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THE INFLUENCE OF PKA DIRECTION ON DISPLACEMENT CASCADE EVOLUTION

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ABSTRACT

An extensive database of atomic displacement cascades in iron has been developed using molecular dynamic 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 influence of PKA direction in low energy simulations. For primary knockon (PKA) directions that lie in the close-packed {110} planes, the cascade tends to be constrained to develop in only two dimensions. This planar “channeling” leads to much higher point defect survival than when a random high-index PKA direction is used to initiate the cascade. For example, the average number of stable Frenkel pair produced in 300 eV cascades is about 2.1 for cascades initiated with a [135] PKA, and 3.2 for [114] cascades. Some influence of this PKA direction effect was observed for energies up to 2 keV. The interstitial clustering behavior also appears to be affected in cascades with high defect survival.

INTRODUCTION

The exposure of materials to irradiation by high-energy particles leads to the formation of atomic displacement cascades. Depending on the energy of the initiating particle, these events involve from a few atoms to a few tens of thousands of atoms, and occur on the time scale of a few pico-seconds. The method of molecular dynamics (MD) was first applied to simulate cascade evolution around 1960 [1], but only in the last ten years have the capabilities provided by modern computers made it possible to simulate the high energy cascades relevant to nuclear energy systems [2-12]. For example, these same computational capabilities have permitted the development of an extensive library of atomic displacement cascade simulations in iron with cascade energies as high as 100 keV [12]. The analysis discussed in Ref. [12] provided a basis to determine the number of simulations required to obtain statistically-relevant mean values for several primary damage parameters as a function of cascade energy and temperature. This database has also permitted meaningful comparisons of primary radiation damage parameters in various irradiation environments to be made [13].

In order to avoid lattice effects such as channeling and directions with particularly low or high displacement thresholds, most MD cascade simulations are initiated using a high index PKA direction. For example, most of the simulations in the database discussed in Ref. [12] were generated using a [135] PKA direction. An initial investigation of PKA direction effects using 1 keV cascades indicated that mean values obtained with [135] PKA should be representative of the average behavior at this energy [10]. However, further analysis of the cascade database revealed unexpected phenomenon in the lower energy cascades that lead to relatively large differences in point defect production. These differences are discussed below, where it will be convenient to use the number of displacements calculated with the standard Norgett-Robinson-Torrens (NRT) model as a normalizing factor [15]. This number of displacements is $\nu_{NRT} = 0.8*T_{dam} / (2*E_d)$, where T_{dam} is the so-called damage energy [15] and E_d is the average displacement threshold, 40 eV for the case of iron [16]. Since the cascade energy is analogous to the damage energy in these MD simulations, the NRT model predicts that 3 stable Frenkel pair should be formed.

EFFECT OF PKA DIRECTION IN 300 eV CASCADES

The statistical analysis in Ref. [12] demonstrated that more simulations are required for low than for high cascade energies to obtain similar fractional standard errors. There were originally sixteen 300 eV cascades included in the database[5,7]. In order to improve the statistics, 24 additional 300 eV cascades were subsequently completed. The mean values for stable defect formation and the fraction of interstitials in clusters were found to be significantly different between these two populations. The differences were traced to an effect of PKA direction. Twelve different PKA directions were used in the initial 16 simulations, but only the [135] direction was used for the second set of 24. A review of the first 16 simulations indicated that simulations using [114] and [121] PKA directions appeared to be responsible for the differences.

In order to verify this observation, 16 additional simulations were carried out using four PKA directions: [135], [114], [121], and [123]. The [123] was added as second, relatively high index point of comparison. The results of these simulations are shown in Figure 1, where the normalized

