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Enhanced calculation of eigen-stress field and elastic energy in atomistic interdiffusion of alloys

José M. Cecilia [a], A.M. Hernández-Díaz [a,*,1], Pedro Castrillo [a], J.F. Jiménez-Alonso [b]

[a] Escuela politécnica superior, Universidad Católica de Murcia (UCAM), Spain

[b] Escuela superior de ingeníeros, Universidad de Sevilla, Spain

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ABSTRACT

The structural evolution of alloys is affected by the elastic energy associated to eigen-stress fields. However, efficient calculations of the elastic energy in evolving geometries are actually a great challenge in promising atomistic simulation techniques such as Kinetic Monte Carlo (KMC) methods. In this paper, we report two complementary algorithms to calculate the eigen-stress field by linear superposition (a.k.a. LSA, Lineal Superposition Algorithm) and the elastic energy modification in atomistic interdiffusion of alloys (the Atom Exchange Elastic Energy Evaluation (AE^4) Algorithm). LSA is shown to be appropriated for fast incremental stress calculation in highly nanostructured materials, whereas AE^4 provides the required input for KMC and, additionally, it can be used to evaluate the accuracy of the eigen-stress field calculated by LSA. Consequently, they are suitable to be used on-the-fly with KMC. Both algorithms are massively parallel by their definition and thus well-suited for their parallelization on modern Graphics Processing Units (GPUs). Our computational studies confirm that we can obtain significant improvements compared to conventional Finite Element Methods, and the utilization of GPUs opens up new possibilities for the development of these methods in atomistic simulation of materials.

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1. Introduction

Eigen-stress fields are generated by the matching conditions of different constituents in material systems [1,2]. In particular, inhomogeneous crystal alloys with composition-dependent lattice parameter are subjected to intrinsic eigen-stress fields, which depend on the spatial composition distribution. This distribution could be rather complex in some cases, such as spinodal decomposed metal alloys [3] or alloy-based nanostructured semiconductors [4].

Predictive simulation of the time-evolution of material nanostructure is critical in certain scenarios such as structural steels in nuclear plants [5] or state-of-the-art integrated circuits during front-end processing [6]. Such evolution is affected by the elastic energy associated to eigen-stress fields [7,8]. However, efficient calculations of the elastic energy in evolving geometries are actually a great challenge for promising simulation techniques such as Kinetic Monte Carlo (KMC) methods [9,10]. In most cases, numerical solutions to this problem have been proposed by using Finite Element Methods (FEM) [11,12]. Nevertheless, the use of both KMC methods and on-the-fly FEM calculations is nowadays computationally prohibitive. Indeed, FEM represents an approach for the solution of a weak form and, hence, any modification of the system configuration implies the whole resolution of the resulting new algebraic system of equations [13]. Consequently, the process would be too time-consuming for estimating the "instantaneous" eigen-stress field in evolving systems.

Eigen-stress fields may be also approximated in the context of the linear elastic theory within the small strain limit [14]. Within this framework, the final configuration coincides with the reference configuration (small displacement hypothesis) and the strain is linear with stress [14]. Therefore, superposition can be applied. In this work, we propose an algorithm based on the superposition of the eigen-stress fields associated to elementary contributions. Within the same context, the elastic energy modifications associated to atom-scale changes can be also estimated from stress field modifications. Our proposal offers several advantages compared to previous approaches [7,11,12,15,16]:

1. It allows incremental calculation of the stress field taking into account only local modifications of the alloy structure. This means higher computational efficiency.

* Corresponding author.
E-mail addresses: jmcecilia@ucam.edu (J.M. Cecilia), amhernandez@ucam.edu (A.M. Hernández-Díaz), pcastrillo@ucam.edu (P. Castrillo), jfjimenez@us.es (J.F. Jiménez-Alonso).

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2. The balance between accuracy and efficiency can be tuned by choosing the truncation radius for superposition.
3. It is massively parallel by its definition and, therefore, an additional performance gain can be obtained by using parallel processors.

