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Evaluation of the genetic algorithm performance for the optimization of the grand potential in the cluster variation method

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ABSTRACT

Due to the importance of phase diagrams in a wide range of material based industries, additional efforts should be dedicated to their elaboration techniques. The cluster variation method is a promising technique to model the entropy within different plane lattices and is recognized by the materials physics community as a powerful modeling framework. Motivated by the efficiency of genetic algorithms in solving numerous types of optimization problems, our aim in this work is to investigate their performance in minimizing the grand potential in the context of the cluster variation method. A comparison is conducted with respect to numerical iterative techniques namely the Newton-Raphson and natural iteration methods, where many performance criteria are computed and compared. The obtained results allow the ranking of the considered approaches according to their performance measures and suggest a more profound investigation of metaheuristics particularly for complicated cluster structures in the future.

1. Introduction

The tremendous development of fabrication processes has recognized nowadays a wide deployment of various materials. Such situation has motivated the boost of methodologies for the elaboration of phase diagrams associated to these materials, which allows later a deep understanding of the behavior in addition to different properties of the considered alloy [1–3]. The cluster variation method is a very efficient tool used not only in the computation procedure of alloy phase diagrams but also in many applications of materials science in connection to phase transitions. In fact, such method can be used with a satisfactory accuracy to calculate phase equilibrium configurations in solid solutions characterized by the nature of the involved phases, which varies only in the permutation of atoms and clusters at the level of the lattices sites [4–7].

The cluster variation method has been proposed initially by Kikuchi in a series of pioneering works as an approximate approach to model order-disorder phenomena by providing analytical formulations for the configuration entropy, internal and free energies of the system as a function of the cluster probability variables [8–11]. The choice of the basic cluster is generally guided by the support of maximum number of interactions, where the configuration phase equilibrium is established by the variation of the cluster probabilities (variation principle). The cluster variation method has shown to admit several previous models as special cases. Furthermore, this framework has been accredited due to its success in predicting the behavior and phase diagrams of numerous alloys [12–14]. In order to tackle the computation burdens, Kikuchi has introduced an effective algorithm known as natural iteration method to minimize the grand potential in terms of the cluster probabilities in the context of the cluster variation method [15,16]. The convergence of the natural iteration method has been proved by imposing a sufficient condition on the expansion factors of the cluster entropy, which is verified for a wide range of cluster geometries [17]. Another alternative to remedy the same problem has been proposed using the Newton-Raphson iterative method to solve the minimization problem with respect to the independent variables given by the correlation functions [18–20]. By focusing on both techniques, it is worth mentioning that the natural iteration method in almost all cases converges to a solution independently of the initial conditions except for some lattices for which the convergence rate is slow at the level of certain points. For example, the iterations number needed by the natural iteration method for convergence tends to infinity at the second-order phase transition point. Moreover, at the vicinity of a tricritical point, the natural iteration method convergence is very slow due to the small variation of energy between ordered and disordered phases. It should be mentioned that such convergence behavior of the method may be aggravated when large clusters or low temperatures are considered during the calculation of the cluster variation method [21–23]. Nevertheless, the initial

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solutions for the Newton-Raphson method are of crucial importance since they have an impact on the quality of the obtained solutions, especially with the existence of local optima leading hence to the limitation of the technique performance [24].

Nature inspired metaheuristics have emerged in the last decades as a successful contender to the existing conventional techniques built upon the concept of the gradient of a function or its higher derivatives such as the case of the iterative approaches [25]. Genetic algorithms belong to such class of frameworks and have approved their efficiency in dealing with a large number of sophisticated continuous and discreet optimization problems. The genetic algorithm is a population based technique, where a set of solutions is created using selection, crossover and mutation operators in analogy to the mechanisms of the natural selection. By evaluating the population individuals during the running of the algorithm, it is likely to get a solution that is as close as possible to the global optimal solution [26].

From a computational complexity viewpoint, the Newton-Raphson has a quadratic rate of convergence and it is very fast if the initial solution is not so far of the root. However, some drawbacks can arise such as oscillation or generation of negative values for the probability variables. The natural iteration method insures the convergence of the iteration procedure independently of the initial solution. However, this method is much slower than the Newton-Raphson technique and sometimes the converged state may not be the absolutely stable configuration since in general there are many local minima [27]. Because the genetic algorithm behavior depends on some stochastic operators, it is very difficult to provide compact formulas for time complexity. Only few case studies have been treated in literature where simplifying hypotheses are assumed [28–30].

Our objective in this work is to investigate the capacity of genetic algorithms in the optimization of the grand potential in terms of the correlation functions, which permits later the determination of the mole fractions of different elements in the binary alloy. The motivation behind the choice of such algorithm resides in its gradient free nature in comparison to other conventional iterative techniques like the well-known Newton-Raphson method. Therefore, there is a low probability of being trapped in local optima for the genetic algorithms due to their global exploration of the solution space in addition to the use of several genetic operators. The assessment of the proposed genetic algorithm shows that the probability of such approach for being altered by a convergence drawback is really negligible in comparison to the Newton-Raphson or the natural iteration methods. Furthermore, the calculation of statistical measures indicates that both genetic algorithm and natural iteration method are robust against the selection of the initial solutions.

