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*Invited Speaker

ANALYTICAL DESCRIPTION OF THE SHORT-RANGE ORDER IN ALLOYS WITH MANY-BODY ATOMIC INTERACTIONS

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ABSTRACT

The high-accuracy ring approximation elaborated in [R. V. Chepulskii and V. N. Bugaev, J. Phys. Condens. Matter **10**, 7309; 7327 (1998)] by use of the thermodynamic fluctuation method in the context of the modified thermodynamic perturbation theory as applied to the lattice gas model is generalized for calculation of the short-range order (SRO) parameters and their Fourier transform in disordered binary alloys with many-body atomic interactions of arbitrary order and effective radius of action. On the basis of the comparison with the Monte Carlo simulation data, the numerical accuracy of the derived approximation is studied. It is demonstrated that the temperature dependence of a position in reciprocal space of the SRO Fourier transform's maximums is correctly described within this approximation.

INTRODUCTION

In [1], a number of analytical approximations were elaborated for calculation of the short-range order (SRO) parameters and their Fourier transform in disordered (i.e. without a long-range order) binary alloys with a Bravais crystal lattice and with many-body atomic interactions

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of arbitrary orders and effective radius of action. To achieve this aim, the Krivoglaz approach [2] based on application of the thermodynamic fluctuation method within the mean-field approximation was used. From the all obtained approximations, the generalized spherical model one yielded the highest numerical accuracy of results.

However, within the spherical model approximation it is impossible to describe the phenomenon of temperature dependence of a position in reciprocal space of the SRO Fourier transform's maximum in case of temperature independent atomic interactions. The presence of nonpair atomic interactions has no effect on this conclusion [1]. Thus, the use of this approximation is not adequate when the denoted phenomenon takes place, as, e.g., in Pd-V [3, 4], Cu-Au, Cu-Pd [5]-[9] as well as Pt-V [10]-[12] alloys and in a binary Madelung lattice [4, 13].

In case of *absence* of nonpair atomic interactions in alloy, the denoted temperature dependence can be correctly (see [4]) described using the ring approximation, derived by use of the thermodynamic fluctuation method within the first order of a modified thermodynamic perturbation theory under the choice of the inverse effective number of atoms interacting with one fixed atom as a small parameter of expansion [14, 15]. For such description to be correct also in case of alloys with nonpair atomic interactions (such as Cu-Au and Cu-Pd ones [5]-[7]), it seems to be useful to generalize the ring approximation to this case. The present paper is devoted to the performance of such generalization.

THEORY

In general, in the framework of the lattice gas model, the Hamiltonian H of a two-component A-B alloy with a Bravais crystal lattice and with many-body atomic interactions of arbitrary orders and radius of action can be written in the following form [1]

$$\begin{aligned} H &= N v_0 + \sum_{n=1}^{N} \tfrac{1}{n!} \sum_{\mathbf{R}_1,\mathbf{R}_2,\ldots,\mathbf{R}_n} V^{(n)}_{\mathbf{R}_1,\mathbf{R}_2,\ldots,\mathbf{R}_n} C_{\mathbf{R}_1} C_{\mathbf{R}_2} \ldots C_{\mathbf{R}_n} = \\ &= N v_0 + \sum_{\mathbf{R}} V^{(1)}_{\mathbf{R}} C_{\mathbf{R}} + \tfrac{1}{2} \sum_{\mathbf{R}_1,\mathbf{R}_2} V^{(2)}_{\mathbf{R}_1,\mathbf{R}_2} C_{\mathbf{R}_1} C_{\mathbf{R}_2} + \\ &\quad + \tfrac{1}{6} \sum_{\mathbf{R}_1,\mathbf{R}_2,\mathbf{R}_3} V^{(3)}_{\mathbf{R}_1,\mathbf{R}_2,\mathbf{R}_3} C_{\mathbf{R}_1} C_{\mathbf{R}_2} C_{\mathbf{R}_3} + \ldots . \end{aligned} \tag{1}$$

In Eq. (1): v_0 is the energy per site of "alloy" in which all N sites are occupied by B-type atoms, $V^{(n)}_{\mathbf{R}_1,\mathbf{R}_2,\ldots,\mathbf{R}_n}$ is the mixing potential of n-th order (n=1,2,...,N), $C_{\mathbf{R}}$ takes the values 1 or 0 depending on whether the site $\mathbf{R}$ is occupied by an A- or B-type atom, the summations on the vectors $\mathbf{R}, \mathbf{R}_1, \mathbf{R}_2, \ldots, \mathbf{R}_N$ are carried over all crystal lattice sites. The expression for the grand thermodynamic potential Ω of the system in