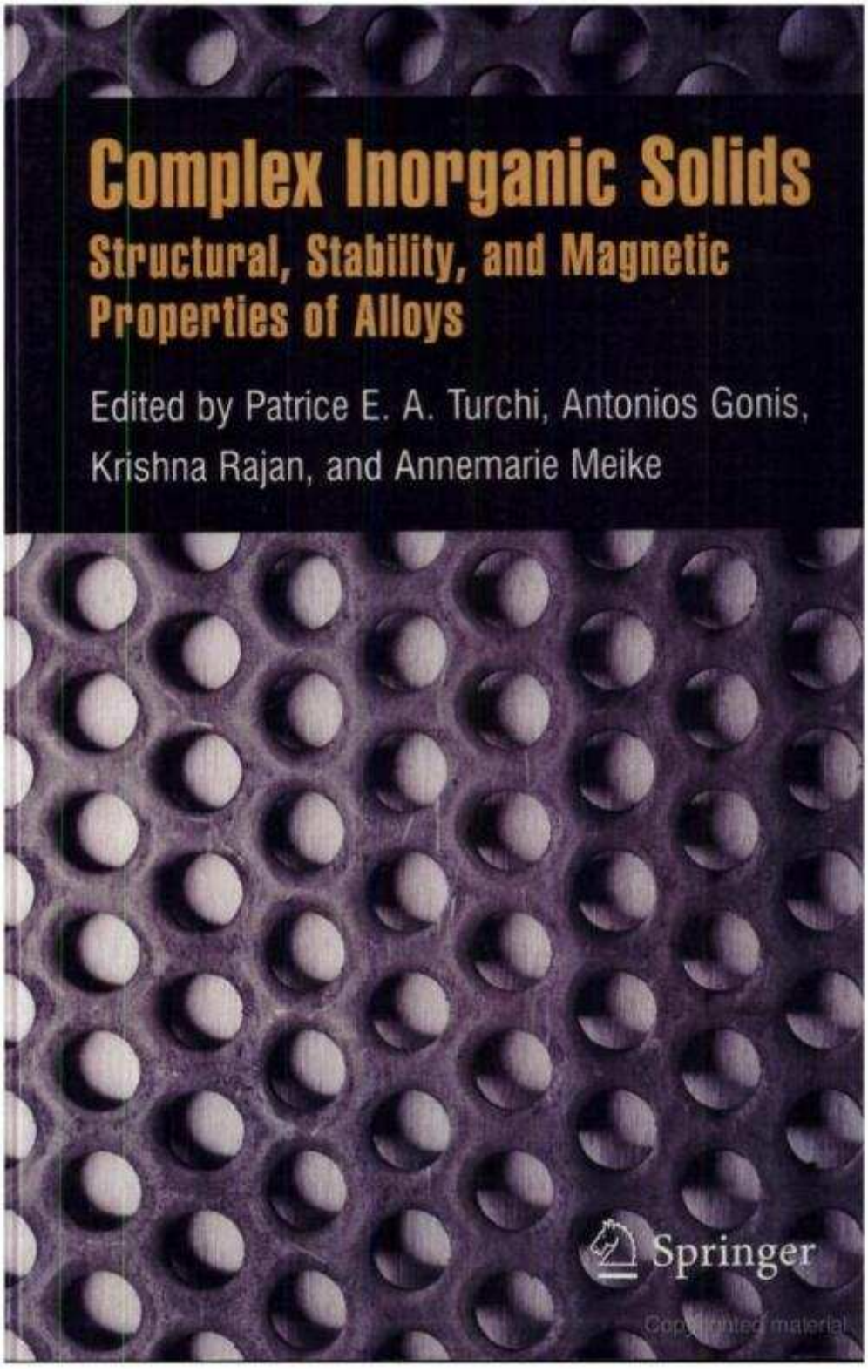
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CALCULATION OF THE PHASE DIAGRAMS OF ALLOYS WITH NONPAIR ATOMIC INTERACTIONS WITHIN THE RING APPROXIMATION

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ABSTRACT

The elaborated in [R. V. Chepulskii, Analytical method for calculation of the phase diagram of a two-component lattice gas, *Solid State Commun.* 115:497 (2000)] analytical method for calculation of the phase diagrams of alloys with *pair* atomic interactions is generalized to the case of many-body atomic interactions of arbitrary orders and effective radii of action. The method is developed within the ring approximation in the context of a modified thermodynamic perturbation theory with the use of the inverse effective number of atoms interacting with one fixed atom as a small parameter of expansion. By a comparison with the results of the Monte Carlo simulation, the high numerical accuracy of the generalized method is demonstrated in a wide concentration interval.

INTRODUCTION

In Ref. 1 the new analytical method for calculation of the phase diagrams of alloys (or more generally of a two-component lattice gas[2]) with arbitrary complex crystal lattice and any long-range order in atomic distribution was developed. The method was elaborated within the ring approximation in the context of a modified thermodynamic perturbation theory with the use of the inverse effective number of atoms interacting with one fixed atom as a small parameter of expansion[3,4]. The numerical accuracy of the method proved to be high in a wide temperature-concentration interval and turns higher with increase of the effective radius of atomic interactions. The consideration of the lattice gas with arbitrarily long-range atomic interactions is possible within the method, because the interaction's parameters appear in the corresponding expressions only through the Fourier transforms of the interatomic potentials. It should be noted the much comparative generality and simplicity of the method in comparison with, *e.g.*, the most widely used Monte Carlo[5] and cluster-variation methods[6].

However, the developed method can be applied in case of alloys with only *pair* atomic interactions. The aim of the present letter is to generalize the method to the case of alloys with many-body atomic interactions of arbitrary orders and effective radii of action.

THEORY

Let us consider a two-component A-B alloy (within the lattice gas model) whose primitive unit cell consists of ν crystal lattice sites. Taking into account the many-body atomic interactions of arbitrary orders and radii of action, the Hamiltonian H of it can be written in the following form[7]

$$\begin{aligned} H &= N\nu_0 + \sum_{n=1}^{N\nu} \frac{1}{n!} \sum_{i_1 i_2 \ldots i_n} \sum_{\mathbf{R}_1, \mathbf{R}_2, \ldots, \mathbf{R}_n} V^{(n)}_{i_1, \mathbf{R}_1 i_2, \mathbf{R}_2 \ldots i_n, \mathbf{R}_n} C_{i_1, \mathbf{R}_1} C_{i_2, \mathbf{R}_2} \ldots C_{i_n, \mathbf{R}_n} \\ &= N\nu_0 + \sum_i V^{(1)}_i \sum_{\mathbf{R}} C_{i, \mathbf{R}} + \frac{1}{2} \sum_{i_1 i_2} \sum_{\mathbf{R}_1, \mathbf{R}_2} V^{(2)}_{i_1, \mathbf{R}_1 i_2, \mathbf{R}_2} C_{i_1, \mathbf{R}_1} C_{i_2, \mathbf{R}_2} \\ &+ \frac{1}{6} \sum_{i_1 i_2 i_3} \sum_{\mathbf{R}_1, \mathbf{R}_2, \mathbf{R}_3} V^{(3)}_{i_1, \mathbf{R}_1 i_2, \mathbf{R}_2 i_3, \mathbf{R}_3} C_{i_1, \mathbf{R}_1} C_{i_2, \mathbf{R}_2} C_{i_3, \mathbf{R}_3} + \ldots . \end{aligned} \tag{1}$$