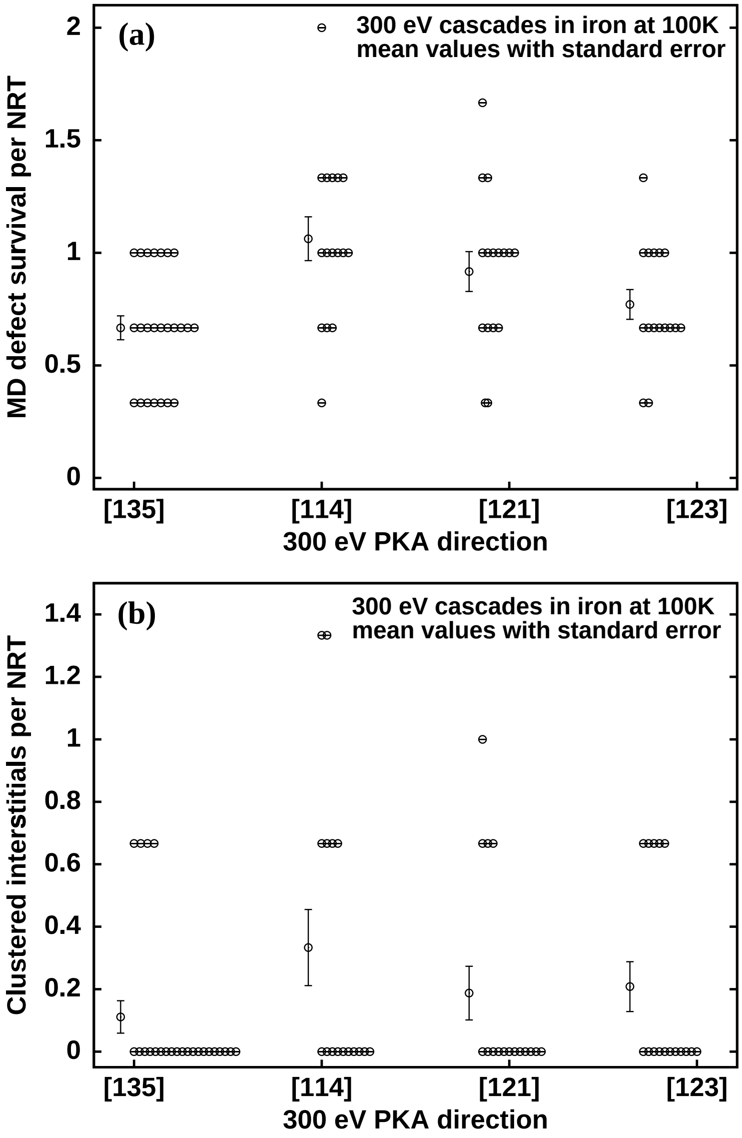

Figure 1. Effect of PKA direction on: (a) the number of stable displacement and, (b) the fraction of interstitials in clusters. Both are normalized using the NRT displacements.

number of stable defects produced is plotted in 1(a) and the normalized number of interstitials in cluster in 1(b). Stable defect survival is significantly greater for the [114] than for the [135] direction. The effect on defect survival is somewhat weaker for the [121] PKA direction, and [123] results are not significantly different than the [135]. The impact of PKA direction on interstitial clustering shown in Figure 1(b) is less systematic since there is more cascade-to-cascade scatter in this parameter than in defect survival [12]. More simulations would be required to establish the statistical significance of the small differences observed in this figure.

The reason for the increased defect survival for the [114] and [121] PKA directions appears to be the formation of a planar cascade morphology when the PKA direction lies in a close-packed {110} plane. A typical cascade using a [135] PKA direction is shown in Figure 2, where the peak damage state is shown in part (a) and the final, stable defect configuration in part (b). The [135] cascades develop isotropically, with a nearly spherical configuration of displaced atoms in the peak damage state shown in Figure 2(a). In this and the subsequent cascade images, the larger and lighter grey spheres are interstitial atoms and the smaller, darker spheres are vacant lattice sites. Only one stable interstitial-vacancy pair are created by the 300 eV cascade in Figure 2. The single interstitial is in the form of a <110> dumbbell.

