Six-Jump-Cycle Mechanism for Collective Correlations in Nonstoichiometric Intermetallic Compounds

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Abstract. The six-jump-cycle (6JC) mechanism is used to derive expressions for collective correlation factors in a nonstoichiometric binary intermetallic compound AB. The 6JC is used as a fundamental unit for the cycle involving a perfectly ordered configuration and a two-jump-cycle (2JC) as a fundamental unit for the cycle involving existing antistructural atoms. The jump frequency for the 6JC is calculated in terms of a four-frequency-model using the mean first passage concept of Arita *et al.*, while the jump frequency for the 2JC is taken to be the harmonic mean of the individual jump frequencies. The expressions for phenomenological transport coefficients are obtained through the linear response approximation using the kinetic equation approach. The results for collective correlation factors are compared with Monte Carlo simulation and are found to be in reasonably good agreement when the ratio of jump frequencies of regular site and antistructural atoms is of the order of 10^{-1} .

Introduction

Intermetallics having the B2 structure such as $M_{1-x}Al_x$ ($M=Fe, Co, Ni$) have a number of attractive properties that motivate their extensive use in industry. The advantages over other materials include higher specific strength as well as improved temperature and oxidation resistance [1]. Despite the simplicity of the intermetallic B2 structures [2], diffusion in these technologically promising alloys, which is generally believed to be diffusion via vacancies, is an intriguing subject since nearest-neighbour sites in these structures are jumps to antistructural sites, hence temporarily disturbing the local order, see, for example, the reviews [3,4]. A number of Monte Carlo simulations of general vacancy models such as the four-frequency model [5,6] and the Ising alloy model [7,8] have shown that the six-jump cycle (6JC) mechanism predominates in highly ordered structures existing at low temperatures and for compositions approaching stoichiometry.

The collective correlation factors f_{ij} [9] appear in combination in the expressions for vacancy-wind factors [10,11] occurring in the diffusion coefficients describing *collective* diffusion processes, for example, the inter-diffusion or chemical diffusion coefficient ($\tilde{D}$) and the intrinsic diffusion coefficients (D_A^I, D_B^I). Murch and Belova [7,11,12] have derived expressions for the

vacancy-wind factors r_A , r_B and S giving their relationship to collective and tracer correlation factors for B1/ B2 ordered alloys.

Using the path probability method [14], Wang and Akbar [13], have calculated the Onsager phenomenological coefficients L_{ij} [15] in the Ising alloy model for B1 and B2 structures. Qin and Allnatt [16] have used a matrix method for the calculation of the collective correlation factors via the collective cosines. Belova and Murch [6] have extended the Manning [17,18] formalism, well known for its description in random alloys, to intermetallic compounds and have given expressions [8] for diagonal and off-diagonal collective correlation factors, in the limit of perfect order, for B2 intermetallic compounds. Recently, Murch and Belova [8,20] have calculated phenomenological coefficients and collective correlation factors using, as an example, the Ising alloy model for non-stoichiometric B2 intermetallic compounds. They considered the antistructural atom as an 'impurity' and, making use of the 6JC as a fundamental diffusion unit, employed an analogue of the five-frequency model for impurity diffusion via vacancy jumps [21]. The results were in excellent agreement with Monte Carlo simulations.

In this paper, we have used a two-sublattice model of an ordered alloy where the correlation factors are partitioned into sublattice correlation factors (e.g., f_{AA} into f_{A1A1} and f_{A2A2} etc). We have calculated the collective correlation factors for nonstoichiometric B2 intermetallic compound using the six-jump-cycle (6JC) as a fundamental unit for the cycle involving atoms on regular sites and a two-jump-cycle (2JC) as a fundamental unit for the cycle involving an antistructural atom at one of the 110- type or 100-type sites. Correlation effects arising from the interference of the antistructural atoms are not taken into account. We have used a kinetic equation approach to describe the random diffusion of 6JC or 2JC as units by taking into account atoms on regular sites as well as antistructural atoms at 110- and 100-type sites.

