8.2 IMPLEMENTATION OF FIRST-PASSAGE TIME APPROACH FOR OBJECT KINETIC MONTE CARLO SIMULATIONS OF IRRADIATION—G. Nandipati, W. Setyawan, H. L. Heinisch, K. J. Roche, R. J. Kurtz (Pacific Northwest National Laboratory) and B. D. Wirth (University of Tennessee)

OBJECTIVE

The objective of the work is to implement a first-passage time (FPT) approach to deal with very fast 1D diffusing SIA clusters in *KSOME* (kinetic simulations of microstructural evolution) [1] to achieve longer time-scales during irradiation damage simulations. The goal is to develop *FPT-KSOME*, which has the same flexibility as *KSOME*.

SUMMARY

This is a work in progress and in this report we present basic implementation details of the first-passage time (FPT) approach to deal with very fast 1D diffusing SIA clusters in *KSOME* (kinetic simulations of microstructural evolution) and the status of its development.

PROGRESS AND STATUS

Introduction

From the test simulations of irradiation in bulk tungsten carried out using the *KSOME* code we find that one-dimensionally (1D) diffusing SIA clusters, due to very low migration barriers, will limit the achievable simulation time and radiation dose. In this case most of the computational time is spent moving around SIA clusters that are far away from other defects, in the empty space of a simulation box. In order to avoid simulating these numerous individual diffusive hops by SIA clusters we let them do multiple nearest neighbor jumps simultaneously, depending on conditions in their neighborhood, and calculate the time for this jump using a well-known analytical expression for mean first-passage time (MFPT) for a 1D diffusing walker. [2, 3] SIA clusters that are very close to other defects and all other types of defects will perform regular KMC moves. A full FPT approach, where all defects are treated using FPT approach was employed previously to accelerate irradiation simulations [4] and we take a similar approach in implementing FPT in *KSOME.* In contrast to previous approaches, to reduce overhead, *FPT-KSOME* will be hybrid of FPT and traditional KMC methods.

Implementation of FPT Approach

In our first-passage-time approach, detailed 1D motion of an SIA cluster is replaced by a calculation of its overall first-passage time for ``absorption'' at the boundaries of an interval whose length is determined based on how far it is from the nearest defect. Diffusive moves of other types of defects with barriers that are significantly higher than the migration barrier for SIA clusters are treated as regular KMC moves. The intent is that the bigger the difference between the migration rates of SIA clusters and other defects in the simulation the bigger will be the gain in decreased simulation time.

A key point is that the use of the FPT approach to accelerate KMC adds significant overhead. Therefore the best approach to achieve significant speedups is to treat only frequently occurring low-barrier events with the FPT approach while other events are treated as regular KMC events [3,4,5]. In addition, only SIA clusters that are farther than a certain user specified distance from a defect are allowed to make multiple nearest neighbor jumps, while other SIA clusters will perform regular KMC hops. Therefore diffusion of an SIA cluster will switch back and forth from multiple hop (FPT) to single hop (KMC) diffusion depending on how far it is from another defect. In order to further reduce the overhead we take the less rigorous approach of using average FPT instead of randomly selecting the FPT from an appropriate probability distribution function.

Calculation of Average First-passage Time For a 1D Diffusing SIA

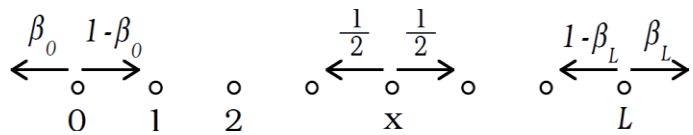

Figure 1. Schematic showing 1D random walker diffusing between partially absorbing boundaries at 0 and L with absorption probabilities β_0 and β_L, respectively [2].

In our case a 1D diffusing SIA cluster is mapped to a 1D random walker diffusing between two boundaries. For a 1D diffusing SIA cluster we treat both of the boundaries of the interval (see Figure 1) as perfectly absorbing, meaning β_0 $(\beta_L) = 1$. Then

$$n(x) = x(L - x) \qquad (1)$$

Where L is the interval length and x is the location of the 1D random walker in the interval. In our implementation we assume for simplicity that SIA clusters are initially always at the middle of the interval, that is at $x = L/2$ i.e., an SIA has equal probability to reach or escape from either end of the interval. The mean first passage time $\tau(x)$ to escape the interval from $[0,L]$ is given by

$$\tau\left(\frac{L}{2}\right) = L^2/8D_{SIA} \qquad (2)$$

Where D_{SIA} is the diffusion rate of an SIA cluster. For verification we can easily see that $L = 2$ and $x = 1$ represents a regular KMC jump. For this case, using Eqs (1) & (2) one can see that $n(1) = 1$ and $\tau(1) = 1/2D_{SIA}$ clearly represents a regular KMC jump.

