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Sink strength calculations of dislocations and loops using OKMC

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HIGHLIGHTS

- The sink strength for dislocations and loops are calculated using OKMC.
- The master curves for the 1D to 3D defect migration transition are well reproduced.
- We find that OKMC and theory are in good agreement for low volume fractions.

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ABSTRACT

We calculate the sink strength of dislocations and toroidal absorbers using Object Kinetic Monte Carlo and compare with the theoretical expressions. We get good agreement for dislocations and loop-shaped absorbers of 3D migrating defects, provided that the volume fraction is low, and fair agreements for dislocations with 1D migrating defects. The master curve for the 3D to 1D transition is well reproduced with loop-shaped absorbers and fairly well with dislocations. We conclude that, on the one hand, the master curve is correct for a wide range of sinks and that, on the other, OKMC techniques inherently take correctly into account the strengths of sinks of any shape, provided that an effective way of appropriately inserting the sinks to be studied can be found.

1. Introduction

Irradiation introduces mobile defects such as self-interstitial atom (SIA) clusters and vacancy clusters in metals. These defects will interact with each other and with the pre-existing microstructure, mainly dislocations, thereby inducing nanostructural changes that will affect the mechanical properties of the material. To fully understand the evolution of the defect populations over time, the rates of these reactions needs to be correctly assessed.

Object Kinetic Monte Carlo (OKMC) is a stochastic simulation method, where the dynamic behaviour of all objects, such as SIA or vacancy clusters, is described by pre-defined probabilities. It is a well-suited technique for simulation of the evolutions of radiation induced defects in iron alloys (see e.g. [1]). The OKMC has been shown to be equivalent to rate theory calculations [2]. It has the advantage of going beyond the mean-field approximation and taking explicitly all spatial correlations, except the elastic interactions, into account.

In mean-field approaches, the rate at which a mobile defect interacts with a cluster or dislocation of a given shape and size, acting as a sink, is given by the sink strength, k^2. This is proportional to the inverse square of the average distance covered by the defects before the interaction, which is normally absorption or clustering. The sink strength is *a priori* affected by the shape and size of the sinks, their number density, their type and orientation. Also, the migration regime of the defects will have an impact: defects that migrate in a 1D fashion are less likely to interact with sinks than defects that migrate in 3D or in a fashion between fully 1D and 3D.

Analytical expressions for different sink shapes, such as spheres, toroids and dislocations have been theoretically obtained in the case of 3D migrating defects and a number of them is reviewed by e.g. Nichols [3]. Barashev et al. derived expressions for fully 1D migrating defects in the case of spherical absorbers, dislocations and grain boundaries [4]. The 3D to 1D transition has been studied by Trinkaus et al., who also proposed a master curve for the transition [5,6]. Malerba et al. [7] showed that OKMC calculations of the sink strength for spherical sinks and grain boundaries show good agreement with analytical expressions used in rate theory and that also the 3D to 1D defect migration regime transition with spherical absorbers can be reproduced using OKMC. These

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results simultaneously corroborate the theory and show the equivalence between OKMC and mean-field approaches.

In this work, we extend the study by Malerba et al. [7], where spherical absorbers were considered, to also calculate the sink strength for dislocation lines and toroidal absorbers, the latter corresponding to dislocation loops, and compare the results with analytical expressions available from rate theory. The structure of this paper is as follows: In Section 2, we describe our methodology. In Section 3.1 we compare the sink strength of dislocations obtained by OKMC to rate theory expressions, in the limits of 3D and 1D migration, and in Section 3.2, we do the same with toroidal absorbers. Finally, in Section 3.3, we study the transition of the migration regime from 3D to 1D of defects absorbed by dislocations and toroidal sinks and compare with the theoretical master curve. The discussion and conclusions are found in Sections 4 and 5, respectively.

2. Computation method

We have estimated the sink strength of straight dislocations and dislocation loops using the same methods as in [7] (where spherical absorbers were considered), which is here briefly recalled. For our calculation we use the OKMC code LAKIMOCA [8]. The probabilities for migration jumps of defects in the simulations are given in terms of Arrhenius frequencies for thermally activated events, $\Gamma_i = \nu_i \exp\left(\frac{-E_{a,i}}{k_B T}\right)$, where ν_i is the attempt frequency, $E_{a,i}$ the activation energy for the process, k_B Boltzmann's constant and T the temperature. Events are randomly chosen according to their probability, following the Monte Carlo algorithm [9]. The simulated time is increased according to the resident time algorithm [10] with $\Delta t = 1/\left(\sum_{i=1}^{N_{int}} \Gamma_i + \sum_{j=1}^{N_{ext}} P_j\right)$, where N_{int} is the number of internal events such as defect jumps and N_{ext} the number of external events, such as cascades or Frenkel pair creation, with P_j being the probabilities for the external events. In the long term, this equation substitutes $\Delta t' = -\ln u \Delta t$, which is fully exact by including the stochasticity due to the Poisson distribution [11]. u is here a uniform random number between 1 and 0.

