

## The effect of nonpair atomic interactions on the short-range order in disordered alloys

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**Abstract.** The high numerical accuracy of the recently developed (Chepulsii R V 1999 *J. Phys.: Condens. Matter* **11** 8645–60) generalized ring approximation for analytical description of the short-range order (SRO) in disordered alloys with many-body atomic interactions of arbitrary orders is revealed through comparison with the corresponding data of the Monte Carlo simulation. It is shown that this accuracy rises with an increase of the characteristic radius of atomic interactions. By the example of both the simplest model systems and Ni–V alloy, we demonstrate that, within the generalized ring approximation, it is possible to describe the phenomenon of the temperature dependence of a position in reciprocal space of the SRO Fourier transform's maximum at temperature independent atomic interactions. The analytical description of the effect of nonpair atomic interactions on the Fourier transform of the SRO parameters is performed in case of Ni–V alloy.

### 1. Introduction

In [1, 2], the following analytical approximations for calculation of the Fourier transform  $\alpha_k$  of the short-range order (SRO) Warren–Cowley parameters [3, 4] were obtained for the case of a two-component disordered (i.e. without a long-range order) alloy with many-body atomic interactions of arbitrary orders and radii of action, whose  $N$  sites form a Bravais crystal lattice:

(1) within the generalized spherical model approximation

$$\alpha_k = \left[ 1 + \frac{c(1-c)}{k_B T} (\mu + \tilde{V}_k^{\text{eff}}) \right]^{-1} \quad (1.1)$$

where

$$\tilde{V}_k^{\text{eff}} = \sum_{m=0}^{N-2} \frac{c^m}{m!} \tilde{V}_{k, \mathbf{0}, \mathbf{0}, \dots, \mathbf{0}}^{(2+m)} = \tilde{V}_k^{(2)} + c \tilde{V}_{k, \mathbf{0}}^{(3)} + \frac{c^2}{2} \tilde{V}_{k, \mathbf{0}, \mathbf{0}}^{(4)} + \dots \quad (1.2)$$

$c$  is the concentration,  $k_B$  is the Boltzmann constant,  $T$  is the absolute temperature,  $\tilde{V}_{k_1, k_2, \dots, k_{t-1}}^{(t)}$  is the Fourier transform of the mixing potential of  $t$ th order ( $t = 1, 2, \dots, N$ );

(2) within the generalized ring approximation

$$\alpha_k = \left[ 1 + \frac{c(1-c)}{k_B T} (\mu + \tilde{V}_k^{\text{eff}} + \tilde{V}_k^{\text{ring}}) \right]^{-1} \quad (1.3)$$

where

$$\tilde{V}_k^{\text{ring}} = \frac{1}{N} \sum_q \left\{ \frac{c(1-c)\phi_{q,k-k}^{(4)}/2 + (1-2c)\phi_{q,k-q}^{(3)} - \phi_q^{(2)}}{1 + \phi_q^{(2)}c(1-c)/(k_B T)} - \frac{[c(1-c)\phi_{q,k-q}^{(3)}]^2 + 2c(1-c)(1-2c)\phi_q^{(2)}\phi_{q,k-q}^{(3)} + (1-2c)^2\phi_q^{(2)}\phi_{k-q}^{(2)}}{2k_B T[1 + \phi_q^{(2)}c(1-c)/(k_B T)][1 + \phi_{k-q}^{(2)}c(1-c)/(k_B T)]} \right\} \quad (1.4)$$

and, taking account of only pair, triplet and quadruplet atomic interactions,

$$\phi_k^{(2)} = \mu + \tilde{V}_k^{\text{eff}} = \mu + V_k^{(2)} + cV_{k,0}^{(3)} + c^2/2V_{k,0,0}^{(4)} \quad (1.5)$$

$$\phi_{k_1,k_2}^{(3)} = V_{k_1,k_2}^{(3)} + cV_{k_1,k_2,0}^{(4)} \quad (1.6)$$

$$\phi_{k_1,k_2,k_3}^{(4)} = V_{k_1,k_2,k_3}^{(4)}. \quad (1.7)$$

$\mu$  is the quantity to be found from the equation of the following form common for both approximations (1.1) and (1.3)

