get an expression for f. HU [7] derived f also. His result was not obtained as an analytical expression, but was computed numerically. Recently MEHRER [8] included the effect of a long range Coulomb interaction between a charged impurity and a vacancy with opposite charge.

Since there are some errors in the latter treatment, we thought it worthwhile to reconsider the problem.

Calculation of the Correlation Factor

For diffusion in cubic structures D and so f is isotropic. Therefore it is sufficient to consider migration in a particular direction, e. g. along an X-axis. It can be shown that for a single vacancy mechanism of diffusion f is given by [9, 10]

$$f = (1+t)/(1-t), \tag{2}$$

where

$$t = P_+ - P_-. \tag{3}$$

P_+ is the probability that after a tracer jump the next tracer jump is in the same direction compared with that initial jump, P_- is the probability for the inverse direction. The calculation of f in the f.c.c. structure can be simplified by considering migration perpendicular to a mirror plane [4, 11]. Contrary to MEHRER [8] we shall not make use of this possibility for the diamond structure.

As an X-axis we have chosen the [100] direction. Let the tracer be situated in the origin T as shown in Figure 1.

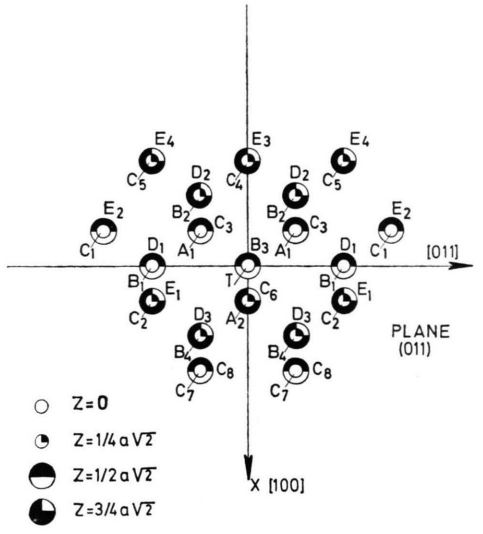

Fig. 1. Classification of lattice sites. Projections on the (011)-plane of sites with $Z \geqq 0$ are given for T-, A-, B-, C- and some D- and E-sites.

Now we classify lattice sites into coordination shells in the following way: sites, the tracer needs only one jump to arrive at are called A-sites, two jumps B-sites, etc. A-sites are nearest neighbours of T, B-sites are second nearest neighbours, among C-sites we notice third as well as fifth nearest neighbours.

By inspection of the lattice we find that not all sites in a coordination shell have equal probability of being occupied by the vacancy after a specified number of jumps. Therefore we classify sites into sets with equal occupation probability. In this way there are two sets of A-sites (A_1 and A_2, both existing of two sites), four B-sets, eight C-sets, etc.

We assume that the tracer has just made a jump along the negative X-direction into the origin. Immediately after such a jump the vacancy will be at one of the positions A_2. Both positions will have the same probability of being occupied by the tracer (namely $\frac{1}{2}$ for each A_2 site).

Now the vacancy may exchange position with the tracer immediately, or it may jump to a B-position and then start a walk through the lattice. It will be possible that the vacancy after such a detour returns to an A-position to cause the next tracer jump.

However, when the vacancy passes a boundary far from the tracer, we shall consider it as "effectively lost", i. e. then the vacancy will be supposed not to arrive at T at all, or to arrive at this position from random direction. The number of sites within the boundary determines the numerical accuracy of a calculation of f. The farther from the impurity the boundary is chosen the better the accuracy is.

In this calculation we shall consider sites as far as the F-coordination shell and moreover G-sites as far as they are 13-th nearest neighbours of T (from all the G-sites they will not only contribute most to the correlationfactor, but also they will be more important than other G-sites when Coulomb interaction between tracer and vacancy is included).

For reasons of clearness only a small number of sites is drawn in Figure 1.

Only sites with positive Z-coordinate are given, because sites with negative Z-coordinate are easily found by reflection in the (011)-mirror plane.

Furthermore we shall distinguish five disturbed atom-vacancy exchange rates. Following Mehrer we shall denote by w_{1T} the exchange rate of the vacancy with the impurity, by w_{12} the exchange rate of the vacancy from first to second nearest neighbour of the tracer and by a similar definition w_{21} (from B to A-sites), w_{23} (from B to third nearest neighbouring C-sites) and w_{25} (from B to fifth nearest neighbouring C-sites). Other vacancy jumps are assumed to occur with the selfdiffusion exchange rate w_0.