Objects, such as defects or clusters, in the model are described as geometrical objects, such as spheres, toroids or cylinders. Reactions between objects take place when these overlap geometrically. Reactions could be annihilations or clustering. In this study, the only reaction considered is absorption, where the reacting defect will not change the volume of the absorbing objects.

The straight dislocation was simulated as an immobile cylinder-shaped sink whose two opposite faces touch the faces of a non-cubic simulation box. No defect can ever impinge on the cylinder from one of the faces, as no defect is allowed to be outside the box, so this is an effective way to simulate an infinitely long straight dislocation. However, since periodic boundary conditions are applied in all direction, we are in practice simulating a regular array of infinitely long straight dislocations: this must be taken into account to rationalize the results and certainly when choosing the theoretical expression to which the simulation results are to be compared. (On the other hand, as discussed by Brailsford and Bullough [12], there is no real theoretical expression for the sink strength of an array of dislocations significantly different from a lattice and for real random arrays the Z factor of proportionality with the dislocation density should be regarded as an empirical parameter.)

The simulation box with the dislocation is pictorially represented in Fig. 1. Different dislocation densities and capture radii, r_d (as in Fig. 1) were explored. With reference to Fig. 1, the dislocation density, ρ_d, was changed by varying l_y and l_z: $\rho_d = (l_y l_z)^{-1}$, for a fixed $l_x = 100a_0$ (since iron is taken as materials of reference, the underlying lattice is body-centred-cubic (bcc) and the lattice

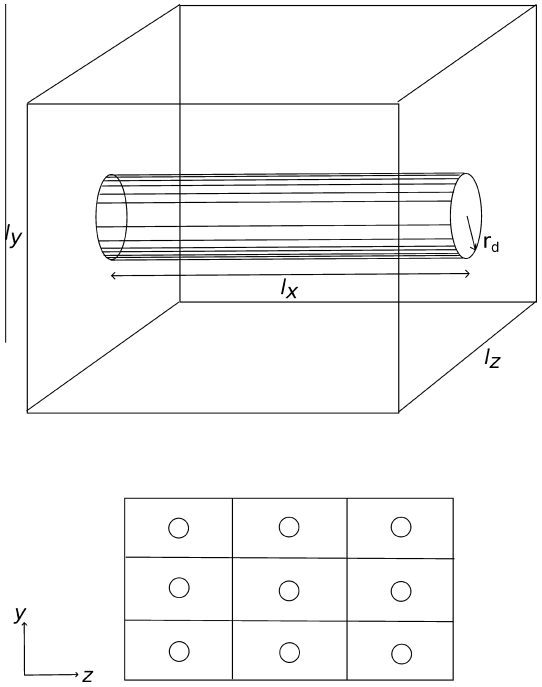

Fig. 1. Upper side: Pictorial representation of the non-cubic simulation box and the cylinder mimicking the sink effect of a straight dislocation. Lower side: view normal to x axis of the simulation box and image boxes corresponding to applying periodic boundary conditions: the image dislocations effectively create a regular array.

parameter is $a_0 = 2.87$ Å), with $l_x \neq l_y \neq l_z$. Dislocation densities were varied between 10^{14} and 10^{15} m^{-2}, capture radii, r_d, between 2 and 9 nm (smaller densities, down to 5×10^{13} m^{-2}, were also considered in the 3D limit only; simulations with smaller radii, 0.5 and 1 nm, for $\rho_d = 10^{14}$ m^{-2} did not provide sufficient statistics to be fully acceptable in the 1D limit). The simulation temperature was arbitrarily set to 573 K, but it does not have any influence on the sink strength calculation.

Dislocation loops are simulated by immobile sinks of toroidal shape, depicted in Fig. 2, and characterized by the major radius, R, the minor radius r_t and their orientation with four possible [1 1 1] Burgers vectors. Toroidal sinks with the same R and r were randomly distributed in the simulation box with random orientations for a given number density. The simulation box size used for the loop sink strength calculations were $300 \times 350 \times 400a_0^3$, except in Sections 3.2.4 and 3.3, were smaller box sizes of $150 \times 200 \times 250a_0^3$ and $250 \times 300 \times 350a_0^3$, respectively, were used

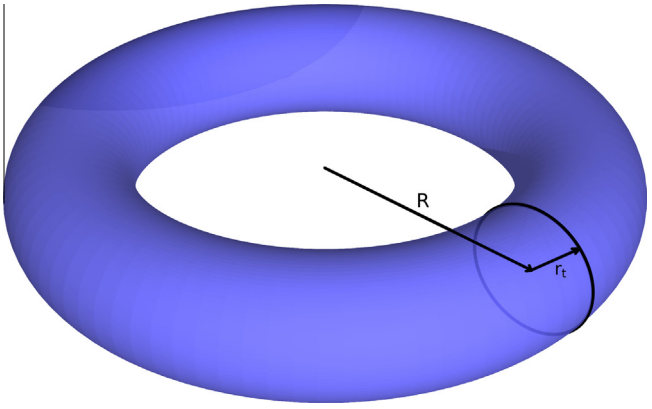

Fig. 2. Depiction of a toroid with the major radius R and the minor radius r_t.