STATISTICAL ANALYSIS OF A LIBRARY OF MOLECULAR DYNAMICS CASCADE SIMULATIONS IN IRON AT 100 K – R. E. Stoller (Oak Ridge National Laboratory) and A. F. Calder (University of Liverpool)

Extended Abstract (the full paper will be published in the Journal of Nuclear Materials as Proceedings of the Ninth International Conference on Fusion Reactor Materials, October 10-15, 1999, Colorado Springs, Colorado).

An extensive database of atomic displacement cascades in iron has been developed using molecular dynamics simulations. Simulations have been carried out at temperatures of 100, 600, and 900K, and at energies between 0.10 and 50 keV. The results presented here focus on the simulations conducted at 100K. A sufficient number of cascades have been completed under each condition of cascade energy and temperature to obtain statistically significant average values for the primary damage production parameters. The cascade database is summarized in Table 1. This statistical analysis has been used to examine the influence of primary knockon direction, simulation cell size, periodic boundary conditions, and lattice heating by the high-energy recoil.

The 100K cascade database can be used to at least partially answer several questions regarding MD cascade simulations. These questions include: what is the effect of PKA direction, how many simulations are required to obtain meaningful average quantities for a given condition, how significant is the effect of periodic boundary conditions, and what is the impact of lattice heating due to the PKA energy input? The first two questions are related, since more simulations are required at energies where the effect of PKA direction is strong. Although the validity of these answers have only been demonstrated for the particular iron potential employed in this work, they should provide useful guidance to investigations of primary damage formation in other materials. A more detailed analysis of these results will be published when a set of 100 keV cascades has been completed and the 600 and 900K simulations have been fully analyzed.

Table 1. Summary of iron cascade database at 100K
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MD cascade energy (keV)	NRT displacements	Number of simulations*	multiple of standard error to obtain indicated confidence level:	
			90%	95%
0.1	1	40	1.685	2.023
0.2	2	32	1.696	2.040
0.3	3	104	1.660	1.983
0.5	5	20	1.729	2.093
1.0	10	12	1.796	2.201
2.0	20	10	1.833	2.262
5.0	50	9	1.860	2.306
10.0	100	15	1.761	2.145
20.0	200	10	1.833	2.262
30.0	300	10	1.833	2.262
40.0	400	8	1.895	2.365
50.0	500	9	1.860	2.306

* more simulations have been completed, this is the number used in the average values shown in Figure 1

The data indicate that some dependence on PKA direction persists up about 1 keV. For the PKA directions used in this work, the maximum difference in defect survival occurred when comparing the [135] and [114] directions. The difference between the [135] and [114] averages are statistically significant at the 95% confidence level for the 0.3 keV simulations, but not at higher energies. For example, although the [114] defect survival was 15% higher than [135] at 2 keV, this difference is not statistically significant at the lower 90% confidence level. These results suggest the necessity of conducting low-energy simulations in a variety of high and low index directions to characterize defect survival before choosing a single direction for high energy simulations. It is interesting to note that the PKA directions that gave higher than average survival were not necessarily directions with a low displacement threshold. Interstitial clustering appears to be somewhat less sensitive to PKA direction than does defect survival.

Using 40 simulations and 12 PKA directions yielded a standard error that was 6% of the average defect survival at 100 eV. A similar value of 8.7% was obtained from the initial 16 simulations and 12 directions at 300 eV. At higher energies, there is a trend supporting the need for fewer simulations, e.g. the ratio of standard error to average value is 6.5% with 12 simulations at 1 keV, less than 5% with 10 simulations at 20 and 30 keV and as small as 2.5% with 9 simulations at 50 keV.

An evaluation of the effect of periodic boundary conditions can be made based on these results. At both 0.5 and 1.0 keV, a set of simulations was carried out in which the PKA was chosen to ensure that the cascade spilled through one face of the simulation cell and reentered the opposing face. The defect survival fraction and the interstitial clustering fraction were not affected. The same result was obtained when 10 keV simulations carried out in 128,000 and 250,000 atom simulation cells were compared. Simulations in the smaller atom block spilled through the periodic boundary in most cases, but the primary damage parameters were not significantly affected. This result holds as long as the recoils that exit and reenter the block do not travel far enough to encounter the cascade region.

A comparison of 0.3 and 10 keV simulations using different atom blocks sizes to reduce heating did not reveal a significant effect. Defect survival is unchanged, while interstitial clustering is slightly greater in the cooler block at 0.3 keV and slightly lower in the cooler block at 10 keV. The change is not statistically significant in either case at the 90% confidence level.

Finally, the results of this analysis confirm an effect of subcascade formation that we have previously reported. The ratio of surviving point defects to the number calculated by the NRT displacement model passes through a minimum value at about 20 keV, and the statistical significance of this minimum seems established. The increase above this value is reflected in the change in slope of the defect survival curve at 20 keV in Figure 1. The reason for the increase is still under investigation but it appears to be related to the spacing between the subcascades at higher energies. Inspection of the cascades indicates that point defects created in regions between subcascades have a higher probability of survival because the defect density in these regions is relatively low, similar to low energy cascades. Such regions of higher defect survival occur with greater frequency at the higher energies, giving rise to the greater-than-linear energy dependence. Initial analysis of a limited number of 100 keV cascades suggests that this effect may be saturating.

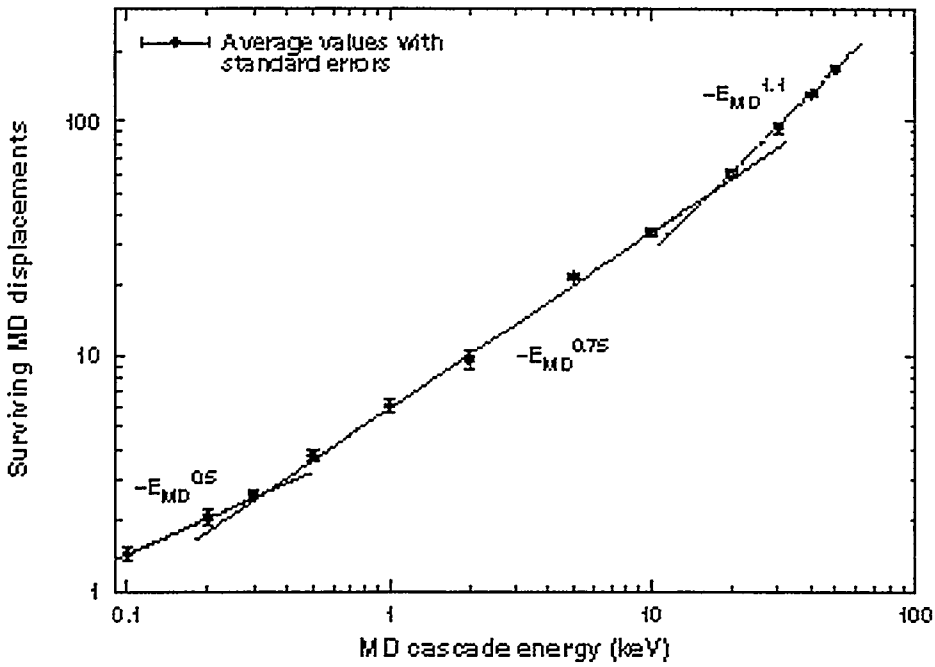

Figure 1. Number of surviving displacements in iron MD cascade simulations at 100K.