

### [3] Tracer Diffusion in Nonstoichiometric Intermetallic Compounds with Random Mixing on Each Sublattice

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**Abstract.** Tracer diffusion by way of vacancies is investigated in B2 intermetallics AB by means of a kinetic equation approach. The model used is one with four inter-sub-lattice frequencies where each sub-lattice is treated as a random alloy. Coupling is achieved between the two types of cycles, *i.e.*, with the vacancy starting on one sub-lattice and finishing on either sub-lattice and with a vacancy starting on the other sub-lattice and finishing on either sub-lattice. An expression for the tracer correlation factor is derived in terms of atom vacancy exchange frequencies and atomic concentrations. Results from this expression are compared with Monte Carlo calculations and also results from a previous Manning-type random alloy approach to the problem.

#### Introduction

Intermetallic compounds form when two unlike metals diffuse into one another with individual elements taking up preferred positions within the crystal structure. Unlike conventional alloys that have no definite atomic formula, these compounds have a definite stoichiometry with a limited composition range. Recently, there has been considerable interest in the study of diffusion kinetics in intermetallic compounds because of their applications in modern technology: some of these compounds offer low density, a high strength at elevated temperatures and a high corrosion resistance.

Since an extensive review on diffusion kinetics calculations in intermetallics has been provided very recently [1], in the following we will give only a very brief coverage and then only of tracer diffusion. It was recognized very early in the literature on diffusion in intermetallics that a vacancy moving on a sequence of jumps in random directions, as in a pure metal, would soon leave a trail of extensive disorder in its wake. To avoid this difficulty, a vacancy must inevitably be confined to an ever-smaller set of lower energy penalty jump sequences as the overall order increases. At the limit of perfect order, we have the six-jump-cycle (6JC) mechanism [2]. In this mechanism, starting from a fully ordered configuration for a stoichiometric AB alloy taking the B2 structure the vacancy progressively disorders the structure in its first three *effective* jumps. In its following three effective jumps the vacancy progressively re-orders the lattice resulting in the fully ordered configuration once again. By the end of the sequence of six (effective) vacancy jumps, tracer diffusion has occurred. Punctuating this sequence are of course numerous jump reversals caused by many of the antistructural atoms formed during the sequence returning immediately to their original sites. Belova and Murch [3] have shown in computer simulations that the 6JC mechanism certainly operates at high levels of order and at the stoichiometric composition. With the pure 6JC mechanism, tracer diffusion at non-

stoichiometric compositions does not allow for the participation of anti-structural atoms produced by non-stoichiometry. Furthermore, there is no means for switching between the two types of cycles, that is a 6JC with the vacancy starting and finishing on one sub-lattice and a 6JC with a vacancy starting and finishing on the other sub-lattice. Belova and Murch [4-6] extended the idea of the 6JC to non-stoichiometric compositions using an analogue of the five-frequency model for impurity diffusion via vacancy jumps. They derived expressions for tracer correlation factors and tracer diffusivities and verified the expressions by Monte Carlo computer simulation of the well-known Ising alloy model.

The Ising model itself has been used on a number of occasions to provide analytical expressions for the tracer diffusion coefficients in intermetallics [7-9]. Such calculations do not include the 6JC mechanism explicitly but attempt to imply it at high levels of order. In general, when compared with results of Monte Carlo computer simulations these calculations do quite well at low levels of order but tend to fail at high levels of order when the 6JC operates. The Ising model describes the jump frequencies in terms of (specified) atomic interactions. A different model, which directly specifies the frequencies for a limited number of types of jumps, has also been introduced [10-14]. In its form for the B2 structure there are four atom-vacancy exchange frequencies for the various inter-sublattice jumps (intra-sublattice jumps can be ignored for this particular structure if the intermetallic being addressed exhibits primarily antistructural disorder). These calculations use an extension of Manning's diffusion kinetics formalism for the random alloy. Similar to the calculations for the Ising model, the calculations are in good agreement with computer simulations at low levels of order but there are considerable deviations at high levels of order. Avenues for improvement are limited. In the present paper we adopt the four frequency model but use a different approach that is based on kinetic equations. This approach has an advantage in its transparency which will allow for systematic improvement in due course.