Jump Frequencies for 6JC and 2JC

Considering the two-sublattice model of a B2 ordered alloy [6,22], we take sublattice-1 as the 'home' sublattice of atoms of kind B and sublattice-2 as the 'home' sublattice of atoms of kind A. We consider the four-frequency model where the jump frequency of atom B from sublattice-1 to sublattice-2 with the exchange with a vacancy is represented by $W_{B1} \equiv W_B^{1 \rightarrow 2}$. Similarly, we define $W_{B2} \equiv W_B^{2 \rightarrow 1}$, $W_{A1} \equiv W_A^{1 \rightarrow 2}$, $W_{A2} \equiv W_A^{2 \rightarrow 1}$. The site fractions C_{A1} , C_{A2} , C_{B1} and C_{B2} can be obtained easily in terms of the composition of A or B atoms and the jump frequencies [6,24]. For a fully ordered configuration, the average jump frequency of a single *isolated* 6JC can be calculated following the method of Arita *et al.* [23] and using the four-frequency model [6] as:

$$\nu_{B1} \equiv \nu_{A2} = \frac{\alpha^3 (3 + 6\alpha + 4\alpha^2)}{(288 + 1152\alpha + 2232\alpha^2 + 2325\alpha^3 + 1360\alpha^4 + 364\alpha^5 + 48\alpha^6 + 4\alpha^7)} \quad (1)$$

Here, W_{B1} and W_{A2} are the jump frequencies of atoms from the 'right' to 'wrong' sublattice, whereas W_{A1} and W_{B2} are the jump frequencies of atoms from the 'wrong' to 'right' sublattice. The ratio of the two is denoted as:

$$\alpha = \frac{W_{B1}}{W_{B2}} = \frac{W_{A2}}{W_{A1}} \quad (2)$$

When an antistructural atom itself is at a 110-type or 100-type site relative to the vacancy then, after the first two jumps of vacancy, the resulting configuration has the same energy as the initial one and the net displacement of the antistructural atom is non-zero. By its very nature, the frequency of this 2JC is much greater than that of the 6JC. The jump frequency for the [110]-2JC or

the [100]-2JC cycle involving two similar atoms can be taken to be the harmonic mean of the individual jump frequencies, say W_{A1} and W_{A2} of the two A atoms [22]. Thus we have that:

$$\nu_{A1} \equiv \nu_{B2} = \frac{2\alpha}{(1+\alpha)} \quad (3)$$

Phenomenological coefficients

Uncorrelated Phenomenological Coefficients. When collective diffusion is investigated by the 6JC or 2JC mechanism, diffusion on the two sublattices is independent of each other since a vacancy on a particular sublattice has no means of switching over to the other sublattice. Therefore, we shall calculate phenomenological coefficients for the sublattice-1 only.

In the 6JC mechanism, we have [110]-, [100]-straight and [100]-bent cycles for perfectly ordered configuration of B2 intermetallic compounds [23,25]. We consider that the jump frequencies for the regular site atom B1 for all the three kinds of cycles are equal and are given by ν_{B1} . In the linear-response approximation [15], the uncorrelated part of the phenomenological coefficient (considering all three types of 6JC) is then given by:

$$\begin{aligned} L_{B1B1}^{(0)} &= \frac{N}{6k_B T} (Z_1 S_1^2 + 2Z_0 S_0^2) C_{V1} C_{B1} \nu_{B1} \\ &= \left(\frac{6Na^2}{k_B T} \right) C_{V1} C_{B1} \nu_{B1} \end{aligned} \quad (4a)$$

The factor 2 in the second term is due to two types of [100] cycles- straight and bent. Here Z_1 is the coordination number for [110]-sites and Z_0 is the coordination number for [100]-sites; C_{V1} , C_{B1} denote site-fractions of vacancy and atoms of the B kind; $S_1 = \sqrt{2}a$ and $S_0 = a$ are the collective displacements on the completion of the [110]- and [100]-cycles; a is the cell length; N is the number of sites per unit volume; and k_B and T have their usual meanings.

For an antistructural A atom, two A atoms undergo nearest-neighbour displacements and the *collective* displacement of A atoms is again S_1 or S_0 when it is at 110-type or at 100-type sites respectively. Also, the 2JC frequency of the antistructured atom is the same whether it is at 110-type site or at 100-type site. Further, the 100-type displacement of the antistructural A atom can take place in *two* ways as compared to the 110-type displacement. Thus, the uncorrelated part of the phenomenological coefficient $L_{A1A1}^{(0)}$ can be written as:

$$L_{A1A1}^{(0)} = \left(\frac{6Na^2}{k_B T} \right) C_{V1} C_{A1} \nu_{A1} \quad (4b)$$