These advantages together offer a great opportunity to have a very efficient algorithm to calculate the elastic energy modifications related to atomistic diffusion events, which are an input to the KMC algorithm for every attempt of interdiffusion event (i.e. after every few Monte Carlo steps).

The paper is structured as follows. After this introduction, Section 2 describes the underlying linear superposition model and the method to calculate the energy modifications associated with the eigen-stress. Based on this model, Section 3 shows the corresponding algorithms and their parallelization on modern processors, whereas Section 4 shows the performance and quality evaluation of our algorithm. Finally, we outline the conclusions and some directions for future work.

2. Model

Let us consider an $A_{1-X}B_X$ binary alloy with orthotropic crystal structure, where X is the molar fraction of B atoms, which is a dimensionless measure of alloy composition. Assuming a linear dependence of lattice parameter a with alloy composition (Vegard's law), the lattice parameter can be expressed as:

$$a(X) = a(0) + (a(1) - a(0))X, \tag{1}$$

where a(0) and a(1) are the lattice parameters of the pure constituents of the alloy. The maximum lattice mismatch in the alloy is $\epsilon_{max} = (a(1) - a(0))/a(0.5)$. The spatial composition dependence is accounted dividing the simulation domain into a nanometer-sized uniform cubic mesh. We denote by $\mathbf{n} = (n_x, n_y, n_z)$ the vector index of each mesh element, with n_x, n_y, n_z being integer numbers. Within an atomistic framework, each mesh element has an integer number of alloy atoms, $N_{at} \simeq C_{at}\Omega$, where C_{at} is the atom density of the alloy and Ω is the volume of each mesh element. Likewise, it verifies $N_{at} = N_A + N_B$, with $X = N_B/N_{at}$, where N_A and N_B are, respectively, the integer number of A and B atoms in each mesh element. If moderated lattice mismatch ($|\epsilon_{max}| \ll 1$) and low defect concentration are assumed, N_{at} can be approximated to be constant in all mesh elements. Usual mesh spacing for atomistic simulations are within the nanometer scale and N_{at} is typically ranging from few tens to several hundreds.

In this context, the minimum composition variation in an element will be given by:

$$\delta X = \frac{1}{N_{at}}, \tag{2}$$

and, thus, the elementary eigen-expansion ratio, related to a composition change of δX will be:

$$\delta\epsilon = \frac{\epsilon_{max}}{N_{at}}. \tag{3}$$

Let us consider now the tensor stress field $\delta\bar{\bar{\sigma}}(\mathbf{n})$ generated by an elementary eigen-expansion $\delta\epsilon$ in the reference mesh-element located at (0, 0, 0) over an infinite (and otherwise unstressed and homogeneous) domain. We will refer to $\delta\bar{\bar{\sigma}}(\mathbf{n})$ as elementary stress field. An analytic solution for $\delta\bar{\bar{\sigma}}(\mathbf{n})$ could be found if the expanded element would have spherical geometry and the material would be isotropic. However, no analytic solution is available in our case, where the expanded mesh element is cubic (instead of spherical) and the material is orthotropic (instead of isotropic). Alternatively, a numerical estimation of $\delta\bar{\bar{\sigma}}(\mathbf{n})$ can be obtained using FEM. Notice that the magnitude of the components of the elementary stress tensor $\delta\bar{\bar{\sigma}}(\mathbf{n})$ are inversely proportional to the mesh element volume Ω. Hence, the product $\Omega\delta\bar{\bar{\sigma}}(\mathbf{n})$ is independent on the mesh spacing and it could be estimated "once and forever" for each material.