In marked contrast to the isotropic [135] cascade, the morphology of the [114] cascade shown at the peak damage state in Figure 3 is completely planar. Two alternate projections are displayed in parts (a) and (b). All of the displaced atoms lie in the $(1\bar{1}0)$ plane, which contains the [114] PKA direction. Since the PKA energy is dissipated two-dimensionally, the vacancies and interstitials are separated to a greater extent and a larger fraction of the displaced atoms fail to recombine. As shown in Figure 3(c), six interstitial-vacancy pair are created by this cascade. Four of the interstitials (2/3 of the total) are in a single cluster of <111> dumbbells and crowdions. Although this was the only one of the sixteen [114] cascades that was perfectly constrained within a single plane, the morphology of all the [114] cascades tended to be disk-like. Similar observations were made when viewing the [121] cascades. One out sixteen was perfectly constrained to the $(10\bar{1})$ plane which contains the [121] direction. By analogy with its one-dimensional counterpart, the behavior observed in these cascades can be described as a planar channeling.

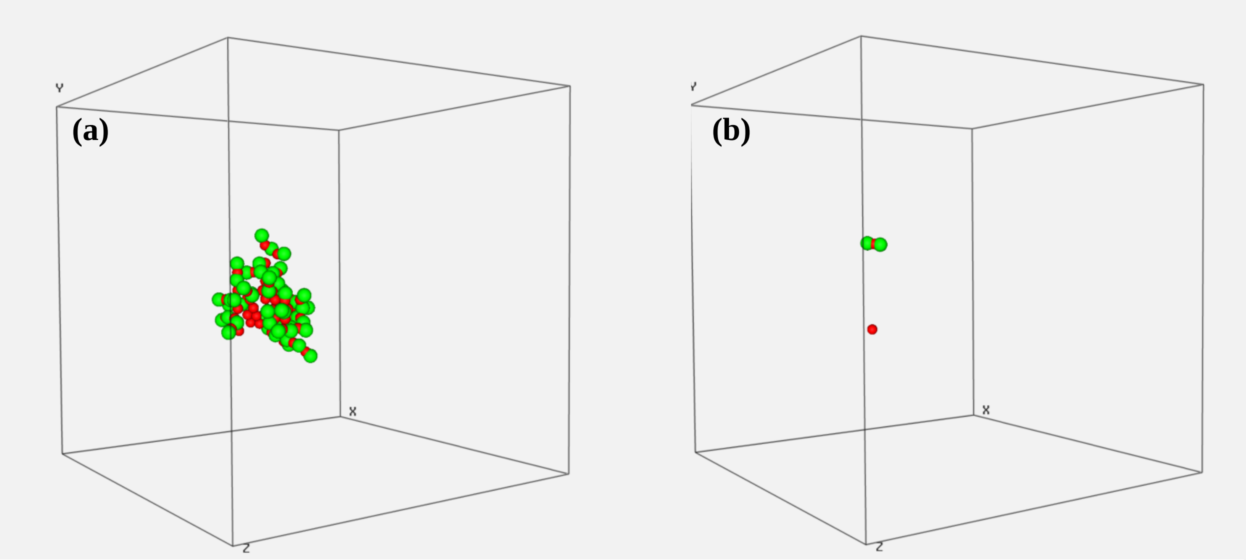

Figure 2. Typical cascade morphology for 300 eV cascade in iron at 100K using a [135] PKA direction. Peak damage state is shown in (a) and final defect configuration in (b).

