Computational Materials Science 120 (2016) 43–52

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

Synchronous parallel spatially resolved stochastic cluster dynamics

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ARTICLE INFO

Article history:
Received 7 December 2015
Received in revised form 7 March 2016
Accepted 9 April 2016
Available online 23 April 2016

Keywords:
Cluster dynamics
kinetic Monte Carlo
Parallel

ABSTRACT

In this study, a spatially resolved stochastic cluster dynamics (SRSCD) model for radiation damage accumulation in metals is implemented using a synchronous parallel kinetic Monte Carlo algorithm. The parallel algorithm is shown to significantly increase the size of representative volumes achievable in SRSCD simulations of radiation damage accumulation. Weak scaling performance of the method is tested in two cases: (1) an idealized case of Frenkel pair diffusion and annihilation, and (2) a characteristic example problem including defect cluster formation and growth in α-Fe. For the latter case, weak scaling is tested using both Frenkel pair and displacement cascade damage. To improve scaling of simulations with cascade damage, an explicit cascade implantation scheme is developed for cases in which fast-moving defects are created in displacement cascades. For the first time, simulation of radiation damage accumulation in nanopolycrystals can be achieved with a three dimensional rendition of the microstructure, allowing demonstration of the effect of grain size on defect accumulation in Frenkel pair-irradiated α-Fe.

1. Introduction

Structural materials in nuclear reactors are subjected to extreme environments including radiation damage and high temperatures [1,2]. In addition, materials to be used in future nuclear reactors need to withstand even greater radiation doses and temperature ranges than those in current reactors [1,3–6]. Recently, several types of radiation-resistant materials have been designed with microstructures that allow increased recombination of radiation damage [7–9]. Materials with microstructure length scales on the order of tens to hundreds of nanometers have shown increased resistance to radiation damage. Examples such as nano-grained and nano-laminate materials show higher radiation tolerance with increasing interface-to-volume ratio [8,10–13]. Several studies have investigated the role of interfaces in mitigating radiation damage accumulation in metals [13–15]. However, models that can explicitly represent nanoscale microstructures and can simulate radiation damage accumulation to doses and timescales that are directly comparable to experiments have not yet been developed.

Techniques such as cluster dynamics (CD) [16–24] and kinetic Monte Carlo (KMC) [16,17,25–30] based methods have led to a greater understanding of the effect of irradiation on microstructure evolution in a variety of materials and irradiation conditions. In CD-based methods, populations of radiation-induced defects are tracked via rate equations that represent the concentration evolution of defects of a given type in the material. These rate equations are solved deterministically. By contrast, KMC-based methods such as object kinetic Monte Carlo (OKMC) represent a stochastic approach for simulating defect evolution. These methods track the diffusion and interaction of individual defects inside simulated volumes, according to Arrhenius laws governing their diffusion and binding behavior. Both CD and KMC methods derive their input parameters such as binding and migration energies from a combination of experimental, atomistic, and ab initio results and have been shown to produce similar results for defect evolution in simplified cases [16,17,31,32]. However, the benefits and limitations of each method are quite different. CD models are typically very computationally efficient and can model large doses and timescales, and grouping schemes such as that of Golubov et al. [33] allow simulation of very large clusters. However, these methods are typically limited to modeling systems with only a few mobile defects and chemical species, limiting the number of reactions that can occur between defects [16,17,20–22,32]. KMC models can model very complex defect behaviors and can capture such effects as spatial correlations between defects [34], but are typically limited by computation time and simulation volumes used for complex

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http://dx.doi.org/10.1016/j.commatsci.2016.04.013
0927-0256/

studies such as cascade damage accumulation are typically limited to approximately 100 nm in length [25,28,29].

Spatially resolved stochastic cluster dynamics (SRSCD) [35] has recently been developed as an alternate method for simulating defect accumulation in irradiated materials. In SRSCD, defects are assumed to be homogeneously distributed within volume elements and the reaction rates for allowed reactions such as clustering, dissociation, and diffusion between volume elements are derived from classical CD methods. However, reactions and time steps are chosen according to a classical kinetic Monte Carlo algorithm. It therefore avoids limitations of CD in the complexity of the allowed defects and behaviors while reducing the computational demands compared to OKMC, which tracks all defect positions within a volume at every step.

To reach large simulation volumes one necessarily needs to implement these tools in parallel. In a deterministic model, such implementation is straightforward as each parallel domain will explicitly march in time with the same time step. However, in the case of kinetic Monte Carlo approaches the problem is far more complex because the time increment at each step is a weighted random choice based on the allowed reactions in the system. Therefore, domains running in parallel may become asynchronous, making reactions such as defect diffusion from one to the other difficult to properly carry out. In order to address this problem, a synchronous parallel kinetic Monte Carlo algorithm has been developed by Martínez et al. [36] in which a single time increment is chosen for all processors and the possibility of choosing null events is added to the KMC algorithm. Although this algorithm has been implemented for OKMC and lattice kinetic Monte Carlo (LKMC) systems [36–38], it has not been applied to the SRSCD methodology. The objective of the present study is to introduce a parallel implementation of the SRSCD scheme and to assess the numerical performance of the approach as well as its ability to simulate, for the first time, irradiation in polycrystals.