$$N^{-1} \sum_q \alpha_q = 1 \quad (1.8)$$

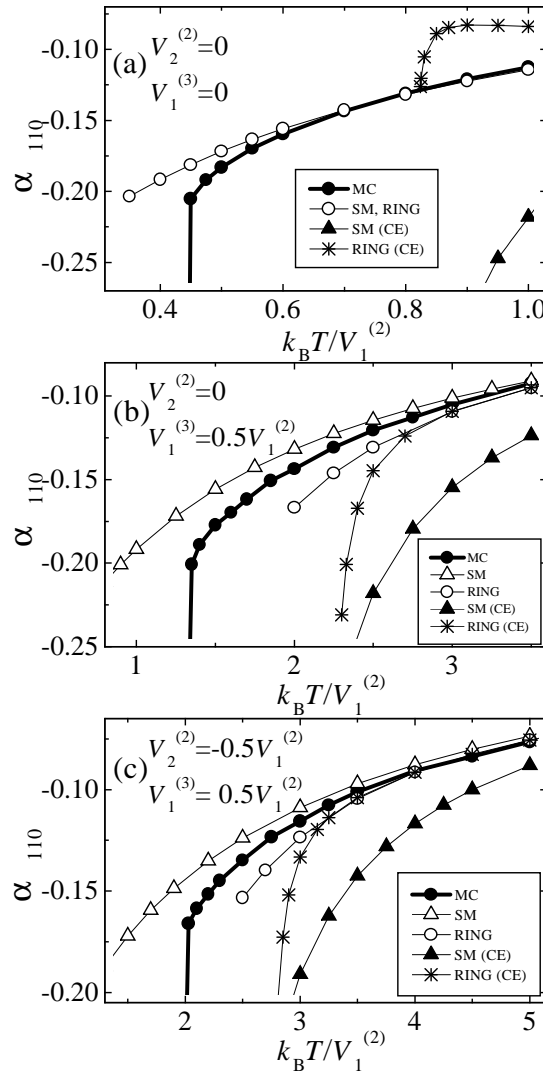
on substitution of the function  $\alpha_k$  corresponding to each approximation. The summations in (1.4) and (1.8) over the wave vectors  $q$  are carried over all points in the first Brillouin zone specified by the cyclic boundary conditions.

In [1], the high numerical accuracy of results of the generalized spherical model approximation in wide temperature and concentration intervals was revealed. However, from the corresponding expression (1.1), it is evident that, within this approximation, the position of the maximum of the function  $\alpha_k$  in reciprocal space coincides with the position of the minimum of the function  $\tilde{V}_k^{\text{eff}}$  at arbitrary values of concentration and temperature. Taking into account (1.2), one may conclude that, within the generalized spherical model approximation, it is impossible to describe the phenomenon of the temperature dependence of a position in reciprocal space of the SRO Fourier transform's maximum at temperature independent atomic interactions, which takes place in a number of alloys (see, e.g. [5–15]).

At the same time, from the corresponding expressions (1.3) and (1.4), it follows that, within the generalized ring approximation, the description of the denoted phenomenon is possible in principle. The aim of the present paper is a comparative study of the numerical accuracies of the generalized spherical model and ring approximations in the case of both the simplest model systems (section 2) and actual alloys for which the necessary information concerning atomic interactions is available (section 3). Our main interest concerns the qualitative adequacy of a description of the SRO Fourier transform within the generalized ring approximation, in particular, the possibility of realization of the above mentioned phenomenon within this approximation.