Let us now proceed to the calculation of f.

By following the wandering vacancy we shall find the probabilities that after the initial tracer jump the vacancy will arrive once, twice etc. at the sites A_2 and A_1 without having exchanged position with the tracer. By multiplying these results by the probability that the tracer exchanges position with the vacancy at A, we shall obtain expressions for P_- and P_+, respectively and so for f.

We define the occupation probability row matrix $[\boldsymbol{p}_0(\mathrm{A})]$

$$[\boldsymbol{p}_0(\mathrm{A})] \equiv (p_0(\mathrm{A}_1), p_0(\mathrm{A}_2)) \tag{4}$$

where $p_0(\mathrm{A}_i)$ is the probability that the vacancy occupies a single A_i-site immediately after the initial tracer jump, so

$$[\boldsymbol{p}_0(\mathrm{A})] = (0, \tfrac{1}{2}) . \tag{5}$$

In a similar way we define the row matrix $[\boldsymbol{p}_n(\mathrm{A})]$, an element $p_n(\mathrm{A}_i)$ of which is the probability that, given the vacancy has been n times available at the single A_i-site to cause the next tracer jump, it is once more available at this A_i. Then we write

$$[\boldsymbol{p}_n(\mathrm{A})] = [\boldsymbol{p}_{n-1}(\mathrm{A})]\, \mathbf{p}_1(\mathrm{AA}) \tag{6}$$

where an element $p_1(\mathrm{A}_k\mathrm{A}_l)$ of the transition probability matrix $p_1(\mathrm{AA})$ is the probability that the vacancy arrives at a specified A_l-site, starting from any site of the set A_k, multiplied by the number of A_k-sites. Thus

$$p_1(\mathrm{A}_k\mathrm{A}_l) = \sum_{i,j} q(\mathrm{A}_k\mathrm{B}_i)\, P(\mathrm{B}_i\mathrm{B}_j)\, q(\mathrm{B}_j\mathrm{A}_l) . \tag{7}$$

$q(X, Y)$ is the probability that the vacancy arrives at a specified site Y *in one jump*, starting from any site of the set X, multiplied by the number of X-sites, whereas $P(\mathrm{B}_i\mathrm{B}_j)$ is the *sum* of the probabilities that the vacancy (avoiding the A-shell) arrives once, twice, etc. at the specified B_j-site, starting from any site of the set B_i, multiplied by the number of B_i-sites.

In matrix notation (see [4])

$$p_1(\mathrm{A}_k\mathrm{A}_l) = [\boldsymbol{q}(\mathrm{A}_k\mathrm{B})]\, \mathbf{P}(\mathrm{BB})\, \{\boldsymbol{q}(\mathrm{BA}_l)\} . \tag{8}$$

From Eq. (6) we find

$$[\boldsymbol{p}_n(\mathrm{A})] = [\boldsymbol{p}_0(\mathrm{A})]\, \mathbf{p}_1{}^n(\mathrm{AA}) . \tag{9}$$

If $P(\mathrm{A}_i)$ is the total probability that the vacancy is available at A_i for the next tracer jump, then

$$[\boldsymbol{P}(\mathrm{A})] \equiv \sum_{n=0}^{\infty} [\boldsymbol{p}_n(\mathrm{A})] = \sum_{n=0}^{\infty} [\boldsymbol{p}_0(\mathrm{A})]\, \mathbf{p}_1{}^n(\mathrm{AA}) = [\boldsymbol{p}_0(\mathrm{A})]\, (\mathbf{I} - \mathbf{p}_1(\mathrm{AA}))^{-1} . \tag{10}$$

$\mathbf{I}$ is the unit matrix.