Furthermore,

$$L_{A1B1}^{(0)} = L_{B1A1}^{(0)} = 0 \quad (4c)$$

Correlated Phenomenological Coefficients. For the random diffusion of a vacancy through the 6JC or 2JC on sublattice-1, the regular site and antistructural atoms can be treated on the same footing except that they are displaced (through S_1 or S_0) with effective jump frequencies ν_{B1} and ν_{A1} respectively. It may be noted that whilst calculating the jump frequency of a single isolated 6JC, using the mean first passage concept of Arita *et al.* [23], the 110-type sites and 100-type sites are coupled together and the average 6JC frequency for the regular site atom (or 2JC for the

antistructural atom) is the same when it is at either of the two sites. This means that starting from a given initial configuration after time t the atom can be either at 110-type sites or at 100-type sites with respect to the vacancy. Thus, taking into account all the initial and final configurations, the correlated part of the phenomenological coefficients $L_{ijl}^{(1)}$ can be expressed as:

$$L_{ijl}^{(1)} = (1 - 2\delta_{ij}) \left(\frac{N v_{il} v_{jl}}{3k_B T} \right) \left[\sum_{S_1, S_1^0} S_1 \cdot S_1^0 \varphi(S_1 : S_1^0) + 2 \sum_{S_1, S_0^0} S_1 \cdot S_0^0 \varphi(S_1 : S_0^0) \right. \\ \left. + 2 \sum_{S_0, S_1^0} S_0 \cdot S_1^0 \varphi(S_0 : S_1^0) + 4 \sum_{S_0, S_0^0} S_0 \cdot S_0^0 \varphi(S_0 : S_0^0) \right] \quad (5)$$

where we have defined, for example:

$$\varphi(S_1 : S_0^0) = \int_0^\infty dt \sum_{\lambda} \psi_{V1A1:V1A1}(\lambda, \lambda - S_1; t; \lambda_0, \lambda_0 - S_0^0; t=0) \quad (6)$$

Here $\psi_{V1A1:V1A1}(\lambda, \lambda - S_1; t; \lambda_0, \lambda_0 - S_0^0; t=0)$ is the conditional probability of finding at time t the vacancy at site λ and A atom at its 110-type site $(\lambda - S_1)$ when initially the vacancy was at any site λ_0 and A atom at 100-type site $(\lambda_0 - S_0^0)$ on the same sublattice-1. In deriving Eq. 5, we have used the fact that at low vacancy compositions the nearest neighbour sites of a vacancy can either be occupied by an A atom or by a B atom. Then all probability functions containing B atoms can be changed to the probability functions containing A atoms only, resulting in Eq. 5.

Chaturvedi and Allnatt [26,27] and Sharma *et al.* [28,29] have shown that instead of solving the correlated part in real space it is much more convenient to work in Fourier space. For this purpose, we define the Fourier transform as:

$$\tilde{\varphi}(\mathbf{k} : \mathbf{S}^0) = \sum_{\mathbf{r}} e^{i\mathbf{k} \cdot \mathbf{r}} \varphi(\mathbf{r} : \mathbf{S}^0) \quad (7)$$

and express Eq. 5 as:

$$L_{ijl}^{(1)} = (1 - 2\delta_{ij}) \left(\frac{2Na^2}{k_B T} \right) v_{il} v_{jl} \left[4U'(:S_1^0) + 2U'(:S_0^0) + 2U(:S_1^0) + U(:S_0^0) \right] \quad (8)$$

where we have used symmetry of the integrals and fixed a particular value of the initial vectors S_1^0 and S_0^0 , say $S_1^0 = a(\hat{x} + \hat{y})$ and $S_0^0 = a\hat{x}$. The U-functions are defined as, for example:

$$U(:S_0^0) = 8i \left(\frac{a}{2\pi} \right)^3 \int d^3\mathbf{k} \sin k_x a \tilde{\varphi}(\mathbf{k} : S_0^0) \quad (9a)$$

$$U'(:S_1^0) = 8i \left(\frac{a}{2\pi} \right)^3 \int d^3\mathbf{k} \sin k_x a \cos k_y a \tilde{\varphi}(\mathbf{k} : S_1^0) \quad (9b)$$