If L is too short we may not see any significant speed up due to the overhead, but if it is too large we may miss important reaction events. The design of the simulation code has to be such that an appropriate interval length L is determined for each individual SIA cluster depending on its neighborhood. We use the distance of an SIA from its nearest defect and the sum of their capture radii to determine the interval length L. Each L is calculated as

$$\boldsymbol{L} = \boldsymbol{R} - (\boldsymbol{R_a} + \boldsymbol{R_b}) \qquad (3)$$

where R is the distance of the SIA from its nearest defect, while $\boldsymbol{R_a}$ and $\boldsymbol{R_b}$ are the capture radii of the SIA cluster and its closest neighbor respectively. This condition ensures that the capture radii of the SIA and its nearest defect never touch or overlap. Note that although the length of the interval is L, an SIA cluster will only move a distance of $L/2$ from its present location. Then the average first-passage time $\boldsymbol{\tau}\left(\frac{\boldsymbol{L}}{2}\right)$ for the diffusion event along with times for all other possible processes an SIA cluster can perform are calculated. The SIA is moved to either end of the interval with equal probability if $\boldsymbol{\tau}\left(\frac{\boldsymbol{L}}{2}\right)$ is the smallest time and the simulation clock is updated to $\boldsymbol{\tau}\left(\frac{\boldsymbol{L}}{2}\right)$**.** If a non-diffusive process is selected then the position of the SIA cluster is updated within its interval before the non-diffusive process is performed and then a new interval length and $\boldsymbol{\tau}\left(\frac{\boldsymbol{L}}{2}\right)$ are calculated. An SIA can perform two non-diffusive processes, emission and rotation. As mentioned earlier only SIAs that are far away from other defects are allowed to perform FPT moves while others will perform regular KMC moves. Accordingly, as SIA clusters move away from other defects they switch from KMC to FPT diffusion and if they move closer to other defects then it switches back from FPT to KMC diffusion. This switch from FPT to KMC diffusion and back is necessary to take care of reaction events properly.

Time-based KMC

Only hops to direct nearest neighbors *(L = 2)* are exponentially distributed. The lack of an exponential probability distribution disqualifies FPT diffusion steps to be used in the classical KMC algorithm (rate-based approach). [3] In order to implement the FPT approach we will use a time-based rather than a rate-based KMC method. [2,4] In this case events are chronologically ordered and the event with smallest time is executed. Each individual 1D diffusing SIA cluster has its own time. In addition to maintaining a list of first-passage times for all 1D diffusing SIA clusters, after each event we also update the total rate for all regular KMC moves $\boldsymbol{R_{KMC}} = \sum \boldsymbol{n_i}\, \boldsymbol{R_i}$ (where $\boldsymbol{R_i}$ is the rate for a process of type *i*, and $\boldsymbol{n_i}$ is the number of processes of this type). This rate is then used to calculate the time before the next regular KMC event given by $\boldsymbol{\Delta t_{KMC}} = -\mathbf{ln}(\xi)/\boldsymbol{R_{KMC}}$, where ξ= a uniform random number between [0,1]. This time is then compared with the time of the earliest FPT event (which will be selected using another binary tree). If the event type corresponds to a regular KMC event, then the specific event is selected randomly from all of the possible events of this type.

Benchmarking Tests

The basic *FPT-KSOME* code has been completed and it is being tested and benchmarked using data from single cascade annealing in tungsten at various PKA energies and temperatures obtained using *KSOME.* [6] Figure 2 compares the results from *KSOME* and *FPT-KSOME* for surviving fraction of defects during single cascade annealing in bulk tungsten at 300 K for PKA energies of 60 and 75 keV. L_{max} represents the maximum allowable interval length (L), which is a user-defined parameter. Each data point is an average of 300 runs. As can be seen from Figure 2 we have obtained reasonable agreement between FPT and regular KMC results.