If we multiply $P(\mathrm{A}_i)$ by the probability $q(\mathrm{A}_i\mathrm{T})$ that the tracer exchanges position with the vacancy at A_i we find P_+ and P_- (for $i=1$ and $i=2$ respectively). So the expression for t becomes

$$t \equiv P_+ - P_- = P(\mathrm{A}_1)\, q(\mathrm{A}_1\mathrm{T}) - P(\mathrm{A}_2)\, q(\mathrm{A}_2\mathrm{T}) . \tag{11}$$

By inspection of the lattice we find

$$q(\mathrm{A}_i\mathrm{T}) = \frac{2\, w_{1\mathrm{T}}}{w_{1\mathrm{T}} + 3\, w_{12}} . \tag{12}$$

From symmetry-arguments we have the equalities

$$p_1(\mathrm{A}_1\mathrm{A}_2) = p_1(\mathrm{A}_2\mathrm{A}_1) , \tag{13}$$

$$p_1(\mathrm{A}_1\mathrm{A}_1) = p_1(\mathrm{A}_2\mathrm{A}_2) . \tag{14}$$

Using Eqs. (5), (10) to (14) we then get

$$t = -\frac{1}{1 - p_1(\mathrm{A}_2\mathrm{A}_2) + p_1(\mathrm{A}_2\mathrm{A}_1)} \frac{w_{1\mathrm{T}}}{w_{1\mathrm{T}} + 3\, w_{12}} . \tag{15}$$

We can calculate $p_1(\mathrm{A}_2\mathrm{A}_2)$ and $p_1(\mathrm{A}_2\mathrm{A}_1)$ by use of Eq. (8)

$$p_1(\mathrm{A}_2\mathrm{A}_2) = \frac{w_{12}}{3\, w_{12} + w_{1\mathrm{T}}} \{P(\mathrm{B}_3\mathrm{B}_3) + 2\, P(\mathrm{B}_3\mathrm{B}_4) + P(\mathrm{B}_4\mathrm{B}_3) + 2\, P(\mathrm{B}_4\mathrm{B}_4)\} \cdot \frac{w_{21}}{w_{21} + 2\, w_{23} + w_{25}} , \tag{16}$$

$$p_1(\mathrm{A}_2\mathrm{A}_1) = \frac{w_{12}}{3\, w_{12} + w_{1\mathrm{T}}} \{P(\mathrm{B}_3\mathrm{B}_1) + 2\, P(\mathrm{B}_3\mathrm{B}_2) + P(\mathrm{B}_4\mathrm{B}_1) + 2\, P(\mathrm{B}_4\mathrm{B}_2)\} \cdot \frac{w_{21}}{w_{21} + 2\, w_{23} + w_{25}} . \tag{17}$$

To find the elements $P(\mathrm{B}_i\mathrm{B}_j)$ of $\mathbf{P}(\mathrm{BB})$ we proceed as follows.

As before we define the row matrices

$$[\boldsymbol{p}_n(\mathrm{B})] = (p_n(\mathrm{B}_1), p_n(\mathrm{B}_2), \ldots,) , \quad n = 0, 1, 2, \ldots . \tag{18}$$

An element $p_n(\mathrm{B}_i)$ is the probability that, if the vacancy has been n times available at the single B_i-site for a jump to the A-shell, it is once more available at this B_i.

We write

$$[\boldsymbol{p}_n(\mathrm{B})] = [\boldsymbol{p}_{n-1}(\mathrm{B})]\, \mathbf{p}_1(\mathrm{BB}) \tag{19}$$

where an element $p_1(\mathrm{B}_k\mathrm{B}_l)$ of the square matrix $\mathbf{p}_1(\mathrm{BB})$ is the probability that the vacancy arrives at the single B_l-site along any path (only avoiding the A-shell), starting from any site of the set B_k, multiplied by the number of B_k-sites.

Again the vacancy can arrive at B_l only after a detour via the $C(D, \ldots)$ shell, thus

$$p_1(\mathrm{B}_k\mathrm{B}_l) = [\boldsymbol{q}(\mathrm{B}_k\mathrm{C})] \cdot \mathbf{P}(\mathrm{CC}) \cdot \{\boldsymbol{q}(\mathrm{CB}_l)\} . \tag{20}$$

An element $P(C_iC_j)$ of the square matrix $\mathbf{P}(CC)$ is the sum of the probabilities that the vacancy arrives at the specified C_j-site once, twice etc. (along any path, but avoiding the B-shell), starting from any site of the set C_i, multiplied by the number of C_j-sites.