Kinetic Equation

In order to know the probability functions ψ or φ , we use the kinetic equation approach. The function $\psi_{V1A1}(\lambda, \lambda - \mathbf{r})$ represents the conditional probability of finding at time t the vacancy at site λ and the atom A at site $(\lambda - \mathbf{r})$ on the same sublattice when the system was in a given initial state. The site $(\lambda - \mathbf{r})$ includes 110-type and 100-type sites (as only these sites are involved

in the 6JC or 2JC). Then considering the 6JC or 2JC as fundamental units for diffusion, the rate equation for the probability function $\psi_{V1A1}(\lambda, \lambda - \mathbf{r})$ can be written as:

$$\begin{aligned} \frac{d\psi_{V1A1}(\lambda, \lambda - \mathbf{r})}{dt} = & v_{A1} \{ \theta_1(\mathbf{r}) + 2\theta_0(\mathbf{r}) \} [\psi_{V1A1}(\lambda - \mathbf{r}, \lambda) - \psi_{V1A1}(\lambda, \lambda - \mathbf{r})] \\ & + \sum_p \nu_{p1} \sum_{\mathbf{r}' \neq \mathbf{r}} \{ \theta_1(\mathbf{r}') + 2\theta_0(\mathbf{r}') \} [\psi_{V1A1p1}(\lambda - \mathbf{r}', \lambda - \mathbf{r}, \lambda) - \psi_{V1A1p1}(\lambda, \lambda - \mathbf{r}, \lambda - \mathbf{r}')] \end{aligned} \quad (10)$$

Here $p = A, B$. $\theta_1(\mathbf{r})$ is the step function which is unity when $\mathbf{r} = \mathbf{S}_1$ and zero otherwise. Similarly, $\theta_0(\mathbf{r})$ is the step function which is unity when $\mathbf{r} = \mathbf{S}_0$ and zero otherwise. In the above, for convenience, we have omitted the initial conditions since they are the same for all the probability functions.

The kinetic equation (Eq. 10) can be put into closed form by a suitable approximation to the three-site probability functions. In the lowest order of approximation [30,31], we neglect the terms that are in second order in fluctuations in the occupancy variables for the atoms. Then add and subtract terms with $\mathbf{r}' = \mathbf{r}$, integrate with respect to t and sum over λ , we finally obtain:

$$\begin{aligned} - \sum_{\lambda} \psi_{V1A1}(\lambda, \lambda - \mathbf{r}; t = 0) = & \theta(\mathbf{r}) [v_1 \varphi(-\mathbf{r}) - (v_1 - v_{V1}) \varphi(\mathbf{r})] \\ & + C_{A1} (v_{A1} - v_{B1}) \sum_{\mathbf{r}'} \theta(\mathbf{r}') [\varphi(-\mathbf{r}') - \varphi(\mathbf{r}')] \\ & + v_{V1} \sum_{\mathbf{r}'} \theta(\mathbf{r}') [\varphi(\mathbf{r} - \mathbf{r}') - \varphi(\mathbf{r})] \end{aligned} \quad (11)$$

In the above, we have used the short notation:

$$\theta(\mathbf{r}) = \{ \theta_1(\mathbf{r}) + 2\theta_0(\mathbf{r}) \} \quad (12a)$$

and have defined the vacancy escape frequency as:

$$v_{V1} = C_{A1} v_{A1} + C_{B1} v_{B1} \quad (12b)$$

and

$$v_1 = C_{A1} v_{B1} + C_{B1} v_{A1} \quad (12c)$$

Now, multiply both sides of Eq. 11 by $e^{i\mathbf{k} \cdot \mathbf{r}}$ and summing over $\mathbf{r}$, we get:

$$\begin{aligned} \tilde{\varphi}(\mathbf{k}) = & \frac{1}{v_{V1} \{Z - \tilde{\theta}(\mathbf{k})\}} \left[\sum_{\lambda} \psi_{V1A1}(\lambda, \lambda - \mathbf{r}; t = 0) \right. \\ & \left. + \left(\frac{a}{2\pi} \right)^3 \int d^3 \mathbf{k}' \{ v_1 \tilde{\theta}(\mathbf{k} + \mathbf{k}') - (v_{V1} - v_1) \tilde{\theta}(\mathbf{k} - \mathbf{k}') \} \tilde{\varphi}(\mathbf{k}') \right] \end{aligned} \quad (13)$$