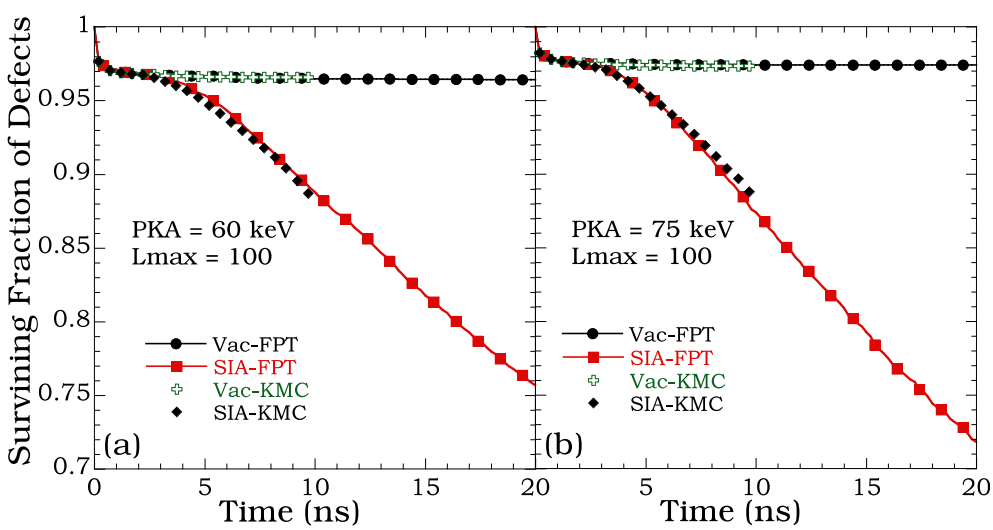

Figure 2. Comparison of regular OKMC and FPT OKMC for surviving fraction of defects during annealing of single cascades in tungsten at 300 K for PKA energies of (a) 60 and (b) 75 keV.

For the two cases shown in Figure 2 an average of 1.5 X 10^6 diffusive steps are performed to reach a simulation time of 10 ns. In case of *FPT-KSOME*, the same simulation time is reached on average a sum of 4 x 10^4 diffusive steps. Further reduction in the number of diffusive steps can be obtained if L_{max} is increased further than 100. As expected due to overhead resulting from additional bookkeeping associated with determining interval length and calculation of first-passage times, for annealing simulations of single cascade we have not seen a significant speed up compared to regular KMC simulations. A small speed up of 1.6X was obtained. However for irradiation simulations, which require achieving much longer times and involve a significant number of KMC steps compared to single cascade aging simulations, we expect to see significant speed up compared to regular KMC simulations.

FUTURE WORK

FPT-KSOME requires further testing of various aspects of the code. It been tested at 300 K where the rotation and dissociation of SIA clusters is negligible and therefore further testing is required to make sure that the code performs correctly at all temperatures. It also requires further testing to determine the optimum criteria to determine when to switch SIA diffusion from FPT-to-KMC and back to make sure that reaction events are properly handled. Note that we have conservatively chosen the length of the interval to be the distance between an SIA cluster and its nearest neighbor minus the sum of their capture radii, but the maximum allowable interval length is twice this value. Therefore we plan to carryout test simulations to determine the optimum value of L_{max} to obtain maximum computational efficiency.

Once the code is completely tested and benchmarked, it will be used to perform long-time scale irradiation simulations in bulk tungsten at various PKA energies and temperatures using the same database of cascades used in the cascade aging simulations.

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REFERENCES

[1] G. Nandipati *et al* Semiannual Progress Report DOE/ER-0313/54, June 2013, 179-183.

[2] A. El-shehawey, J. Phys. A 33, 9005 (2000).

[3] G. Nandipati, Y. Shim, and J. G. Amar, Phys. Rev. B 81, 235415 (2010).

[4] A. Donev, *et al*, J. Comput. Phys. 229, 3214 (2010).

[5] A. Bezzola, B. B. Bales, R. C. Alkire, and L. R. Petzold, J. Comput. Phys. 256, 183 (2014).

[6] G. Nandipati et al., Semiannual Progress Report DOE/ER-0313/55, December 2013, 161-166.