As we assumed the influence of the impurity not to extend beyond the C-shell we can write

$$\mathbf{P}(CC) = (\mathbf{I} - \mathbf{\Gamma})^{-1}. \tag{21}$$

$\mathbf{\Gamma}$ is a one-jump transition probability matrix, an element Γ_{ij} of which is the probability that the vacancy occupies the particular site j after n jumps, given unit occupation probability after $n-1$ jumps for all sites of the i-set. Calculation of $\mathbf{P}(CC)$ can be performed numerically by an electronic computer. Furthermore, in a similar way as was done for the A-shell in Eq. (10), we get [4]

$$[\boldsymbol{P}(B)] \equiv \sum_{n=0}^{\infty} [\boldsymbol{p}_n(B)] = [\boldsymbol{p}_0(B)]\,(\mathbf{I} - \mathbf{p}_1(BB))^{-1}. \tag{22}$$

By definition

$$[\boldsymbol{P}(B)] = [\boldsymbol{p}_0(B)]\,\mathbf{P}(BB) \tag{23}$$

This results in

$$\mathbf{P}(BB) = (\mathbf{I} - \mathbf{p}_1(BB))^{-1}. \tag{24}$$

From Eq. (20) we obtain the expressions for the elements of $\mathbf{p}_1(BB)$, for example

$$p_1(B_1B_1) = \frac{w_{23}\{P(C_2C_1) + 2\,P(C_2C_2)\}\,\frac{1}{4}}{w_{21} + 2\,w_{23} + w_{25}} + \frac{w_{25}\{P(C_1C_1) + 2\,P(C_1C_2)\}\,\frac{1}{4}}{w_{21} + 2\,w_{23} + w_{25}}. \tag{25}$$

Taking $x \equiv w_{23}/w_{21}$ and $y \equiv w_{25}/w_{21}$, substitution of the $P(CC)$ values gives

$$p_1(B_1B_1) = \frac{w_{21}}{w_{21} + 2\,w_{23} + w_{25}}\,(0.62093\,x + 0.34593\,y) \tag{26}$$

etc.

This leads to

$$t = \frac{-w_{1T}}{w_{1T} + 3\,F\,w_{12}}, \tag{27}$$

$$f = \frac{3\,F\,w_{12}}{2\,w_{1T} + 3\,F\,w_{12}}, \tag{28}$$

$$F = 1 - \frac{g_1(x,y)}{3\,g_2(x,y)}. \tag{29}$$

$g_1(x,y)$ and $g_2(x,y)$ are polynomials of the third and fourth degree respectively

$$g_1(x,y) = \sum_{0 \leq i+j \leq 3} \beta_{ij}\,x^i\,y^j, \tag{30}$$

$$g_2(x,y) = \sum_{0 \leq i+j \leq 4} \gamma_{ij}\,x^i\,y^j. \tag{31}$$

The coefficients β_{ij} and γ_{ij} are given in Table 1 $(c/kT = 0)$.

The expression for F looks rather complicated, which is due to the fact that we took into account a fifth distinct jump frequency, viz. w_{25}. MANNING [5, 6] and MEHRER [8] take $w_{25} = w_{23}$ and $x(=y) = \alpha^{-1}$. With this approximation we get

$$F = \frac{6.39\,\alpha^3 + 32.32\,\alpha^2 + 52.11\,\alpha + 26.83}{3\,\alpha^4 + 21.75\,\alpha^3 + 57.39\,\alpha^2 + 65.16\,\alpha + 26.83}. \tag{32}$$

So another remarkable difference between the expressions of Manning and Mehrer is the occurrence of a higher power of α in both denominator and numerator. However, when values for α are substituted in Eq. (32) it turns out that our result is not much different from theirs. For $\alpha = 1$ we have $F = 0.6757$, which is 1.3% higher than the exact value of $2/3$ [12], while the error in f is 0.7%.

Calculation of the Correlation Factor Including Coulomb Interaction

In this section we shall consider the influence upon the correlation factor of a long range electrostatic interaction between an impurity-tracer with a charge e and a vacancy with a charge $-e$. Such a situation occurs in germanium and silicon for diffusion of group V impurities, which behave as donors in these materials.

