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Parallel kinetic Monte Carlo simulation of Al_3Sc precipitation

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Abstract

The present paper reports the precipitation process of Al_3Sc structures in an aluminum scandium alloy, which has been simulated with a synchronous parallel kinetic Monte Carlo (spkMC) algorithm. The spkMC implementation is based on the vacancy diffusion mechanism. To filter the raw data generated by the spkMC simulations, the density-based clustering with noise (DBSCAN) method has been employed. spkMC and DBSCAN algorithms were implemented in the C language and using MPI library. The simulations were conducted in the SeARCH cluster located at the University of Minho. The Al_3Sc precipitation was successfully simulated at the atomistic scale with spkMC. DBSCAN proved to be a valuable aid to identify the precipitates by performing a cluster analysis of the simulation results. The achieved simulations results are in good agreement with those reported in the literature under sequential kinetic Monte Carlo simulations (kMC). The parallel implementation of kMC has provided a 4x speedup over the sequential version.

Keywords: Al_3Sc precipitation; vacancy diffusion; kinetic Monte Carlo; spkMC; MPI.

1. Introduction

In material sciences, precipitated structures acquire a fundamental role due to the ability of imposing enormous obstacles for dislocation movements within the material structure. The knowledge and application of statistical mechanics, namely the kinetic Monte Carlo method (kMC) [1], will be the prime focus of this paper. kMC will be applied in studying the precipitation phenomenon on an aluminum scandium alloy [2]. The documented work, tackles kMC focusing on parallelism, synchronization between processes, and communication with message passing interface (MPI).

The outcome is a set of software applications that allows us (i) to run kMC simulations on a single or multiple processors, (ii) to apply Density Based Spatial Clustering of Applications with Noise (DBSCAN) technique for data mining outputs [3], and (iii) to perform a comparison between the results obtained with the MC simulations and the values predicted by classical nucleation theory (CNT). The practical results of these applications are (i) simulation reports, (ii) DBSCAN reports about clusters and precipitates, (iii) files for 3D visualization of the simulation (at various simulation stages - snapshots), and (iv) files for 3D visualization of the precipitates.

Therefore the main contributions of the present work to the reviewed literature are, besides the mentioned applications, an accelerated simulation algorithm through the parallelization of kMC with MPI.

2. Background and motivation

The constant increase in available computational resources has been accompanied by a growing interest in modeling and simulation of precipitation at different scales, each one with its own advantages. The number of publications and studies related to the topic of precipitation kinetics at the atomic level has increased too [4]. Examples of materials subjected to such studies are alloy materials, such as Fe-Cu [5], Fe-P-C [6], Fe-Cu-Ni-Si [7], Al-Cu [8]. Aluminum alloys

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have also their share of published studies and our contribution will focus on the study of an Al-Sc alloy.
The literature has documented the enormous potential of the addition of scandium to aluminum alloys for the use mainly in aerospace and automotive applications as it benefits the alloy in recrystallization inhibition, strength increase, grain size refinement as well as the reduction and elimination of hot cracking in welding [9].
Monte Carlo (MC) simulations have also been used on the study of other phenomena [10], such as grain growth [11], abnormal grain growth [12], thin film deposition and growth [13][14], sintering for nuclear fuel aging [15], and bubble formation in nuclear fuels [16].
There are also several published works on parallel kinetic MC simulations, namely the works reported in [17], [18], [19], [20], [21], [22], and [23].