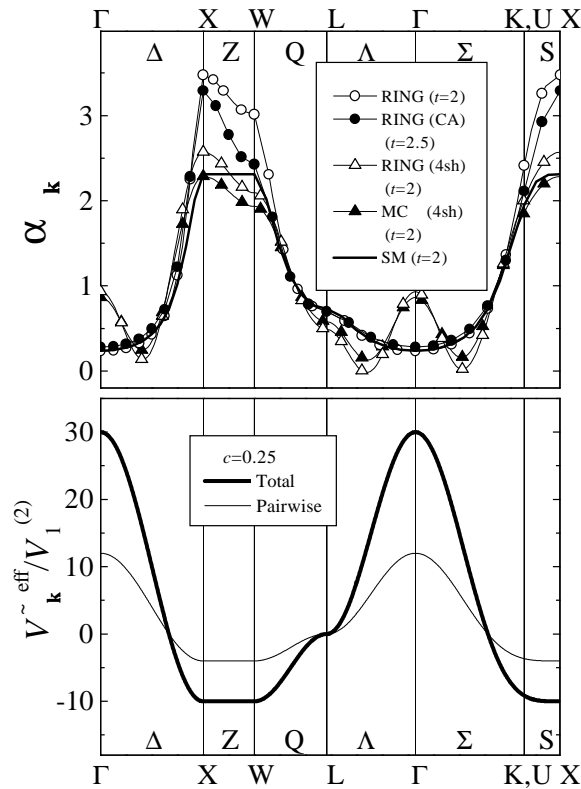
## 2. Case of model alloys

Firstly, we considered the same model alloys as in [1]. In all these alloys with the f.c.c. crystal lattice only the pair and triplet atomic interactions for the first one or two coordination shells are taking into account. In figure 1, the SRO data for the first coordination shell obtained by the Monte Carlo simulation [1] as well as within the generalized spherical model (1.1) and ring (1.3) approximations are shown in three cases all corresponding to  $c = 0.75$ . The choice of such concentration for presentation in figure 1 is not principal and corresponds to



**Figure 1.** The dependencies of the SRO parameter for the first coordination shell of the f.c.c. crystal lattice on the reduced temperature that were calculated through the Monte Carlo simulation (MC) as well as within the generalized spherical model (1.1) (SM) and ring (1.3) (RING) approximations at  $c = 0.75$ ,  $V_1^{(2)} > 0$  and (a)  $V_2^{(2)} = 0$ ,  $V_1^{(3)} = 0$ ; (b)  $V_2^{(2)} = 0$ ,  $V_1^{(3)} = 0.5V_1^{(2)}$ ; (c)  $V_2^{(2)} = -0.5V_1^{(2)}$ ,  $V_1^{(3)} = 0.5V_1^{(2)}$ , where  $V_s^{(n)}$  is the value of the mixing potential of  $n$ th order for the  $s$ th coordination shell. The values of the mixing potentials of the other orders and/or coordination shells than the above mentioned ones are identically equal to zero. The designation ‘CE’ corresponds to the use of the canonical ensemble instead of the grand canonical one.

the largest effect of nonpair atomic interactions on the SRO in this case [1]. The point of the order–disorder phase transition in figure 1 corresponds to the abrupt change of the temperature dependence of the SRO parameter obtained by the Monte Carlo simulation. Note that the values of the SRO parameter were not found within the generalized ring approximation below the values 2 and 2.5 of reduced temperature in the cases corresponding to figures 1(b) and 1(c), respectively, because the solving of the equation (1.8) at such temperatures requires significant computational efforts.



**Figure 2.** The dependencies (a) of the SRO Fourier transform  $\alpha_k$  calculated within the same approximations as in figure 1 at  $c = 0.75$ ,  $V_1^{(2)} > 0$ ,  $V_2^{(2)} = 0$ ,  $V_1^{(3)} = 0.5V_1^{(2)}$  and (b) of the reduced function  $\tilde{V}_k^{\text{eff}}$  at  $c = 0.75$ ,  $V_1^{(2)} > 0$ ,  $V_2^{(2)} = 0$  and both  $V_1^{(3)} = 0$  (Pairwise) and  $V_1^{(3)} = 0.5V_1^{(2)}$  (Total) with respect to the wave vector along the high-symmetry lines [18] in the corresponding first Brillouin zone. The designation ‘4sh’ means that the corresponding Fourier transform was calculated through the data on the SRO parameters for the first four coordination shells only. The designation ‘CE’ corresponds to the use of the canonical ensemble instead of the grand canonical one. The reduced temperature  $t = k_B T / V_1^{(2)}$ .

