Cluster Dynamics Modeling of Cavity and Loop Microstructure under Irradiation

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The simulation of the loop and cavity microstructure evolution over long time scales requires efficient coarse grained methods. Cluster dynamics belongs to this class of methods, inasmuch as doses of around 100 dpa can be simulated in reasonable computation times. When switching to coarser grain scales, one often needs to resort to some approximations, either in the physical model or in the modeling techniques. Obviously these approximations must be controlled as carefully as possible in order to preserve the same degree of reliability from one scale to the other.

In the case of cluster dynamics, the method operating at finer scale is object kinetic Monte Carlo (OKMC), which considers the microstructure as a collection of objects interacting with each other. The physical model is the same as cluster dynamics but the modeling technique is very different: in the case of OKMC, clusters are explicitly considered, whereas in cluster dynamics, only cluster concentrations are retained. Under thermal aging, as long as clusters can be considered as uniformly distributed in a representative volume, OKMC and cluster dynamics are shown to be rigorously equivalent.

Under ion or neutron irradiation, displacement cascades are generated, which results in significant spatial correlations between defects. The simulation of such irradiation conditions is straightforward in OKMC, but is often seen as the crux of the problem in cluster dynamics. It is all the more important as physical results are often very sensitive to the irradiation term, since it can control entirely the cluster density through the nucleation of clusters inside cascades. To solve this problem, we have recently proposed a method to introduce cascades in cluster dynamics without loss of information compared to OKMC [1]. This method is based on a homogenization technique which makes use of a modified version of OKMC (Figure 1). The modified OKMC provides an effective source term for cluster dynamics, which is shown to reproduce satisfactorily reference calculations performed with full OKMC calculations.

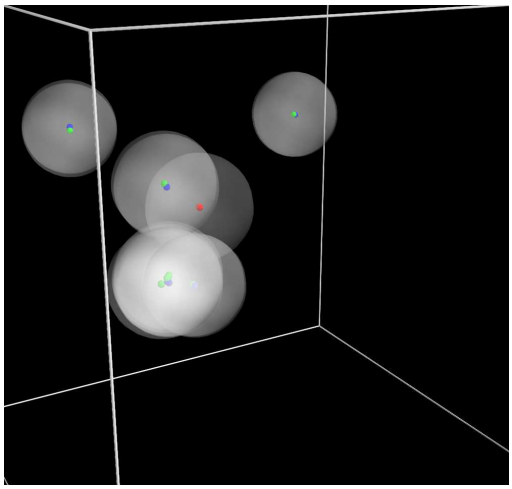

Figure 1: Snapshot of a modified OKMC simulation used to homogenize a cascade. The defects are the small colored spheres.

References

[1] T. Jourdan and J.-P. Crocombette, “Rate theory cluster dynamics simulations including spatial correlations within displacement cascades”, Phys. Rev. B 86 (2012) 054113.