### The Tracer Correlation Factor

We consider a B2 type AB intermetallic compound where 1 constitutes the home sub-lattice of atoms of B kind and 2 is the home sub-lattice of atoms of A kind. Let  $B_1$  and  $A_1$  respectively denote the regular and antistructural atoms on sublattice-1 and  $A_2$ ,  $B_2$  respectively denote the regular and antistructural atoms on sublattice-2. If the atom-vacancy exchange frequencies depend only on the type of atom jumping and the sub-lattice, there will be four frequencies with two different types of vacancies;  $V_1$  = vacancy on sublattice-1 only and  $V_2$  = vacancy on sublattice-2 only. The four exchange frequencies are  $W_{A_1} \equiv W_A^{1 \rightarrow 2}$ , the atom-vacancy exchange frequency when an A atom is on sublattice-1 and vacancy on sublattice-2. Likewise, we define  $W_{B_1} \equiv W_B^{1 \rightarrow 2}$ ,  $W_{A_2} \equiv W_A^{2 \rightarrow 1}$ ,  $W_{B_2} \equiv W_B^{2 \rightarrow 1}$ . In the case of tracer diffusion, in addition there will formally be two further frequencies  $W_{T_1} \equiv W_T^{1 \rightarrow 2}$  and  $W_{T_2} \equiv W_T^{2 \rightarrow 1}$  for  $T_1$  = tracer on sublattice-1 only and  $T_2$  = tracer on sublattice-2 only, respectively. For very dilute vacancy and tracer components, the species compositions for the four-component system can be written as [10,11]:

$$\begin{aligned}
 C_{A_1} + C_{A_2} &= 2C_A \\
 C_{B_1} + C_{B_2} &= 2C_B \\
 C_{A_i} + C_{B_i} &= 1 \quad , \quad i=1,2 \\
 C_A + C_B &= 1
 \end{aligned} \tag{1}$$

Here  $C_A$  is the fraction of sites occupied by A atoms, etc. For a stoichiometric B2 structure  $C_A$  is equal to  $C_B$ . The compositions and the frequencies are related through detailed balance expressed as:

$$C_{V_1} C_{j_2} W_{j_2} = C_{V_2} C_{j_1} W_{j_1}, \quad j = T, A, B. \quad (2)$$

Following Belova and Murch [15], the phenomenological coefficients for tracer can be expressed as:

$$L_{TT} = L_{T_1T_1} + L_{T_2T_2} + 2L_{T_1T_2} \quad (3)$$

where the Onsager relation ( $L_{T_1T_2} = L_{T_2T_1}$ ) has been used. We can now apply the usual definition (see Allnatt and Lidiard [16]) to express the  $L$ 's as a sum of uncorrelated  $L^{(0)}$  and correlated  $L^{(1)}$  parts as:

$$L_{T_iT_j} = L_{T_iT_j}^{(0)} + L_{T_iT_j}^{(1)}, \quad i, j = 1, 2 \quad (4)$$

The uncorrelated parts can be expressed as:

$$L_{T_iT_j}^{(0)} = \delta_{ij} C_{V_k} C_{T_j} W_{T_j} NZS^2 / 6k_B T \quad ; k \neq j \quad (5)$$

where  $N$  is the number of sites per unit volume,  $Z$  is the coordination number,  $S$  is the nearest-neighbour (n-n) jump distance and  $k_B$  and  $T$  have their usual meanings. From the equilibrium condition (Eq. 2) it can be seen that:

$$L_{T_1T_1}^{(0)} = L_{T_2T_2}^{(0)} = 0.5 L_{TT}^{(0)} \quad (6)$$

The correlated parts can be expressed as:

$$L_{T_iT_j}^{(1)} = - \left( \frac{NZS^2}{3KT} \right) W_{T_i} W_{T_j} \sum_S \left( \frac{S \cdot S_0}{S^2} \right) \phi_{v_i, v_j}(S, S_0) \quad (7)$$

where, for example:

$$\phi_{v_1, v_2}(S; S_0) = \int_0^\infty dt \sum_\ell \psi_{v_1T_2, v_2T_1}(\ell, \ell - S; t; \ell_0, \ell_0 - S_0; t = 0) \quad (8)$$