Accepting the results of the Monte Carlo simulation as a standard, on the basis of the data presented in figure 1, one may conclude the following. The numerical accuracies of both the generalized spherical model and ring approximations decreases when the triplet atomic interactions are taken into account (compare figures 1(a) and 1(b)). By contrast, the numerical accuracies of both these approximations have the opposite tendency if one considers them within the canonical ensemble instead of the grand canonical one (i.e. setting  $\mu$  equal to zero rather than to the solution of the equation (1.8) [2, 16, 17]). The numerical accuracies of all considered analytical approximations rise when the pair atomic interactions on the second coordination shell are taken into account (compare figures 1(b) and 1(c)).

In figure 2, we present the dependencies of the SRO Fourier transform  $\alpha_k$  calculated within the same approximations as in figure 1 with respect to the wave vector along the high-symmetry lines [18] in the corresponding first Brillouin zone in the case corresponding to figure 1(b). The same dependencies of the reduced function  $\tilde{V}_k^{\text{eff}}$  in two cases corresponding to figures 1(a) and 1(b) (i.e. taking and not taking into account the triplet atomic interactions, respectively) are

also shown in figure 2. Besides, in this figure, we include the Fourier transform  $\alpha_k$  obtained, taking into account the SRO parameters only for the first four coordination shells calculated within the generalized ring approximation, with the aim of a correct comparison with the Monte Carlo simulation data obtained in exactly the same manner.

It should be noted that, within the mean-field approximation, as follows from the corresponding expression for the critical temperature  $T_c$  of the order–disorder phase transition in alloy with only pair atomic interactions:

$$k_B T_c = -c(1 - c) \min_k \tilde{V}_k^{(2)} = -c(1 - c) \tilde{V}_{k_0}^{(2)} \quad (2.1)$$

one should investigate the minima of the Fourier transform  $\tilde{V}_k^{(2)}$  of the pair mixing potential, if one wants to find the instability wave vector  $k_0$  [19, 20]. Because the positions of the maxima of the Fourier transform  $\alpha_k$  of the SRO parameters correspond to the instability wave vectors when the temperature approaches its critical value, the above conclusion may be achieved from the following mean-field-like Krivoglaz–Clapp–Moss formula [21–26]

$$\alpha_k = A \left[ 1 + \frac{c(1 - c)}{k_B T} \tilde{V}_k^{(2)} \right]^{-1} \quad (2.2)$$

( $A$  is a normalization factor), within which the positions of the maxima of  $\alpha_k$  coincide with the positions of the minima of  $\tilde{V}_k^{(2)}$  in the reciprocal space at arbitrary values of the concentration and temperature.

In the case of the presence of nonpair atomic interactions in an alloy, the expressions

$$k_B T_c = -c(1 - c) \min_k \tilde{V}_k^{\text{eff}} = -c(1 - c) \tilde{V}_{k_0}^{\text{eff}} \quad (2.3)$$

[1] and (1.1) are the analogies of (2.1) and (2.2), respectively. Therefore, in this case, the function  $\tilde{V}_k^{\text{eff}}$  plays the role of  $\tilde{V}_k^{(2)}$ , and the minima of  $\tilde{V}_k^{\text{eff}}$  rather than of  $\tilde{V}_k^{(2)}$  should be investigated, if one wants to find the instability wave vectors within the mean-field approximation. Thus, in the corresponding figures of the present paper, we show not only the SRO Fourier transform  $\alpha_k$  but also the function  $\tilde{V}_k^{\text{eff}}$  in all considered cases. Note that the information concerning the topology of the function  $\tilde{V}_k^{\text{eff}}$  is also useful for prediction of a high temperature behaviour of the SRO Fourier transform, because, at high temperatures, the generalized spherical model approximation (1.1) demonstrates the high numerical accuracy of results (see figure 1 and [1]).