The manuscript is organized as follows. In Sections 2 and 3, SRSCD and the parallel kinetic Monte Carlo algorithm are described. In Section 4, the parallel scaling of the SRSCD code is investigated in an idealized system with only single vacancies and interstitials as well as in characteristic simulations of Frenkel pair and cascade implantation in α-Fe. Here, an explicit cascade implantation scheme is developed to address problems of poor weak scaling due to fast-moving defects that occur in simulations of cascade damage accumulation. In Section 5, synchronous parallel SRSCD is shown to enable simulations of damage accumulation in nano-grained polycrystalline α-Fe and the effect of grain size on damage accumulation is studied as a model case. The choice of kinetic Monte Carlo domain size is discussed in Section 6. In Section 7 conclusions are discussed including the limitations of the present methodology.

2. Description of SRSCD

2.1. Formulation of stochastic cluster dynamics (SCD)

Stochastic cluster dynamics (SCD) was developed by Marian and Bulatov as an intermediate method between OKMC and CD methods for simulating defect accumulation in irradiated metals [39]. It is based on the work of Gillespie [40], in which an algorithm is presented to simulate the evolution of chemical rate equations in a kinetic Monte Carlo setting. To describe this algorithm in the context of radiation damage, we consider a system containing N defect species $S_i, i \in \{1,\dots,N\}$, with the concentration c_i (in units of atomic fraction, or defects per lattice atom) of species S_i. In typical deterministic rate theory, the first-order rate equation for c_i is in the form:

$$\frac{dc_i}{dt} = \sum_{\mu=1}^{M_i} \pm a_\mu^i(c_1,\dots,c_N) \tag{1}$$

where a_μ^i is the reaction rate of reaction R_μ^i that impacts the population of species S_i (in units of reactions per lattice atom per second) and the $\pm$ symbol indicates whether the reaction adds or subtracts defects of this type from the system. In general, a_μ^i is dependent on the concentration of defects of various types in the system. There are a total of M_i reactions involving species i in this example. To treat a system of coupled rate equations $\frac{dc_i}{dt}$ in a stochastic setting, the concentrations of each species $c_i(t)$ are converted into populations $X_i(t)$ inside a finite volume V by multiplying by the ratio of the chosen volume element size to the atomic volume Ω:

$$\frac{dX_i}{dt} = \sum_{\mu=1}^{M_i} a_\mu^i(X_1,\dots,X_N)\cdot\left(\frac{V}{\Omega}\right) = \sum_{\mu=1}^{M_i} A_\mu^i(X_1,\dots,X_N) \tag{2}$$

Here, reaction rates A_μ^i are in units of reactions per second and represent the rate for the specified reaction R_μ^i to occur inside the chosen volume element V.

At this point, instead of measuring the evolution of the various defect populations X_i through a deterministic solution of the rate equations presented in Eq. (2), we can instead choose a stochastic approach to population evolution. Given a system at time t with volume V and defect populations $\{X_1,\dots,X_N\}$, we can create a list of reaction rates A_μ for all allowed reactions R_μ in the system, $\mu \in \{1,\dots,M\}$. If the populations X_i are known, the rates A_μ are analytically calculable via the terms of Eq. (2). We now restrict ourselves to considering integer populations of each defect species S_i, reducing the number of nonzero reaction rates that must be calculated.

Given such a system, the classical kinetic Monte Carlo algorithm can be applied to choose a time step τ and reaction μ to carry out in the system by choosing two random numbers r_1 and $r_2 \in (0,1)$ and applying the formula [40]:

$$\tau = \frac{1}{A}\ln\left(\frac{1}{r_1}\right), \quad \sum_{\nu=1}^{\mu-1} A_\nu < r_2 A \leqslant \sum_{\nu=1}^{\mu} A_\nu \tag{3}$$

Once reaction R_μ is chosen, the populations of defects X_i in the system are subsequently updated according to the reaction chosen and the changed reaction rates A_μ are recalculated. Therefore, all defects are accounted for at each step and any imbalances in defect populations are due to preferential absorption of defects at sinks, for example due to the greater diffusivity of self-interstitials compared to vacancies. This formalism assumes that when reactions occur, they are carried out instantaneously so that two reactions cannot occur simultaneously. It has been proven [41,42] that the stochastic description of events presented here is equivalent to the deterministic rate theory formulation given in Eq. (1). Note that for a given reaction such as two single vacancies joining to form a cluster, $V + V \rightarrow 2V$, the reverse reaction $2V \rightarrow V + V$ may or may not be allowed, and if it is allowed it may have a different reaction rate than the forward reaction. This reflects the different mechanisms associated with defect clustering and dissociation, and can lead to a system with no equilibrium state in which clusters grow indefinitely.

2.2. Spatially resolved stochastic cluster dynamics

The development of SCD allows simulations of radiation damage accumulation to model more complex systems and defect behaviors than CD because reaction rates A_μ are only calculated for defects present in the volume element V [39]. However, both