As a result of this interaction it will be more difficult for the vacancy to migrate far away from the impurity-tracer, which means more correlation and so a smaller correlation factor. Following Mehrer we shall assume the interaction beyond the C-shell to be of a Coulombic nature. Then, if a matrix atom makes a jump from a position r_j into a vacancy at r_i, the electrostatic energy change between initial and final situation will be

$$e^2/\varepsilon\,r_i - e^2/\varepsilon\,r_j; \tag{33}$$

ε is the dielectric constant of the material. We shall suppose that, when the atom is situated in the saddle point, halfway between both positions, a change of half this amount has occurred. Thus the height of the saddle point barrier will alter with

$$\Delta E_{ij} = \frac{e^2}{2\,\varepsilon}\left(\frac{1}{r_i} - \frac{1}{r_j}\right). \tag{34}$$

This is equivalent with the assumption that, the atom being in the saddle point, the charge $-e$ is distributed equally between the two equilibrium positions (cf. LECLAIRE [13]).

The atom-vacancy exchange rate becomes

$$w_{ij} = w_0 \exp \frac{e^2}{2\,\varepsilon\, k\, T}\left(\frac{1}{r_j} - \frac{1}{r_i}\right). \qquad (35)$$

Now the elements of the large one jump transition probability matrix Γ are changed and are replaced by expressions of the form

$$p_{ij} = \frac{w_{ij}}{\sum\limits_k w_{ik}}. \qquad (36)$$

The sum in the denominator is composed of the four exchange rates of the vacancy at i with its four nearest neighbours. Not only the $P(\mathrm{CC})$ values are now altered, but the $q(\mathrm{CB})$ values are as well. For example we get

$$p_1(\mathrm{B_1B_1}) = \frac{w_{23}\{p_{52}\,P(\mathrm{C_2C_1}) + 2\,p_{32}\,P(\mathrm{C_2C_2})\}}{w_{21}+2\,w_{23}+w_{25}} + \frac{w_{25}\{p_{52}\,P(\mathrm{C_1C_1}) + 2\,p_{32}\,P(\mathrm{C_1C_2})\}}{w_{21}+2\,w_{23}+w_{25}}. \qquad (37)$$

Without Coulomb interaction we have $p_{52} = p_{32} = \frac{1}{4}$ and we recognize Equation (25).

If we substitute

$$c = e^2/2\,\varepsilon\, a \qquad (38)$$

in Eq. (35), a being the cubic lattice constant, we are able to calculate F as a function of c/kT. In Fig. 2 $3F$ is plotted as function of α for various values of c/kT (cf. MEHRER [8]), whereas values of β_{ij} and γ_{ij} are given in Table 1.

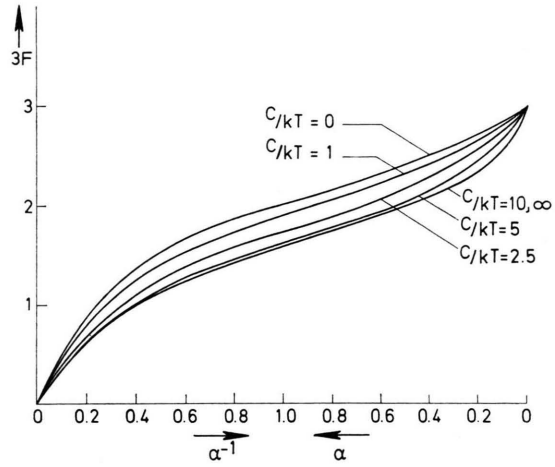

Fig. 2. $3F$ as a function of α for some values of c/kT.

Discussion

If electrostatic interaction is not included in the calculation ($c/kT = 0$), our expression for F differs from Manning's and Mehrer's by the occurrence of a higher power of α.

However, by substituting numerical values for α, it turns out that the final result is not much different from theirs.

Table 1. Coefficients of the polynomials $g_1(x, y)$ (1 a) and $g_2(x, y)$ (1 b) for some values of c/kT.

Table 1 a.

c/kT	β_{00}	β_{10}	β_{01}	β_{20}	β_{11}	β_{02}	β_{30}	β_{21}	β_{12}	β_{03}
0	3	9.59	5.77	9.33	12.07	3.67	2.79	5.73	3.76	0.77
0.5	3	8.56	4.98	7.01	9.17	2.72	1.67	3.58	2.40	0.49
1	3	7.68	4.18	5.21	6.76	1.89	0.94	2.10	1.42	0.28
2.5	3	6.07	2.11	2.37	2.48	0.46	0.13	0.33	0.20	0.03
5	3	5.29	0.50	1.18	0.47	0.02	0.00	0.01	0.00	0.00
10	3	5.04	0.02	0.80	0.02	0.00	0.00	0.00	0.00	0.00
∞	3	5	0	0.75	0	0	0	0	0	0