2. Grand potential modeling using the cluster variation method

In the cluster variation method, a basic cluster including all atomic interactions is defined as a geometric shape with a fixed number of atoms. In the present work, the regular tetrahedron approximation of the cluster variation method in face centered cubic (fcc) lattice is considered the basic cluster as indicated by Fig. 1. Throughout the remaining of this paper, we adopt the Strukturbericht notation for specifying the crystal lattice structure.

The main modeling stages of the grand potential using the cluster variation method are showcased in the following passages. For more detailed developments, interested readers can refer to [31–34].

For the A1 disordered phase, the weight factor denoted g is given by the following formula:

$$g = \left(N! \left[\prod_{ij} (NY_{ij})\ ! \right]^6 \right) \Big/ \left(\left[\prod_{ijkl} (NW_{ijkl})\ ! \right]^2 \left[\prod_{i} (NX_i)\ ! \right]^5 \right) \tag{1}$$

with N represents the number of the lattice positions, X_i denotes the probability of having an atom i on a lattice point, Y_{ij} expresses the probability of locating the atoms i and j on a pair of adjacent sites, W_{ijkl} is the probability to get the atoms i, j, k, and l on the tetrahedron cluster. It should be mentioned that these probabilities are related by the reduction formulas:

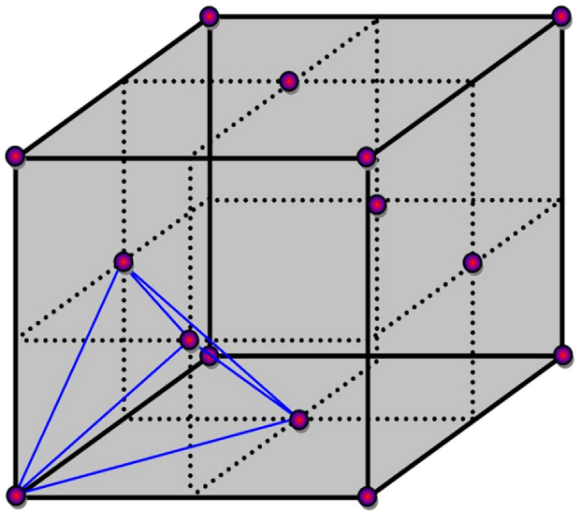

Fig. 1. Illustration of the regular tetrahedron cluster in the face centered cubic lattice.

$$\begin{cases} X_i = \sum_{jkl} W_{ijkl} \\ Y_{ij} = \sum_{kl} W_{ijkl} \end{cases} \tag{2}$$

The configuration entropy in the framework of the cluster variation formalism is specified by multiplying the Boltzmann constant ($k_B = 1.380664 \times 10^{-23}$) with the logarithm of the weight factor:

$$S_{CVM} = k_B \ln(g) \tag{3}$$

Therefore, the configuration entropy associated to the A1disordered phase is:

$$S_{A1} = Nk_B \left[-2 \sum_{ijkl} W_{ijkl} \ln(W_{ijkl}) + 6 \sum_{ij} Y_{ij} \ln(Y_{ij}) - 5 \sum_{i} X_i \ln(X_i) \right] \tag{4}$$

Since a face centered cubic crystal including N lattice points have a total number of $2N$ tetrahedra, the internal energy can be expressed in this case by:

$$U = 2N \sum_{ijkl} W_{ijkl}^{\alpha\beta\gamma\delta} \varepsilon_{ijkl}^{\alpha\beta\gamma\delta} \tag{5}$$

where α, β, γ and δ reflect the lattice locations, $\varepsilon_{ijkl}^{\alpha\beta\gamma\delta}$ is the energy per tetrahedron, which can be written as a function of the pair interactions $\varepsilon_{ij}^{\alpha\beta}$ as:

$$\varepsilon_{ijkl}^{\alpha\beta\gamma\delta} = \frac{1}{2} (\varepsilon_{ij}^{\alpha\beta} + \varepsilon_{ik}^{\alpha\gamma} + \varepsilon_{il}^{\alpha\delta} + \varepsilon_{jk}^{\beta\gamma} + \varepsilon_{jl}^{\beta\delta} + \varepsilon_{kl}^{\gamma\delta}) \tag{6}$$

Accordingly, the Helmholtz free energy can be developed as:

$$F = U - TS \tag{7}$$

Hence, we deduce the grand potential provided by the relation:

$$\Omega = F - \sum_{i} \mu_i^* x_i \tag{8}$$

subject to the condition ($\sum_i \mu_i^* = 0$), which relates the effective chemical potentials associated to elements i.

3. Minimization of the grand potential

In what follows, we consider the mathematical formulation of the minimization problem of the grand potential in terms of the correlation