Here

$$\tilde{\theta}(\mathbf{k}) = \sum_{\mathbf{r}} e^{i\mathbf{k} \cdot \mathbf{r}} \theta(\mathbf{r}) \quad (14a)$$

and

$$Z = Z_1 + Z_0 \quad (14b)$$

In order to solve for U and U' , defined through Eqs. 9a and 9b, we first multiply Eq. 13 by $(8i \sin k_x a)$, and then integrate over k . With the use of symmetry of integrals this finally yield linear equations in U and U' for two initial configurations as:

$$a_1 U(:S_0^0) + a'_1 U'(:S_0^0) = -JC_{V1}C_{A1}C_{B1} \quad (15a)$$

$$a_1 U(:S_1^0) + a'_1 U'(:S_1^0) = -J'C_{V1}C_{A1}C_{B1} \quad (15b)$$

Here

$$a_1 = \left(1 - \frac{J}{2}\right)v_{V1} + v_1 J \quad (16a)$$

$$a'_1 = -(v_{V1} - 2v_1)J' \quad (16b)$$

The values of J and J' can be calculated from the following integral:

$$\left(\frac{a}{2\pi}\right)^3 \int d^3\mathbf{k} \frac{\sin^2 k_x a}{[Z - \tilde{\theta}(\mathbf{k})]} e(\mathbf{k}) \quad (17)$$

if we replace $e(\mathbf{k})$ by 1 and $\cos k_y a$ respectively. The values comes out to be $J=0.2416$ and $J'=0.0259$.

Similarly, we multiply Eq. 13 by $(8i \sin k_x a \cos k_y a)$ and integrate over k . This further yields two linear equations for U and U' as:

$$b_1 U(:S_0^0) + b'_1 U'(:S_0^0) = -J'C_{V1}C_{A1}C_{B1} \quad (18a)$$

$$b_1 U(:S_1^0) + b'_1 U'(:S_1^0) = -J''C_{V1}C_{A1}C_{B1} \quad (18b)$$

Here

$$b_1 = -\frac{1}{2}(v_{V1} - 2v_1)J' \quad (19a)$$

$$b'_1 = (1 - J'')v_{V1} + 2v_1 J'' \quad (19b)$$

The value of J'' can be calculated from Eq. 17 if we replace $e(\mathbf{k})$ by $\cos^2 k_y a$. This results $J''=0.1253$. From Eqs. 15 and 18 U and U' can be calculated for a given initial state. The resulting expressions when substituted in Eq. 8 yields:

$$L_{iljl}^{(1)} = (1 - 2\delta_{ij}) \left(\frac{2Na^2}{k_B T} \right) \frac{v_{il}v_{jl}C_{V1}C_{il}(1 - C_{il})}{(a_1 b'_1 - a'_1 b_1)} \times [(2J' + J)(b'_1 - 2b_1) - (2J'' + J')(a'_1 - 2a_1)] \quad (20)$$

The collective correlation factors for sublattice-1 are given by:

$$f_{A1A1} = 1 - \frac{v_{A1}C_{B1}}{3(a_1 b'_1 - a'_1 b_1)} [(2J' + J)(b'_1 - 2b_1) - (2J'' + J')(a'_1 - 2a_1)] \quad (21a)$$

$$f_{A1B1}^{(j)} = \frac{L_{A1B1}^{(1)}}{L_{j1j1}^{(0)}} = \frac{v_{A1}v_{B1}C_{A1}C_{B1}}{3(a_1 b'_1 - a'_1 b_1) v_{j1}C_{j1}} [(2J' + J)(b'_1 - 2b_1) - (2J'' + J')(a'_1 - 2a_1)] \quad (21b)$$

The expressions for f_{B1B1} and $f_{B1A1}^{(j)}$ can be obtained by interchanging A and B in Eqs. 21a and 21b. We see that $f_{A1B1}^{(j)} = f_{B1A1}^{(j)}$ satisfy the Onsager reciprocity theorem.

The collective correlation factors for sublattice-2 can be obtained by changing the subscript 1 with 2 in Eqs. 21a and 21b. The collective correlation factors for the intermetallic alloy are obtained by taking the harmonic mean of the partial correlation factors for the two sublattices, *i.e.*,

$$\frac{1}{f_{ij}^{(j)}} = \frac{1}{2} \left[\frac{1}{f_{i1j1}^{(j)}} + \frac{1}{f_{i2j2}^{(j)}} \right] \quad (22)$$

The superscript j is omitted when $i = j$.