Table 1 b.

c/kT	γ_{00}	γ_{10}	γ_{01}	γ_{20}	γ_{11}	γ_{02}	γ_{30}	γ_{21}	γ_{12}	γ_{03}	γ_{40}	γ_{31}	γ_{22}	γ_{13}	γ_{04}
0	1	4.75	2.50	7.95	8.85	2.34	5.49	9.79	5.47	0.97	1.33	3.34	3.00	1.12	0.15
0.5	1	4.34	2.14	6.45	6.89	1.70	3.76	6.71	3.61	0.60	0.73	1.91	1.72	0.62	0.08
1	1	4.00	1.77	5.27	5.22	1.16	2.52	4.48	2.23	0.33	0.38	1.01	0.91	0.31	0.04
2.5	1	3.39	0.85	3.34	2.08	0.26	0.79	1.25	0.40	0.03	0.04	0.12	0.10	0.02	0.00
5	1	3.10	0.19	2.53	0.41	0.01	0.19	0.20	0.01	0.00	0.00	0.00	0.00	0.00	0.00
10	1	3.01	0.01	2.28	0.02	0.00	0.02	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00
∞	1	3	0	2.25	0	0	0	0	0	0	0	0	0	0	0

Furthermore we should like to remark that Mehrer's claim to more generality, by taking into consideration vacancy jump frequencies w_{32} and w_{52} explicitly, is not correct.

This would introduce quite a number of transition probabilities of the type

$$p_{36} = \frac{w_0}{2\,w_0 + 2\,w_{32}} \tag{39}$$

etc. and

$$p_{56} = \frac{w_0}{3\,w_0 + w_{52}} \tag{40}$$

etc.

into the large C – D – E . . . matrix, which makes a numerical inversion of $(\mathbf{I} - \mathbf{T})$ [8] almost impracticable. Such an inversion would result in the occurrence of high powers of w_{52} and w_{32} in the coefficients in Mehrer's Eqs. (6.2) and (6.3).

The above kind of error in the normalisation is far more serious when long range electrostatic interaction is included in the calculation. A normalisation constant of 1/4 as in Mehrer's expression (5.7) is not justified. Normalisation ought to be performed following our Equation (36).

Moreover, we should like to point out that in a four frequency model, in particular the transition probabilities $q(C_i B_k)$ are changed considerably by an electrostatic impurity-vacancy interaction. Furthermore we have objections to the expansion of the exponential function following Mehrer's Equation (5.6), if $c/kT \gg 1$ as is plotted in his Figure 4.

From the foregoing arguments it will be clear, why we arrive at a different (and larger) influence of Coulomb interaction on F (Figure 2).

Finally it is interesting to note that in the case of a strongly bound impurity-vacancy pair ($3\,F\,w_{12} \ll 2\,w_{1T}$) the impurity diffusion coefficient is – apart from the creation probability p_{vi} of a vacancy as a nearest neighbour of the tracer – determined by the quantity $F\,w_{12}$, because then, by inserting Eq. (28) in the expression for D_{imp}

$$D_{imp} \sim f\,w_{1T}\,p_{vi} \approx \tfrac{3}{2}\,F\,w_{12}\,p_{vi}\,. \tag{41}$$

In the opposite limiting case $3\,F\,w_{12} \gg 2\,w_{1T}$ the correlation factor is equal to unity and so

$$D \sim p_{vi}\,w_{1T}\,. \tag{42}$$

More information about the diffusion process of group V elements in germanium and silicon might be obtained by measurements of isotope effects *.

Acknowledgements

We thank Dr. J. R. MANNING for helpful correspondence, Prof. Dr. G. DE VRIES for reading the manuscript, Dr. C. A. J. AMMERLAAN for helpful discussions and Miss A. ABELS for a contribution to the computer programming.

* *Note added in proof:* Following MANNING [14, 15] the order of α, which appears in the numerator and denominator of the expression for F, depends on the number of sets of B-sites one chooses. Manning, distinguishing two independent B-sites, arrives at an expression for F in which α appears to the second power. MANNING [14] points out that dividing both numerator and denominator of our Eq. (32) by $3\,\alpha^2 + 10.87\,\alpha + 8.68$ yields an equation similar to his Equation (32) [15].

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