The Influence of PKA Direction on Displacement Cascade Evolution - Roger E. Stoller (Oak Ridge National Laboratory)

EXTENDED ABSTRACT

An extensive database of atomic displacement cascades in iron has been developed using molecular dynamic (MD) simulations. More than 300 cascades have been completed at 100K at energies between 100 eV and 100 keV, with fewer simulations at 600 and 900K. A systematic evaluation of the database has revealed an unexpected effect of PKA direction in MD simulations of 300 eV cascades in iron at 100K. A type of planar channeling was observed when the PKA direction lies in the close-packed {110} planes. An example of a cascade with a [114] direction is shown in Figure 1. Parts (a) and (b) of this figure show the peak damage condition in two different orientations, and part (c) shows the final configuration of stable defects. In this case, 6 stable vacancies and interstitials were created, whereas the average from a large number of cascades initiated in a high-index direction is about 2. The two-dimensional nature of cascade development leads to more efficient separation of vacancies and interstitials, thereby reducing in-cascade

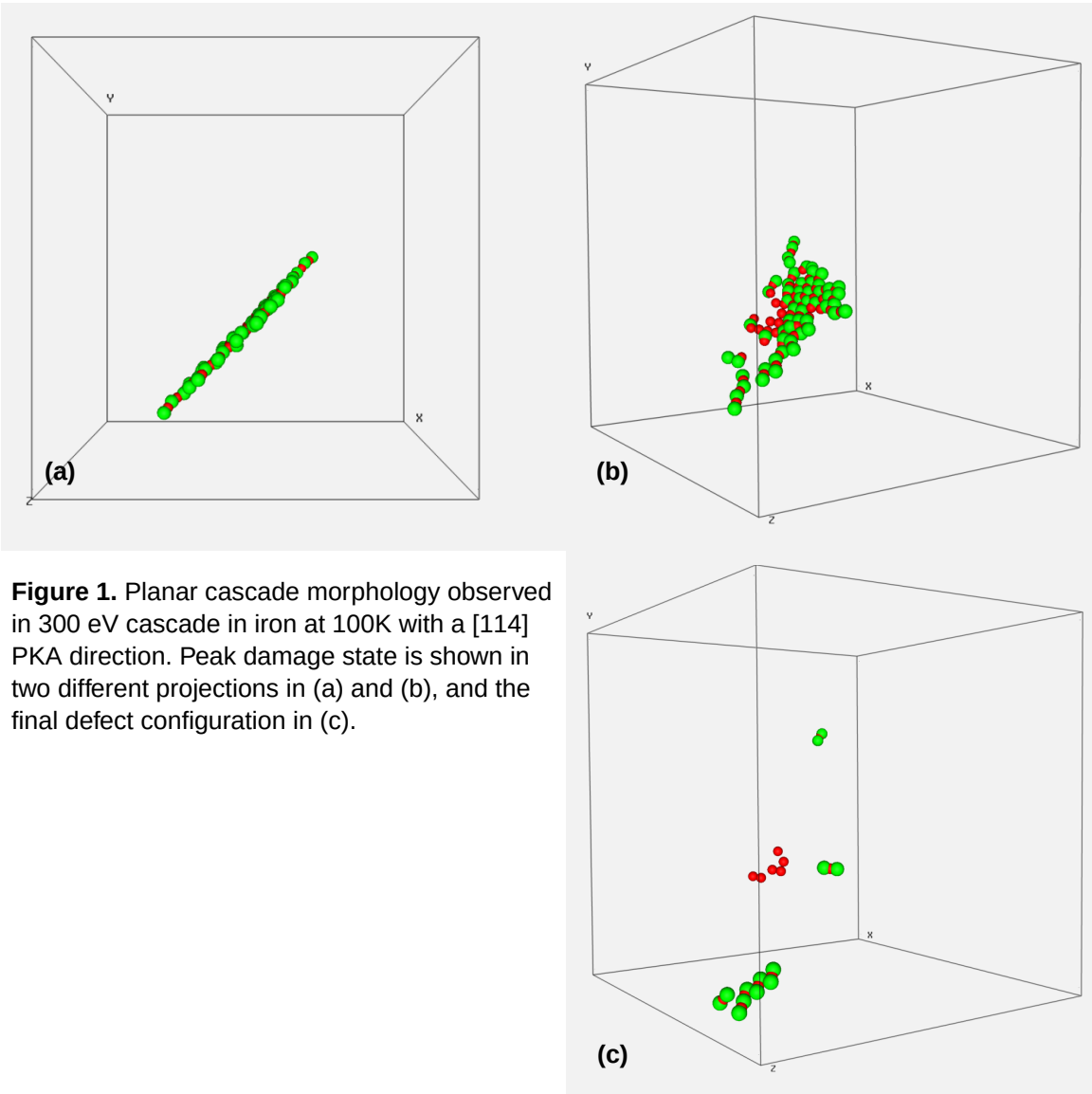

Figure 1. Planar cascade morphology observed in 300 eV cascade in iron at 100K with a [114] PKA direction. Peak damage state is shown in two different projections in (a) and (b), and the final defect configuration in (c).

recombination. Thus, a greater fraction of the radiation-produced interstitials and vacancies survive in cascades with a PKA directions that lies in a {110} plane.