Figure 1. Collective correlation factors f_{AA} , f_{BB} , $f_{AB}^{(A)}$, $f_{AB}^{(B)}$ as a function of A- atom composition C_A for $\alpha = 0.1$: (—) Calculated values, (* * *) Simulation results, (-----) Sandhu *et al.* [24].

Results and Discussion

In this paper, collective correlation factors in a nonstoichiometric B2 intermetallic compound have been derived through a kinetic equation approach and the 6JC and 2JC mechanisms for diffusion. At small deviations from stoichiometry, each antistructural atom is assumed to be isolated *i.e.* the correlation effects arising from the interference of the antistructural atoms are not taken into account. Using the 6JC for a perfectly ordered configuration and the 2JC for the cycle involving an antistructural atom at 110-type or 100-type sites relative to the vacancy, expressions for the partial phenomenological coefficients and collective correlation factors were derived for a given sublattice. The collective correlation factors are then obtained by taking the harmonic mean of the partial correlation factors for the two sublattices.

Figure 2. Collective correlation factors f_{AA} , f_{BB} , $f_{AB}^{(A)}$, $f_{AB}^{(B)}$ as a function of A-atom composition C_A for $\alpha = 0.08$: (—) Calculated values, (* * *) Simulation results, (-----) Sandhu *et al.* [24].

Figure 3. Collective correlation factors f_{AA} , f_{BB} , $f_{AB}^{(A)}$, $f_{AB}^{(B)}$ as a function of A-atom composition C_A for $\alpha = 0.06$: (—) Calculated values, (* * *) Simulation results, (-----) Sandhu *et al.* [24].

Figure 4. Collective correlation factors f_{AA} , f_{BB} , $f_{AB}^{(A)}$, $f_{AB}^{(B)}$ as a function of A-atom composition C_A for $\alpha = 0.04$: (—) Calculated values, * * *) Simulation results, (-----) Sandhu *et al.* [24].

The results for collective correlation factors are shown in Figs. 1-4 as a function of equilibrium composition of A atoms C_A at fixed values of the jump frequencies ratio α . These are compared with the results of Monte Carlo simulation and a previous calculation [24] based on random nearest-neighbour jumps of a vacancy on two sublattices. As compared to Sandhu *et al.* the present results show less variation with C_A and are in rather better agreement with the simulation data. The Monte Carlo simulations at and near stoichiometry were carried out by taking $W_{A1} = W_{B2} = 1$ and $W_{A2} = W_{B1} = \alpha$ for the values of $\alpha = 0.1, 0.08, 0.06, 0.04$. We can see that for $\alpha = 0.04$ (Fig. 4) in the nearest neighbour jump model, as C_A decreases f_{AA} tends towards negative and f_{BB} becomes larger whereas the present results show qualitative agreement with the simulation data. The cross correlation factors $f_{AB}^{(A)}$ and $f_{AB}^{(B)}$ are much smaller and are of the order of 10^{-2} . The results of Sandhu *et al.* [24] are in much better agreement with the simulation up to $\alpha = 0.08$. However, at $\alpha = 0.04$, our results are in close agreement with the simulation data but this could be fortuitous.

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Figure Captions.

Figure 1. Collective correlation factors f_{AA} , f_{BB} , $f_{AB}^{(A)}$, $f_{AB}^{(B)}$ as a function of A- atom composition C_A for $\alpha = 0.1$: (—) Calculated values, (* * *) Simulation results, (-----) Sandhu *et al.* [24].

Figure 2. Collective correlation factors f_{AA} , f_{BB} , $f_{AB}^{(A)}$, $f_{AB}^{(B)}$ as a function of A-atom composition C_A for $\alpha = 0.08$: (—) Calculated values, * * *) Simulation results, (-----) Sandhu *et al.* [24].

Figure 3. Collective correlation factors f_{AA} , f_{BB} , $f_{AB}^{(A)}$, $f_{AB}^{(B)}$ as a function of A-atom composition C_A for $\alpha = 0.06$: (—) Calculated values, * * *) Simulation results, (-----) Sandhu *et al.* [24].

Figure 4. Collective correlation factors f_{AA} , f_{BB} , $f_{AB}^{(A)}$, $f_{AB}^{(B)}$ as a function of A-atom composition C_A for $\alpha = 0.04$: (—) Calculated values, * * *) Simulation results, (-----) Sandhu *et al.* [24].

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