We shall call two wave vectors  $k_1$  and  $k_2$  energetically and/or statistically (within one or another approximation) equivalent if  $\tilde{V}_{k_1}^{\text{eff}} = \tilde{V}_{k_2}^{\text{eff}}$  and/or  $\alpha_{k_1} = \alpha_{k_2}$ , respectively. So, from the forms of the function  $\tilde{V}_k^{\text{eff}}$  shown in figure 2(b), it follows that all points belonging to the  $Z(0, 1, h)$  high-symmetry line in reciprocal space are energetically equivalent in both presented cases. (Here and below, we present the Cartesian coordinates of points in reciprocal space in units of  $2\pi/a$ , where  $a$  is the lattice parameter). Accordingly, as directly follows from (1.1), those points are also equivalent statistically within the generalized spherical model approximation (see, also, figure 2(a)). In contrast, within both the generalized ring approximation and Monte Carlo simulation the absolute maximum of the Fourier transform  $\alpha_k$  corresponds exclusively to the  $X(1, 0, 0)$  point.

Note that the account of only the first four coordination shells of the SRO parameters in calculation of the Fourier transform  $\alpha_k$  results in an artificial maximum of this Fourier transform at the point  $\Gamma(0, 0, 0)$  (compare curves RING, RING (4sh) and MC (4sh) in figure 2(a)).

### 3. Case of Ni–V alloy

Secondly, we considered the case of Ni–V alloy. The parameters of atomic interactions for this alloy were calculated by the Connolly–Williams method in [27] and are presented in table 1. By use of these parameters, the behaviour of the Fourier transform  $\alpha_k$  of the SRO parameters was investigated in Ni<sub>3</sub>V ( $c = 0.25$ ) and NiV ( $c = 0.50$ ) disordered alloys within the generalized spherical model (1.1) and ring (1.3) approximations. The obtained results are presented in figures 3–5.

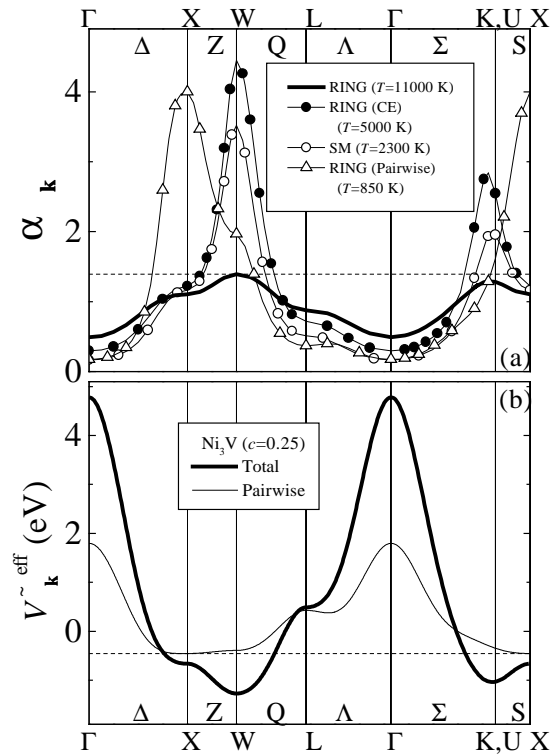
**Table 1.** The values of the mixing potentials  $V$  and  $J$  (see section 3 in [1]) in the case of Ni–V alloy calculated by the Connolly–Williams method in [27].  $n$  is the order of the mixing potential,  $s$  is the number of coordination shell corresponding (see section 4 in [1]) to the sites whose Cartesian coordinates (in units of  $a/2$ , where  $a$  is the lattice parameter) are presented in the third column ‘Sites’. All energy quantities are in units of meV. The values of  $J_s^{(n)}$  in the ‘Pairwise’ column correspond to a setting to zero of the values of both triplet and quadruplet  $J$  mixing potentials. Note that, in contrast to our presentation, the corresponding values of  $J_s^{(n)}$  presented in [27] are in units of meV/atom and include the degeneracy factor.