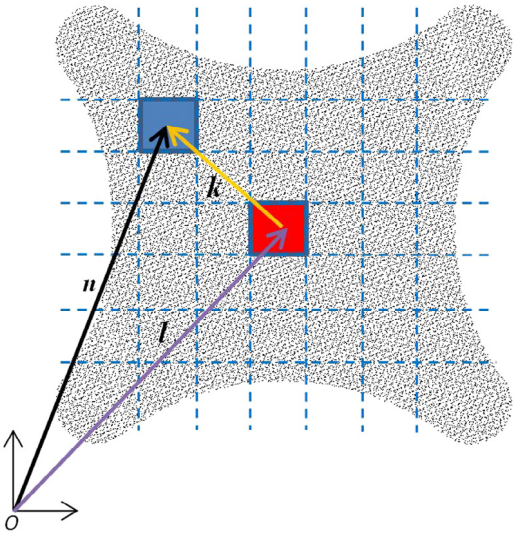

Fig. 1. Schematics of the contribution to the stress $\bar{\bar{\sigma}}$ in a mesh element $\boldsymbol{n}$, induced by an elementary composition variation δX at mesh element $\boldsymbol{l}$. The shadowed region symbolizes the orthotropic stress-field $\delta\bar{\bar{\sigma}}$ related to this δX. The local contribution on element $\boldsymbol{n}$ depends on the relative position vector $\boldsymbol{k} = \boldsymbol{n} - \boldsymbol{l}$.

Consequently, for a non-uniform $X(\mathbf{n})$ alloy composition, the total eigen-stress field $\bar{\bar{\sigma}}(\mathbf{n})$ may be expressed, considering elastic linear superposition, as (see Fig. 1):

$$\bar{\bar{\sigma}}(\boldsymbol{n}) = \sum_{\boldsymbol{l}} \frac{X(\boldsymbol{l}) - \langle X\rangle}{\delta X}\delta\bar{\bar{\sigma}}(\boldsymbol{n} - \boldsymbol{l}). \tag{4}$$

Eq. (4) accounts for the contribution of mesh element $\boldsymbol{l}$ on the stress field at the mesh element $\boldsymbol{n}$. In this sense, $\boldsymbol{n}-\boldsymbol{l}$ represents the vector index of each element relative to the location of the elementary expansion (Fig. 1). Denoting $\langle X\rangle$ the average alloy composition of the system, the magnitude of the eigen-stress field due to element $\boldsymbol{l}$ is proportional to the difference $X(\boldsymbol{l}) - \langle X\rangle$. Under the above mentioned assumptions (and in absence of applied external forces), a mesh element with alloy composition equal to $\langle X\rangle$ does not contribute to the stress field. Since we consider a bulk material, periodic boundary conditions are appropriate and, hence, cyclic values are adopted for the vector $\boldsymbol{n} - \boldsymbol{l}$ in terms of the considered domain.

If the faraway elementary contributions could be neglected, the sum in Eq. (4) may be truncated to small values of $||\boldsymbol{n} - \boldsymbol{l}||$, with $||\,||$ being a norm of the integer vector. For convenience, the relative vector index $\boldsymbol{k} = \boldsymbol{n} - \boldsymbol{l}$ can be adopted (see Fig. 1) and, then, Eq. (4) can be rewritten as:

$$\bar{\bar{\sigma}}(\boldsymbol{n}) = \sum_{\substack{\boldsymbol{k}\\ ||\boldsymbol{k}||\le k_{max}}} \frac{X(\boldsymbol{n} - \boldsymbol{k}) - \langle X\rangle}{\delta X}\delta\bar{\bar{\sigma}}(\boldsymbol{k}). \tag{5}$$

For simplicity, the norm we use is $||\boldsymbol{k}|| = max\{|k_x|, |k_y|, |k_z|\}$. Therefore, the condition $||\boldsymbol{k}|| \le k_{max}$ corresponds to a cube with $(2k_{max}+1)^3$ mesh elements. Notice that, in previous equations, the elementary stress tensor $\delta\bar{\bar{\sigma}}(\mathbf{k})$ represents an input of the model and it can be extracted from the previously calculated $\Omega\delta\bar{\bar{\sigma}}(\mathbf{k})$.

Crystal alloy evolution is known to be driven by mobile native defects [17]. Assuming low defect concentration, alloy interdiffusion and precipitation have been modeled as a sequence of defect-driven exchanges of pairs of A–B atoms of neighboring mesh elements [18,19]. A great computational advantage of the

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