Here  $\psi$  is the conditional probability of finding at time  $t$  the vacancy at site  $\ell$  on sublattice-1 and the tracer at its nearest neighbour(n-n) site ( $\ell - S$ ) on the sublattice-2, when initially the vacancy was at any site  $\ell_0$  on sublattice-2 and tracer at its n-n site ( $\ell_0 - S_0$ ) on sublattice-1. We have used the symmetry available

and have considered any site  $\ell_0$  and its n-n site, say  $S_0 = \frac{a}{2}(1,1,1)$ , where  $a$  is the cubic lattice parameter. The function  $\phi$  depends only on the initial and final jump vectors  $S_0$  and  $S$  respectively. The correlated parts of the phenomenological coefficients depend not only on the  $\phi$ s but also their product with the angle between initial and final jump vectors. Chaturvedi and Allnatt [17,18] have shown that it is much more convenient for such problems to work in Fourier space than in real space. We therefore define the Fourier transform:

$$\tilde{\phi}(K; S_0) = \sum_r e^{-iK \cdot r} \phi(r; S_0) \quad (9)$$

and the inverse transform as:

$$\phi(r, S_0) = \left( \frac{a}{2\pi} \right)^3 \int d^3K e^{iK \cdot r} \tilde{\phi}(K; S_0) \quad (10)$$

The integrations are over the Brillouin zones in the cubic lattice. We can then write:

$$\sum_S \left( \frac{S \cdot S_0}{S^2} \right) \phi_{V_i:V_j}(S : S_0) = 8i \left( \frac{a}{2\pi} \right)^3 \int d^3K \sin K_x \cos K_y \cos K_z \tilde{\phi}_{V_i:V_j}(K : S_0) = U_{ij} \quad (11)$$

We have used here, for convenience, the shorthand notation  $K_x \equiv K_x \frac{a}{2}$ , etc. Using Eq.11 in Eq.7 we obtain the tracer correlation factor with the usual definition ( $f_T = \frac{L_{TT}}{L_{TT}^{(0)}}$ ) as

$$f_T = 1 - \left( \frac{1}{C_{V_2} C_{T_1} W_{T_1}} \right) \sum_{i,j} W_{T_1} W_{T_j} U_{ij} \quad (12)$$

### The Kinetic Equation

In order to calculate  $U_{ij}$ , we use the kinetic equation approach for the probability function  $\psi_{V_1T_2}(\ell, \ell-r)$ , which is the probability of finding at time  $t$  the vacancy at site  $\ell$  on sublattice-1 and the tracer at site  $(\ell-r)$  on sublattice-2, when the system was in a given initial state. By using the arguments of gain and loss in the probability during the time interval  $dt$ , the kinetic equation for  $\psi_{V_1T_2}(\ell, \ell-r)$  can be written as

$$\begin{aligned} \frac{d\psi_{V_1T_2}(\ell, \ell-r)}{dt} = & \theta(r) [W_{T_1} \psi_{V_2T_1}(\ell-r, \ell) - W_{T_2} \psi_{V_1T_2}(\ell, \ell-r)] \\ & + \sum_{r' \neq r} \theta(r') [W_{A_1} \psi_{V_2T_1A_1}(\ell-r', \ell-r, \ell) - W_{A_2} \psi_{V_1T_2A_2}(\ell, \ell-r, \ell-r')] \\ & + \sum_{r' \neq r} \theta(r') [W_{B_1} \psi_{V_2T_1B_1}(\ell-r', \ell-r, \ell) - W_{B_2} \psi_{V_1T_2B_2}(\ell, \ell-r, \ell-r')] \end{aligned} \quad (13)$$

Here  $\theta(r)$  is a step-function which is unity when  $\mathbf{r}=\mathbf{s}$  and zero otherwise. Eq.13 can be put into closed form by a suitable approximation to the three-site probability functions. In the lowest order of approximation, in the presence of vacancy and tracer we can neglect fluctuations in the occupancy variables for the atoms. That is, for example, we can simply write that:

$$\psi_{V_2T_1A_1}(\ell-r', \ell-r', \ell) = C_{A_1} \psi_{V_2T_1}(\ell-r', \ell-r', \ell) \quad (14)$$

We then make the following operations in Eq.13. Add and subtract terms with  $r'=r$ , integrate with respect to  $t$ , sum over  $\ell$  and then take the Fourier transform on both sides. This then yields:

$$\begin{aligned} \phi_{V_1T_2}^{(0)}(K) = & W_{T_1} \left( \frac{a}{2\pi} \right)^3 \int d^3K^1 \theta(K+K^1) \tilde{\phi}_{V_2T_1}(K^1) \\ & + [W_{V_2} - W_{T_2}] \left( \frac{a}{2\pi} \right)^3 \int d^3K^1 \theta(K-K^1) \tilde{\phi}_{V_1T_2}(K) \\ & + W_{V_1} \theta(K) \tilde{\phi}_{V_2T_1}(K) - W_{V_2} Z \tilde{\phi}_{V_1T_2}(K) \end{aligned} \quad (15)$$

