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Sink strength simulations using the Monte Carlo method: Applied to spherical traps

T. Ahlgren*, L. Bukonte

Department of Physics, University of Helsinki, P.O. Box 43, FI-00014 Helsinki, Finland

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ABSTRACT

The sink strength is an important parameter for the mean-field rate equations to simulate temporal changes in the micro-structure of materials. However, there are noteworthy discrepancies between sink strengths obtained by the Monte Carlo and analytical methods. In this study, we show the reasons for these differences. We present the equations to estimate the statistical error for sink strength calculations and show the way to determine the sink strengths for multiple traps.

We develop a novel, very fast Monte Carlo method to obtain sink strengths. The results show that, in addition to the well-known sink strength dependence of the trap concentration, trap radius and the total sink strength, the sink strength also depends on the defect diffusion jump length and the total trap volume fraction. Taking these factors into account, allows us to obtain a very accurate analytic expression for the sink strength of spherical traps.

1. Introduction

To understand and control the changes in the physical and mechanical properties of materials during ageing or ion irradiation, requires a long time and length scale simulation technique, knowledge of the ion irradiation produced defects, and a complete description of how the formed defects diffuse and interact with each other.

The only simulation techniques that are able to fulfil the long time and length scales are the mean-field rate equations (RE) and kinetic Monte Carlo (KMC) methods. The KMC is a stochastic simulation method, where all the dynamic properties and reactions for all involved defects have to be known. The strengths of this method include the ability to take into account expected and unexpected correlated events, e.g. close Frenkel pair annihilation. However, the time step for the KMC method is inversely proportional to the sum of frequencies of all processes, which is a disadvantage in some cases. For instance in tungsten, where the self-interstitial atom moves very fast [1], the KMC time step, even with only one SIA present, might be of the order of 10^{-11} s. Clearly, this restricts the accessible time and defect concentrations for the method.

In the mean-field rate equations (RE) [2,4,5] the defects and other objects are treated as concentrations (number/vol) which interact with each other in space and time. This interaction is described by a parameter called the sink strength, which determines the probability for mobile defects to interact with any other point or extended defect in the material. The sink strength has to be determined for each mobile defect separately and it is proportional to the square of the inverse mean distance covered by the defect before it is absorbed, trapped or annihilated. The sink strength is the single most important parameter in RE simulations and is a function of the geometry, size and concentration of sinks, dimensionality of the diffusion, and, as we will show in this study, the sink strength also depends on the diffusion jump length of the defect.

Sink strengths have been determined for various symmetric traps including spherical traps, dislocation lines and loops, and grain boundaries [6–9]. Monovacancies, vacancy clusters, self-interstitial atoms and impurities are usually counted as spherical traps. For arbitrarily shaped traps, methods like the Monte Carlo (MC) method has to be used to determine the sink strength. The MC method seems in principle straight forward to use, but previous studies have shown some inconsistencies for this method. Malerba *et al.* [7] have noticed that the MC method gives smaller sink strengths than the analytic equation for spherical traps in the low trap volume fraction region. On the contrary, for large trap volume

* Corresponding author.
E-mail address: tommy.ahlgren@helsinki.fi (T. Ahlgren).

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fractions, the sink strengths simulated by the MC method are much larger than the analytical ones. Similar results are observed by Hou *et al.* [10], where the analytic equation is modified to give better agreement with the sink strengths obtained by the MC method.

In this study, we show the reasons for the discrepancy between sink strengths obtained analytically and by MC. We introduce a new, much faster MC concept to simulate sink strengths. We further show how the equation of analytical sink strength can be modified so that it can be used in defect and micro structure simulations with any trap volume fraction and defect jump length.

2. Results

The definition of the sink strength includes the inverse mean distance squared a defect diffuses before it gets trapped. The sink strength calculated with the Monte Carlo (MC) method is expressed as [11]:

$$k^2 = \frac{2 \cdot Dim}{\lambda^2 \langle N \rangle}, \tag{1}$$

where Dim is the dimension for the defect diffusion, λ is the jump length and $\langle N \rangle$ is the mean number of jumps the defect makes before it is trapped: $\langle N \rangle = \sum_{i=1}^{M} N_i / M$, where M is the number of defects simulated and N_i is the number of defect i jumps before it is trapped. In Appendix A, we show how the statistical error for determining the sink strength by the MC method depends on the number of defects M simulated as follows:

$$\Delta k^2 = k^2 \frac{\sqrt{\sum_i^M (1 - N_i/\langle N \rangle)^2}}{M} \approx \frac{k^2}{\sqrt{M}}. \tag{2}$$

As a rule of thumb, to obtain the sink strength with an error less than 1% more than 10^4 defects need to be simulated, and for an error less than a per mille (1 ‰) more than 10^6 defects are needed, see Fig. A.10.

In this study, we place one trap in the middle of the simulation cell, which is either spherical or cubic. The trap concentration c_t is controlled by choosing an appropriate simulation cell volume V, $c_t = 1/V$. The trap volume fraction becomes: $VF_t = 4\pi R_t^3/(3V)$. One defect at a time is placed at a random position in the cell, excluding the trap volume. The defect diffusion jumps are counted until it jumps inside the trapping radius R_t, then a new defect is inserted in the cell. At least $M = 10^6$ defects are simulated for each sink strength calculation, resulting in the statistical error of about 1 ‰.