| $n$ | $s$ | Sites                      | $V_s^{(n)}$ | $J_s^{(n)}$ | $J_s^{(n)}$<br>(pairwise) |
|-----|-----|----------------------------|-------------|-------------|---------------------------|
| 2   | 1   | (000), (110)               | 747.7       | 25.3        | 25.3                      |
|     | 2   | (000), (200)               | 154.3       | –6.7        | –6.7                      |
|     | 3   | (000), (211)               | 11.8        | 4.9         | 4.9                       |
|     | 4   | (000), (220)               | 76.5        | 5.6         | 5.6                       |
| 3   | 1   | (000), (110), (101)        | –374.3      | –12.0       | 0                         |
|     | 2   | (000), (110), (200)        | –155.8      | 3.7         | 0                         |
|     | 3   | (000), (110), (211)        | 21.5        | 2.7         | 0                         |
|     | 4   | (000), (110), (220)        | –108.4      | –13.6       | 0                         |
|     | 5   | (000), (110), (002)        | –13.7       | –1.7        | 0                         |
| 4   | 1   | (000), (110), (101), (011) | 0           | 0           | 0                         |
|     | 2   | (000), (110), (101), (200) | 185.5       | 11.6        | 0                         |

From figures 3–5, it follows that, in the case of Ni<sub>3</sub>V ( $c = 0.25$ ) alloy, the account of nonpair atomic interactions results in the energy (i.e. from the point of view of the function  $\tilde{V}_k^{\text{eff}}$  (1.2)) favourability of the W(1,  $\frac{1}{2}$ , 0) point instead of the X(1, 0, 0) one. Accordingly, the SRO Fourier transform  $\alpha_k$  calculated within all the approximations considered has the absolute maximum at W(1,  $\frac{1}{2}$ , 0) and X(1, 0, 0) points when taking and not taking into account the nonpair atomic interactions, respectively. The obtained results are in agreement with those of the Monte Carlo simulation [28, 29].

In the case of NiV ( $c = 0.50$ ) alloy, the X(1, 0, 0) point is energy favourable, although the function  $\tilde{V}_k^{\text{eff}}$  (1.2) has very close values at X(1, 0, 0) and W(1,  $\frac{1}{2}$ , 0) points. Note that in this case (as in any case of  $c = 0.50$ ), the account of nonpair atomic interactions in terms of  $J$  mixing potentials has no effect on the function  $\tilde{V}_k^{\text{eff}}$  (see equation (3.5) in [1]) and, therefore, on the SRO Fourier transform  $\alpha_k$  calculated within the generalized spherical model (1.1) approximation as well. So, the SRO Fourier transform  $\alpha_k$  calculated within the denoted approximation has the absolute maximum at the X(1, 0, 0) point both taking and not taking into account the nonpair atomic interactions.

Within the generalized ring approximation, if one is not taking into account the nonpair atomic interactions in the case of NiV ( $c = 0.50$ ) alloy, one obtains the absolute maximum of the SRO Fourier transform  $\alpha_k$  at the X(1, 0, 0) point. However, when taking such interactions into account, the denoted maximum moves to the nonhigh-symmetry point belonging to the high-symmetry line  $\Sigma(h/\sqrt{2}, h/\sqrt{2}, 0)$ . The last result obtained within the generalized ring



**Figure 3.** The dependencies (a) of the SRO Fourier transform  $\alpha_k$  calculated within the generalized spherical model (1.1) (SM) and ring (1.3) (RING) approximations and (b) of the function  $\tilde{V}_k^{\text{eff}}$  with respect to the wave vector along the high-symmetry lines [18] in the corresponding first Brillouin zone in the case of  $\text{Ni}_3\text{V}$  ( $c = 0.25$ ) alloy. The designation ‘CE’ corresponds to the use of the canonical ensemble instead of the grand canonical one. The designations ‘Total’ and ‘Pairwise’ correspond to the use of the values of the mixing potentials shown in the fourth (or, equivalently, fifth) and sixth columns of table 1, respectively. The absence of both designations ‘Total’ and ‘Pairwise’ corresponds to the ‘Total’ case.

approximation is in agreement with that of the Monte Carlo simulation [28] and in contradiction to the above described result obtained within the generalized spherical model approximation.

In the case of  $c = 0.25$ , the results obtained both within the generalized spherical model and ring approximations as well as by the Monte Carlo simulation are in agreement with those of the diffuse scattering experiments [30]. Unfortunately, a similar comparison in the case of  $c = 0.50$  cannot be performed, because the corresponding experimental data seem to have not been published yet. Note that in [31] the experimental data on diffuse scattering intensity were successfully interpreted in terms of only *pair* atomic interactions by use of the inverse Monte Carlo method. However, this fact cannot be a proof of the absence of nonpair atomic interactions in the alloy, as demonstrated in [29]. This statement is also obvious from the expressions (1.1) and (1.2), from which it follows that the behaviour of the Fourier transform  $\alpha_k$  of the SRO parameters at high temperatures is determined by the effective pair potential  $\tilde{V}_k^{\text{eff}}$  even in the case of the presence of nonpair atomic interactions in the alloy.