Here, we have defined:

$$\begin{aligned}\phi_{V_1T_2}^{(0)}(K) &= \sum_r e^{-iK \cdot r} \sum_{\ell} \psi_{V_1T_2}(\ell, \ell - r; t=0) \\ \theta(K) &= \sum_r e^{-iK \cdot r} \theta(r) = \sum_S e^{-iK \cdot S} \\ W_{Vi} &= C_{A_i} W_{A_i} + C_{B_i} W_{B_i}, \quad i=1, 2\end{aligned}\quad (16)$$

where  $W_{Vi}$  is the vacancy escape jump rate from the  $i^{\text{th}}$  sub-lattice. Similarly, the kinetic equation for the probability function  $\psi_{V_1T_2}(\ell, \ell - r)$  can be obtained, which in fact results from Eq.15 with the interchange of 1 and 2. Adding the two equations, we obtain:

$$\begin{aligned}& [Z - \theta(K)] [W_{V_1} \phi_{V_2T}(K) + W_{V_2} \phi_{V_1T}(K)] \\ &= [\phi_{V_1T_2}^{(0)}(K) + \phi_{V_2T_1}^{(0)}(K)] \\ &+ [W_{V_1} - W_{T_1}] \left(\frac{a}{2\pi}\right)^3 \int d^3K' \theta(K - K') \phi_{V_2T_1}(K') \\ &+ [W_{V_2} - W_{T_2}] \left(\frac{a}{2\pi}\right)^3 \int d^3K' \theta(K - K') \phi_{V_1T_2}(K') \\ &+ W_{T_1} \left(\frac{a}{2\pi}\right)^3 \int d^3K' \theta(K + K') \phi_{V_2T_1}(K') \\ &+ W_{T_2} \left(\frac{a}{2\pi}\right)^3 \int d^3K' \theta(K + K') \phi_{V_1T_2}(K')\end{aligned}\quad (17)$$

Eq. 17 is an integral equation in terms of two unknown  $\phi$  functions. Chaturvedi and Allnatt [17,18] have shown that instead of solving the integral equation it is much more convenient to solve directly for the  $U$  functions defined through Eq. 11, as the integrands in  $K$  and  $K'$  can be decoupled using the symmetry properties of the Brillouin integrals. For example, we can write

$$8i \left(\frac{a}{2\pi}\right)^6 \iint d^3K d^3K' \frac{\sin K_x \cos K_y \cos K_z}{[Z - \theta(K)]} \theta(K \pm K') \phi_{V_1T}(K') = \mp J U_1 \quad (18)$$

in which we have defined  $J$  as

$$J = 8 \left(\frac{a}{2\pi}\right)^3 \int d^3K \frac{[\sin K_x \cos K_y \cos K_z]^2}{[Z \mp \theta(K)]} \quad (19)$$

We note that the numerical values of  $J$  with either plus or minus sign in Eq.19 are the same and are equal to 0.15793. Thus, using Eqs.11 and 18 in Eq.17, we finally obtain two linear equations corresponding to the initial configurations when the vacancy is on sublattice-1 with the tracer on sublattice-2 and the vacancy on sublattice-2 with the tracer on sublattice-1, respectively. This then yields:

$$\begin{aligned}b_2 U_{11} + b_1 U_{21} &= C_{V_1} C_{T_2} J \\ b_2 U_{12} + b_1 U_{22} &= C_{V_2} C_{T_1} J\end{aligned}\quad (20)$$

where

$$b_i = W_{Vi} (1 - J) + 2 W_{T_i} J \quad ; \quad i=1,2 \quad (21)$$

In order to determine all the  $U_{ij}$  functions we can make use of the expression for the tracer correlation factor derived by Bakker [8] using a straightforward method of inspecting all cosines between the first tracer jump and consecutive ones. This expression is:

$$\begin{aligned}
 f_T &= \frac{n_{T2}}{n_{T1} + n_{T2}} \left( 1 + \frac{2}{n_{T2}} \sum_{i=1}^{n_{T2}} \left( \frac{\langle x_i^2 x_{i+1} \rangle}{S^2} + \frac{\langle x_i^2 x_{i+2} \rangle}{S^2} + \dots \right) \right) \\
 &+ \frac{n_{T1}}{n_{T1} + n_{T2}} \left( 1 + \frac{2}{n_{T1}} \sum_{i=1}^{n_{T1}} \left( \frac{\langle x_i^1 x_{i+1} \rangle}{S^2} + \frac{\langle x_i^1 x_{i+2} \rangle}{S^2} + \dots \right) \right) \\
 &= \frac{1 + p_T q_T - p_T - q_T}{1 - p_T q_T}
 \end{aligned} \quad (22)$$

where  $n_{Ti} = C_{V_k} C_{Ti} W_{Ti}$ ,  $x_i^2$  and  $x_i^1$  are the vector-jumps of tracer T of the type 2 and 1 respectively. After mapping the expressions for the average cosines between the first vector-vector and all consecutive ones in Eq.22 with their expressions in terms of  $p_T$  and  $q_T$  (average cosines between the first vector-jump and the second one) and with Eq.12 we soon have the following expressions for  $U_{ij}$ :

$$\begin{aligned}
 U_{11} &= -\frac{q_T p_T n_{T1}}{(1 - q_T p_T) w_{T1}^2}, & U_{22} &= -\frac{q_T p_T n_{T2}}{(1 - q_T p_T) w_{T2}^2}, \\
 U_{12} &= \frac{q_T n_{T2}}{(1 - q_T p_T) w_{T1} w_{T2}}, & U_{21} &= \frac{p_T n_{T1}}{(1 - q_T p_T) w_{T1} w_{T2}}
 \end{aligned} \quad (23)$$

Eq. 23 shows that there is no reciprocity relation  $U_{12} = U_{21}$  for this case. Eqns 23 can be solved together with Eqn 20 to give expressions for  $q_T$  and  $p_T$ :

$$q_T = \frac{J W_{T2}^2}{b_2 W_{T2} - J W_{T1}^2}, \quad p_T = \frac{J W_{T1}^2}{b_1 W_{T1} - J W_{T2}^2} \quad (24)$$

and then finally for  $f_T$  (Eqn 22):

$$f_T = \frac{((1-J)W_{T1}W_{V1} + J(W_{T1}^2 - W_{T2}^2))(J(W_{T1}^2 - W_{T2}^2) - (1-J)W_{T2}W_{V2})}{G} \quad (25)$$

where

$$\begin{aligned}
 G &= 2J^2(W_{T1}^2 - W_{T2}^2)^2 - (1-J)^2 W_{T1} W_{T2} W_{V1} W_{V2} \\
 &+ J(1-J)\{W_{T1} W_{V1}(W_{T1}^2 - 2W_{T2}^2) + W_{T2} W_{V2}(W_{T2}^2 - 2W_{T1}^2)\}
 \end{aligned} \quad (26)$$

## Results and Discussion

In order to test the results of our expressions Monte Carlo simulations for the four frequency model have been carried out at and near the stoichiometric composition using methods described in [10,11]. The equilibrium composition of A atoms was varied from 0.45 to 0.5. The simulation results were controlled by first taking all the jump frequencies to be equal, which results in  $f_B$  and  $f_A$  being equal to  $f_0 = 0.72722$ . Then we varied the ratio of jump frequencies of antistructural and structural atoms. For example, we took  $W_{A1} = W_{B2} = 1$  and  $W_{A2} = W_{B1} = \alpha$  for different values of  $\alpha$ . Results of these simulations for the tracer correlation factor for A are presented in Figures 1 a-d and for B in Figures 2 a-d together with those calculated using Eqs 25-26 (solid lines). The correlation factors decrease with a decrease in the value of  $\alpha$  and become of the order of  $10^{-2}$  when  $\alpha = 0.01$ . Comparison has been made with the results for the same model but using Manning type considerations [10,11]. These are presented as dashed lines in the same figures.

In general there is reasonable agreement with the present approach with results of the Monte Carlo simulations for values of  $\alpha$  greater than about 0.5. It can also be seen that the results using the Manning-type approach gives considerably better agreement. Our results for the tracer correlation factor become

negative as the frequency ratio is changed from 0.4 to 0.3 showing that the random alloy model is overestimating the tracer correlation effects when the formation of antistructural atoms is restricted. This is probably not the influence of the 6JC mechanism which has been shown to be important at a much lower value of  $\alpha$  [19]. The value of the present approach is that it is relatively transparent to understand and to improve and allows the incorporation of other methods for calculating correlation factors.