The cascade shown in Figure 1 is perfectly planar, and the most extreme example out of the sixteen [114] cascades simulated. However, all the cascades were somewhat disk-like, leading to higher average defect survival. The magnitude if this effect is shown in Figure 2, where the average number of stable displacements is plotted for four different PKA directions: [135], [114], [121], and [123]. The [135] and [123] are relatively high index directions and the [114] and [121] lie in {110} planes. The average number of surviving displacements has been normalized by the value predicted by the standard NRT model [1]. The impact of PKA direction on in-cascade point defect clustering is less systematic since there is more cascade-to-cascade scatter in this parameter than in defect survival [2].

The PKA direction effect gradually disappears at higher energies as the atomic recoils have a greater probability of breaking out of the plane and generating a three-dimensional cascade. However, the data indicate that some dependence on PKA direction persists up to about 2 keV. The difference between the [135] and [114] averages is statistically significant at the 95% confidence level for the 300 eV simulations. The [114] defect survival was 15% higher than [135] at 2 keV, although this difference is not statistically significant at the 90% confidence level.

These results are probably most significant for low temperature irradiation conditions because increased thermal motion of the atoms may mitigate the effect at higher temperatures. The influence of irradiation temperature on the observed behavior is under investigation. Since the effect of PKA direction on defect survival persists up to cascade energies as high as 1-2 keV (~2.5 keV PKA energy), a thorough investigation of PKA direction effects in low-energy cascades should be carried out before choosing a single direction for high energy cascade simulations. Finally, it is interesting to note that the PKA directions which gave higher than average survival were not those directions with a low displacement threshold [3]. Thus, this effect should also be considered when interpreting the results of experiments intended to measure atomic displacement thresholds.

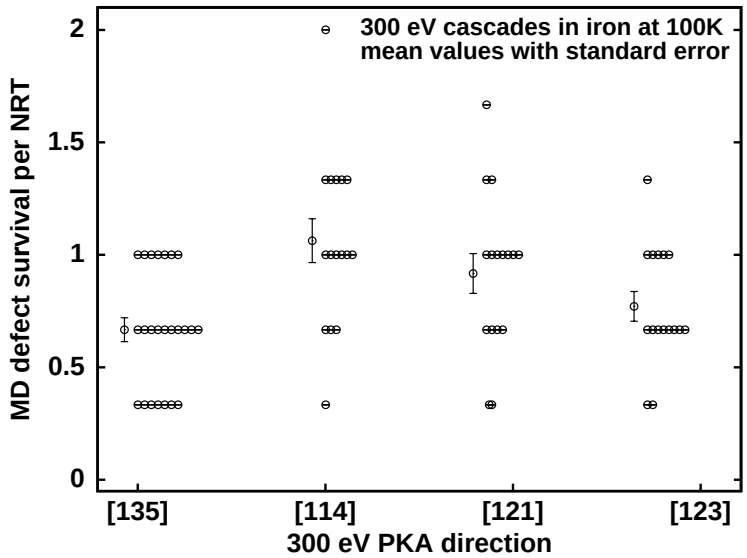

Figure 2. Effect of PKA direction on the number of stable displacements in MD cascade simulations, normalized by the NRT displacements.

ACKNOWLEDGEMENTS

This research was also supported by the Division of Materials Sciences and Engineering, U.S. Department of Energy and the Office of Nuclear Regulatory Research, U.S. Nuclear

Regulatory Commission under interagency agreement DOE 1886-N695-3W with the U.S. Department of Energy, under contract DE-AC05-00OR22725 with UT-Battelle, LLC.

REFERENCES

[1] M. J. Norgett, M. T. Robinson, and I. M. Torrens, Nucl. Eng. and Des. 33 (1975) 50.
[2] R.E. Stoller and A. F. Calder, J. Nucl. Mater., 283-287 (2001) 746.
[3] D. J. Bacon, A. F. Calder, J. M. Harder, and S. J. Wooding, J. Nucl. Mater. 205 (1993) 52.

(extended abstract of paper to be published by Materials Research Society in proceedings of Symposium R: Microstructural Processes in Irradiated Materials, Fall MRS Meeting)