It is the author’s opinion that the question of the presence of nonpair atomic interactions in Ni–V alloy still remains open. One may assume that the first way of resolving this question consists in the consideration of the superstructures with the *same* fixed stoichiometric composition within the Connolly–Williams [32, 33] method, because, in the opposite case,

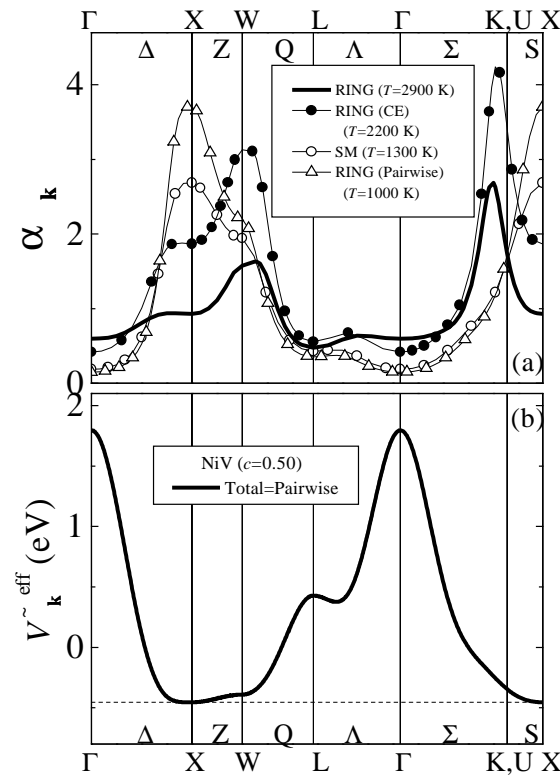
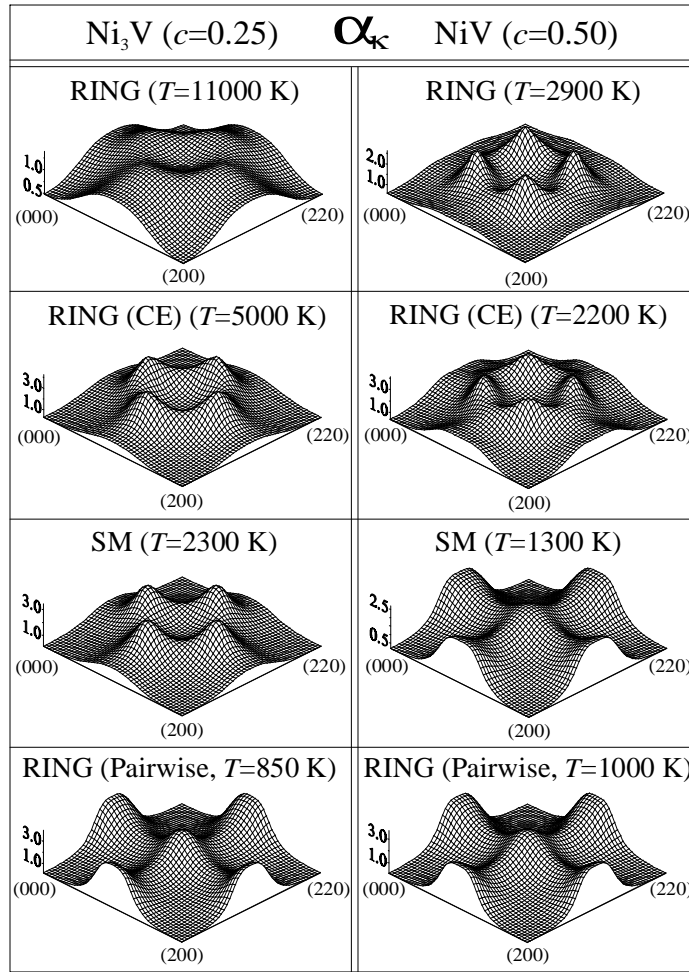