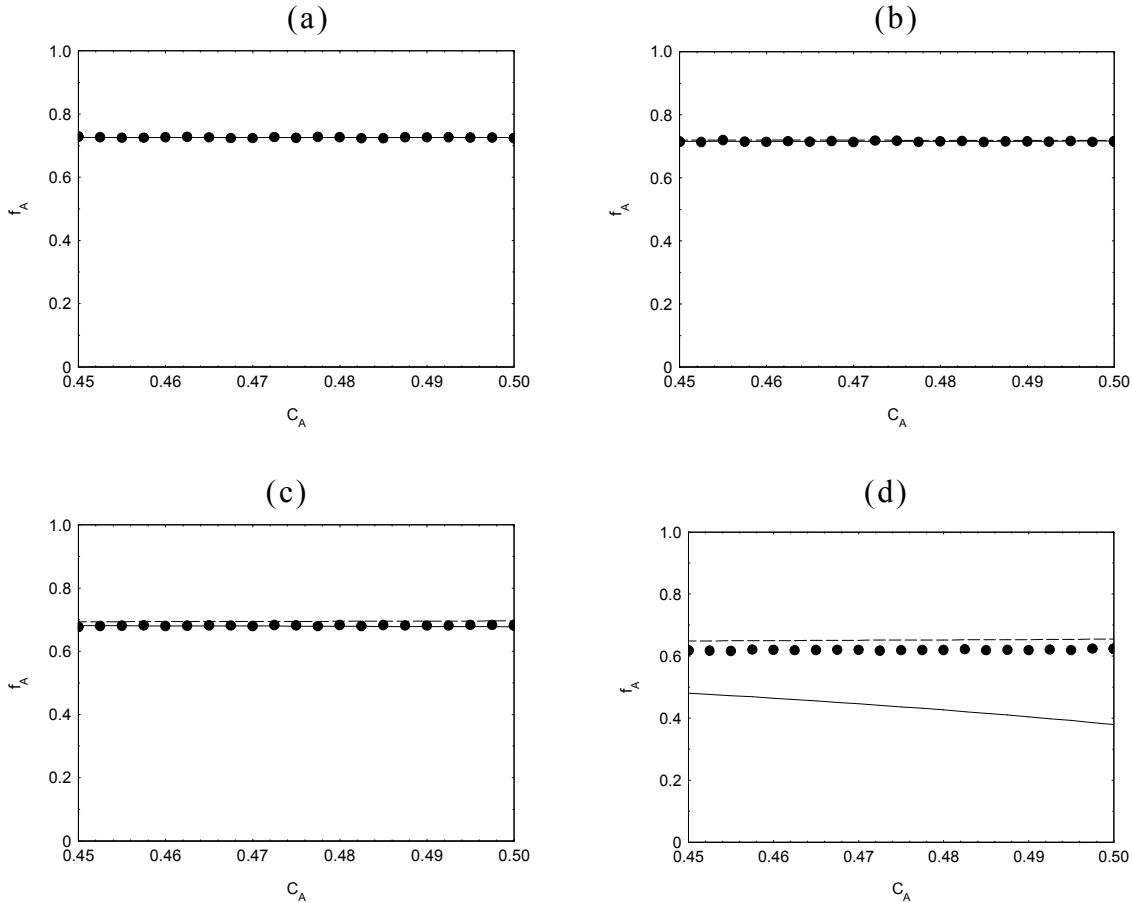
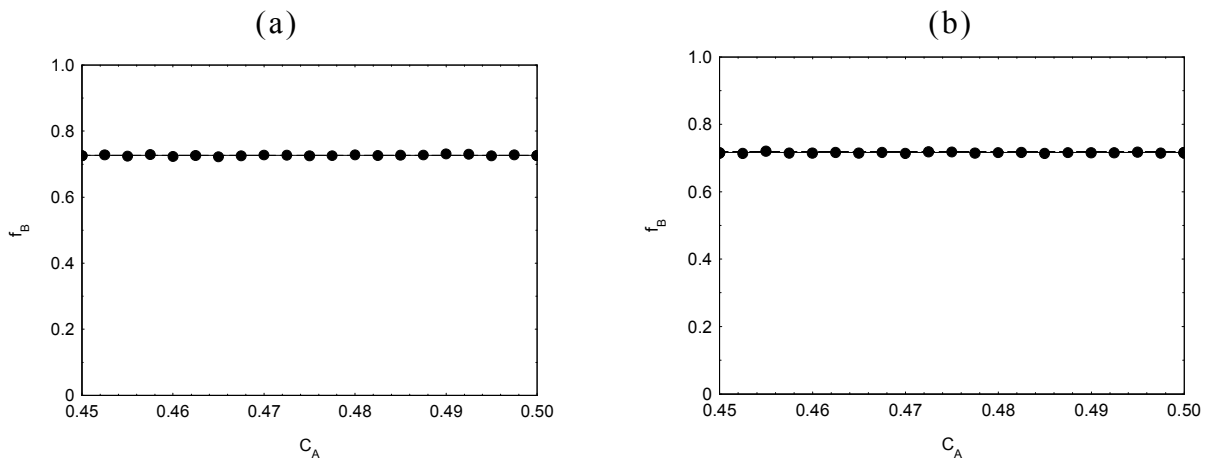