2.1. Improving MC sink strength simulation speed

The MC method for determining the sink strength of systems with quite small trap volume fractions is very inefficient [7]. The reason for this is that the defect can make incredibly large number of jumps before it finds a trap ($k^2 = 6/[\langle N \rangle \lambda^2]$), see Eq. (1). Thus, to find the sink strength for a trap with, let's say, a trap radius $R_t = 0.4$ nm and concentration of $c_t = 10^{-7}$nm^{-3} ($k^2 \approx 4\pi c_t R_t$), for a statistics of 10^6 defects, with jump length $\lambda = 0.1$ nm, we would need about $10^6 \cdot 6/(4\pi 10^{-7} 0.4 \cdot 0.1^2) \approx 10^{15}$ jumps.

In this study, we develop a new and fast MC method to simulate sink strengths, the details are given in Appendix B. The method takes advantage of the fact that if the minimum distance to any trap for the diffusing defect is known (this has to be checked anyway during the MC simulation), the defect cannot be trapped during the following $N^j = floor(D_{\min}/\lambda)$ diffusion jumps, where $D_{\min}$ is the minimum distance to any trap and λ is the jump length. Thus, instead of making N^j diffusion jumps, we can make one jump that gives statistically the same diffusion distance as the N^j individual diffusion jumps would give. This new concept gives surprisingly large improvement in the simulation times. To compare the normal MC with the new (*N-jump*) MC method, we determine the average cpu-time per defect during sink strength simulations for seven different trap volume fractions VF_t: $10^{-1}, 10^{-2}, 10^{-3}, 10^{-4}, 10^{-5}, 10^{-6}$ and 10^{-7}. The trapping radius R_t is 0.5 nm for all simulations. Two different jump lengths $\lambda = 0.2$ and 0.005 nm are chosen for every simulation. The choice of the latter very small jump length will be obvious in the next section where we compare the MC results with analytical sink strengths. Fig. 1 shows the impressive improvement in the simulation times for the *N-jump* MC method. For rather large trap volume fractions VF_t above 10^{-3} and jump length to trapping radius ratio $\lambda/R_t = 0.4$, both methods give similar simulation times. This is expected because the distance to the closest trap is never very large, thus the *N-jump* MC method is seldomly used. However, for smaller trap volume fractions the improvement in simulation time is remarkable. Smaller λ to R_t ratio yields to even more impressive improvement in computational times. For λ to R_t ratio of 5×10^{-3}, the *N-jump* MC method is faster for all trap volume fractions, being a staggering more than four orders of magnitude faster at $VF_t = 10^{-7}$. The new method enables sink strength simulations for smaller trap volume fractions with better statistics. The resulting sink strengths for both normal and *N-jump* MC methods are the same within the statistical error. All the following sink strengths in this study have been calculated with the developed *N-jump* MC method.

2.2. Comparison of the analytical and MC sink strengths

The analytical sink strength for spherical traps under 3D diffusion limit with trap radius R_t and concentration c_t is given by the recursive equation by Brailsford and Bullough [6]:

$$k^2 = 4\pi R_t c_t \left(1 + R_t \sqrt{k^2}\right). \tag{3}$$

In the small trap concentration limit the Eq. (3) is usually truncated to the first order ($n = 1$), $k^2 = 4\pi R_t c_t$. For usual trap concentrations higher order sink strengths ($n = 2, 3, 4, \ldots$) are calculated recursively as $k_n^2 = 4\pi R_t c_t (1 + R_t \sqrt{k_{n-1}^2})$. For $n = \infty$ the solution can be found directly from Eq. (3) as

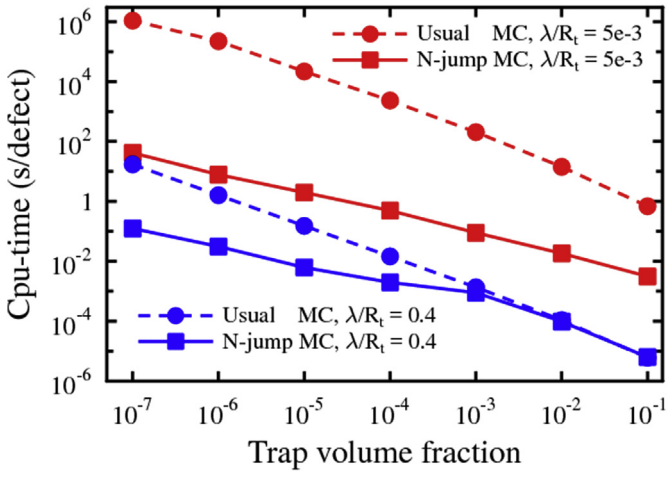

Fig. 1. Comparison of cpu-time per defect for the usual and the developed *N-jump* MC methods for two different jump length to trapping radius ratio and trap volume fractions between 10^{-7}–10^{-1}. The lines are given as guides to the eye.