3. kMC and spkMC theoretical background

The simulation of Al_3Sc precipitation with sequential kMC is fully documented in [2], therefore, this section summarizes the theory as a set of equations, behind the simulation. The transition rate for an *XY* atom to jump into a vacancy, with $XY \in \{Al,Sc\}$, is calculated by Eq. 1.

$$\Gamma_{XY\_V} = \nu_{XY}\, exp\left(-\frac{\Delta E_{XY\_V}}{k_B T}\right) \quad (1)$$

The Al and Sc energy increase, due to the motion from its stable site to the saddle point position, is designated activation energy and is obtained by Eq. 2.

$$\Delta E_{XY\_V} = e_{XY}^{sp} - \sum_{i,n} \varepsilon_{XY\_i}^{(n)} - \sum_{j,n} \varepsilon_{j\_V}^{(n)} \quad (2)$$

As a vacancy site is surrounded by twelve nearest neighbors, twelve jump rates are calculated. They are the jump frequencies Γ_1, Γ_2, until Γ_{12}. One of the twelve frequencies is selected, based on their values and on a random number as expressed by Eq. 3.

$$\sum_{i=1}^{n} \Gamma_i \leq random\ number \leq \sum_{i=1}^{n+1} \Gamma_i \quad (3)$$

Eq. 4 describes the computation of the simulation real time. C_V^{sim} and C_V^{real} are the simulation vacancy concentration and the real vacancy concentration in the Al-Sc alloy, respectively. The ratio of the concentrations is multiplied by the inverse of the accumulated jump frequencies.

$$t_{MC}^{real} = \left(\frac{C_V^{sim}}{C_V^{real}}\right) \times \left(\sum_{i=1}^{12} \Gamma_i\right)^{-1} = \left(\frac{C_V^{sim}}{C_V^{real}}\right) \times t_{MC}^{sim} \quad (4)$$

As it can be observed in eq. 4, the simulation time is rescaled by a factor C_V^{sim}/C_V^{real} to take into account the difference between the simulation and the real vacancy concentrations.

A parallel version of kMC enables multiple events to occur simultaneously. To parallelize kMC we adopted the synchronous parallel generalization of the rejection-free n-fold kMC method documented in [21]. The main steps of spkMC are the following:

1. The accumulated frequency of each sub-domain Ω_k is obtained by Eq. 5 as the sum of n_k individual rates r_{ik}.

$$R_k = \sum_i^{n_k} r_{ik} \quad (5)$$

2. The maximum rate is defined by Eq. 6 and it is also established the relation with the sum of individual rates and the rates of null events (r_{0k}).

$$R_{max} \geq \max_{k=1,\ldots,K} \{R_k\}\ ;\ r_{0k} = R_{max} - R_k \quad (6)$$

The purpose of null events is to eliminate time conflicts between processes in such a way that null events prevent the stochastic trajectory of the simulation to be deeply changed.
Figure 1 shows the frequency rate buildup for several processes. Processes with an accumulated frequency inferior to R_{max} will include null events with rates r_{0k}.

3. The spkMC time increment is defined in Eq. 7, where ξ is a random number between 0 and 1.

$$\delta t_p = -\frac{ln\,\xi}{R_{max}} \quad (7)$$

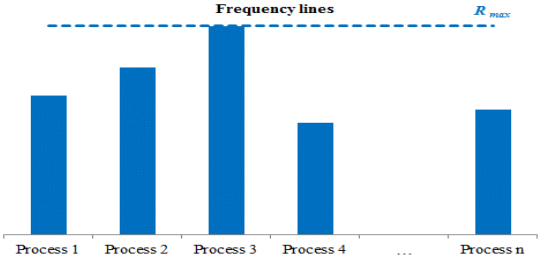

Fig. 1. Sum of frequencies for *n* processes.

4. Implementation of spkMC algorithm

Figure 2 illustrates how the lattice was partitioned into subdomains in spkMC. Each subdomain is further divided into 8 sectors (octants). At the simulation beginning, each sector has a single vacancy. Border conflicts between processes are avoided by a checkerboard scheme. Thus, each sector has a distinct color. The sectors are processed sequentially going through the 8 colors, and always keeping all processes in the sector with the same color. Figure 2 b) illustrates what is designated as the boundary region of a subdomain. The part of a subdomain that is used by other subdomains boundary region is called ghost