Fig 1. Tracer correlation factors  $f_A$  as a function of composition  $C_A$ . a) –  $\alpha = 0.9$ ; b) –  $\alpha = 0.7$ ; c) –  $\alpha = 0.5$ ; d) –  $\alpha = 0.35$ . Symbols: Monte Carlo results; Solid lines: Eqs 25,26; Dashed lines: refs 10,11.





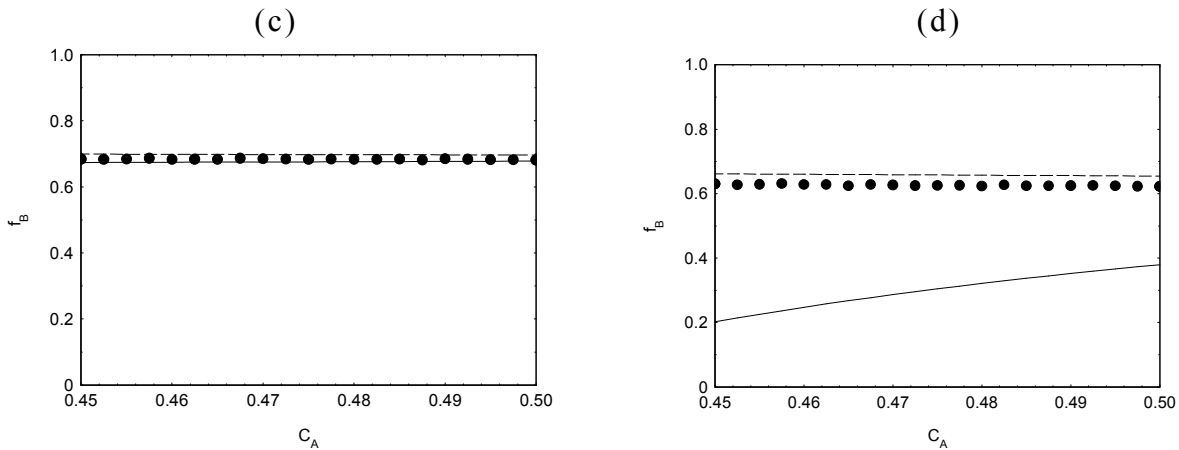


Figure 2. Tracer correlation factors  $f_B$  as a function of composition  $C_A$ . a) –  $\alpha = 0.9$ ; b) –  $\alpha = 0.7$ ; c) –  $\alpha = 0.5$ ; d) –  $\alpha = 0.35$ . Symbols: Monte Carlo results; Solid lines: Eqs 25,26; Dashed lines: refs. 10,11.

### Concluding Remarks

Tracer diffusion by way of vacancies was investigated in B2 intermetallics AB by means of a kinetic equation approach. The model used was one making use of four inter sub-lattice frequencies where each sub-lattice is treated as a random alloy. Coupling was achieved between the two types of cycles, *i.e.*, with the vacancy starting on one sub-lattice and finishing on either sub-lattice and with a vacancy starting on the other sub-lattice and finishing on either sub-lattice. An expression for the tracer correlation factor was derived in terms of atomic jump frequencies and atomic concentrations. Results from this expression were compared with Monte Carlo calculations and also results from a Manning random alloy type approach to the problem.

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