Figure 4. The same as in figure 3, but in the case of NiV ( $c = 0.50$ ) alloy.

the obtained nonpair atomic interactions in the alloy may be no more than the reflection of a concentrational dependence of pair interactions. Secondly, it is desirable to perform the direct estimation of the contribution from the nonpair atomic interactions to the alloy energy by use of the generalized perturbation method [34–37] as well as the mean-field concentration functional theory [38–41] (see also section 8 in [2]). Besides, it would be helpful to elaborate a direct method for extraction of the data on not only pair but also nonpair atomic correlations and interactions in alloy through the data on the diffuse scattering intensity [42] and apply this method in the cases of both  $\text{Ni}_3\text{V}$  and NiV alloys.

#### 4. Conclusions

On the basis of the results obtained in the present work, one may conclude that the description of the SRO Fourier transform in alloys with many-body atomic interactions of arbitrary orders is correct within the generalized ring approximation (1.3), whereas the application of the generalized spherical model (1.1) approximation in some cases may lead to qualitative error. (It seems likely that such cases are characterized by almost equal values of the function  $\tilde{V}_k^{\text{eff}}$  (1.2) in a wide vicinity of the absolute minimum of this function). Namely, within the generalized ring approximation (unlike the generalized spherical model one), it is possible to describe the phenomenon of the temperature dependence of a position in reciprocal space of the SRO Fourier transform's maximum at temperature independent atomic interactions. Note that the knowledge of the correct position of such maximum when the temperature approaches its



**Figure 5.** The same as in figures 3(a) and 4(a), but for the dependencies of the SRO Fourier transform  $\alpha_k$  with respect to the wave vector within the plane  $(h, k, 0)$ .

critical value is helpful for determination of the long-range order superstructure appearing as a result of the order–disorder phase transition, because the position of this maximum characterizes one such superstructure wave vector [19, 20].

In the present paper, it was also demonstrated that under the presence of nonpair atomic interactions in alloy, the correct description may be performed also within the generalized ring approximation elaborated within the canonical ensemble instead of the grand canonical one.

It should be noticed that, within the generalized spherical model and ring approximations, the effective radius of atomic interactions in alloy is not limited *a priori* (in contrast to the widely used Monte Carlo and cluster-variation methods), because only the Fourier transforms of the mixing potentials appear in the corresponding expressions (1.1)–(1.7). Moreover, it was revealed (see section 2) that the numerical accuracies of these approximations become higher with an increase of such effective radius. Thus, the generalized spherical model and ring approximations may be recommended for a description of actual alloys with a long-range character of atomic interactions caused, for example, by the strain-induced (elastic) effects. Note that, within the high-accuracy Tokar–Masanskii–Grishchenko approximation [43, 44]

based on application of the  $\gamma$ -expansion method [45], it is possible to take into account the long-range contributions of the *pair* interatomic potentials, whereas the nonpair atomic interactions are not taken into account within this approximation at all.

As shown in section 8 in [2], the generalized spherical model and ring approximations can be readily applied in combination with such widely used approaches for calculation of interatomic potentials in alloys as the generalized perturbation [34–37] and Connolly–Williams [32, 33] methods as well as the mean-field concentration functional theory [38–41].

The other important advantage of the generalized spherical model and ring approximations is the ability to calculate the Fourier transform of the SRO parameters directly, without neglecting the values of these parameters for coordination shells with large radius, as is done within the Monte Carlo and cluster-variation methods. This is especially important in the case of alloys with long-range atomic interactions and/or of alloys whose temperature is close to the order–disorder phase transition temperature (due to the corresponding increase of the effective radius of interatomic correlations). In the present paper, it was revealed that the above-mentioned neglect may result in a wrong description of the SRO Fourier transform in the vicinity of the origin of reciprocal space (see section 2). Within the generalized spherical model and ring approximations, through the integration of the SRO Fourier transform over the first Brillouin zone, it is possible to calculate the SRO parameter for an *arbitrary* given coordination shell as well.

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