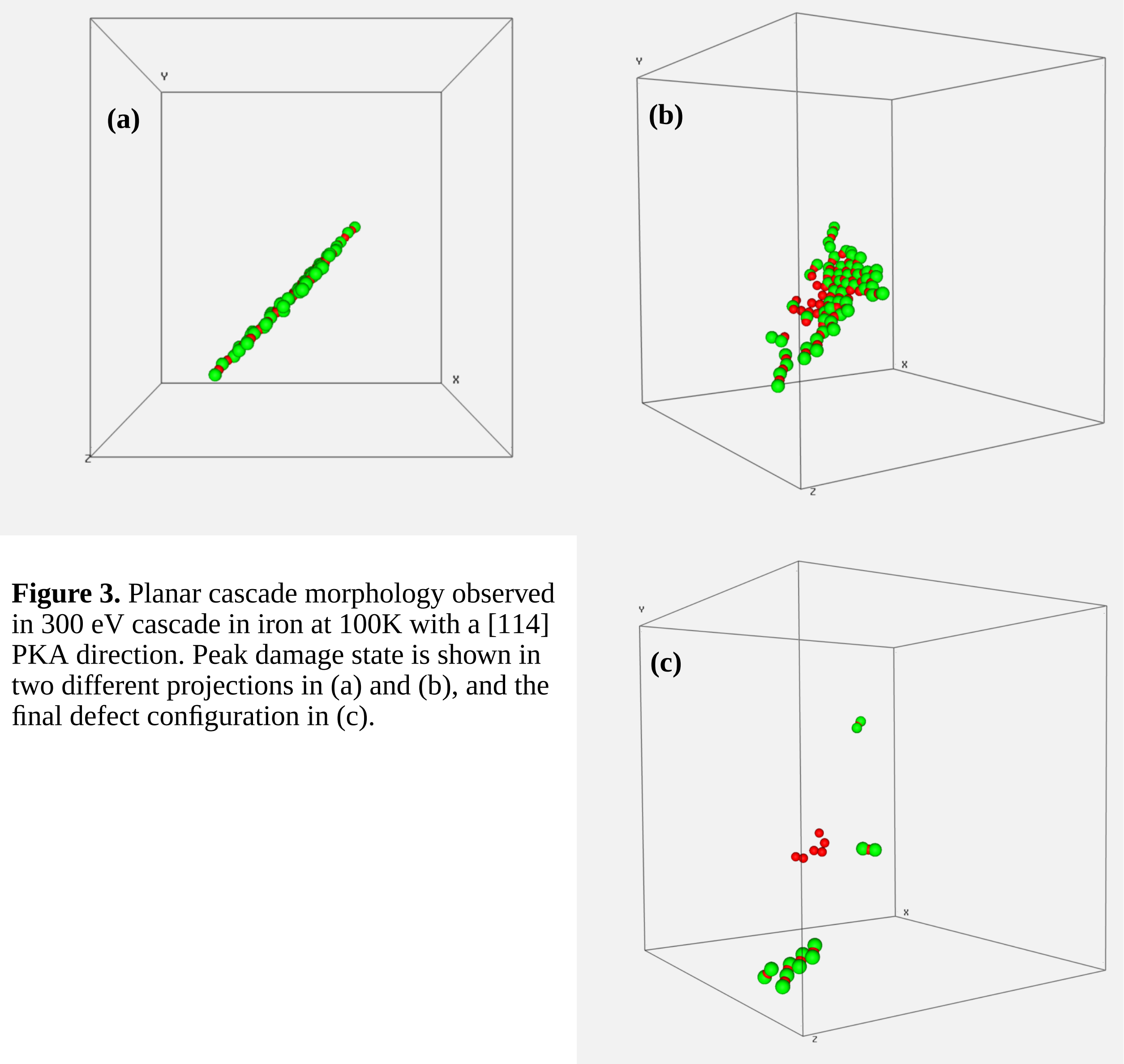

Figure 3. Planar cascade morphology observed in 300 eV cascade in iron at 100K with a [114] PKA direction. Peak damage state is shown in two different projections in (a) and (b), and the final defect configuration in (c).

EFFECT PKA DIRECTION AT HIGHER ENERGIES

It was expected that this planar “channeling” effect would only be observed at relatively low energies since high energy recoils would have a greater probability of transferring sufficient momentum to atoms out of the {110} plane. This was investigated by conducting additional cascade simulations at energies of 0.5, 1.0, 2.0, and 5 keV using the [114] PKA direction for comparison with the results to the [135] cascades completed previously. The normalized defect survival ratios for the highest three energies are shown in Figure 4. It was surprising to observe that the directional effect persists to some degree up to a cascade energy of about 2 keV. The ratio of the defect survival using [114] to that using [135] was 1.59, 1.12, 1.28, 1.15, and 0.995 for cascade energies of 0.3, 0.5, 1.0, 2.0 and 5.0 keV, respectively. Based on the number of simulations completed, the differences observed in the 1.0 keV simulations are significant at the 90% confidence level, while those at 2.0 keV are not.

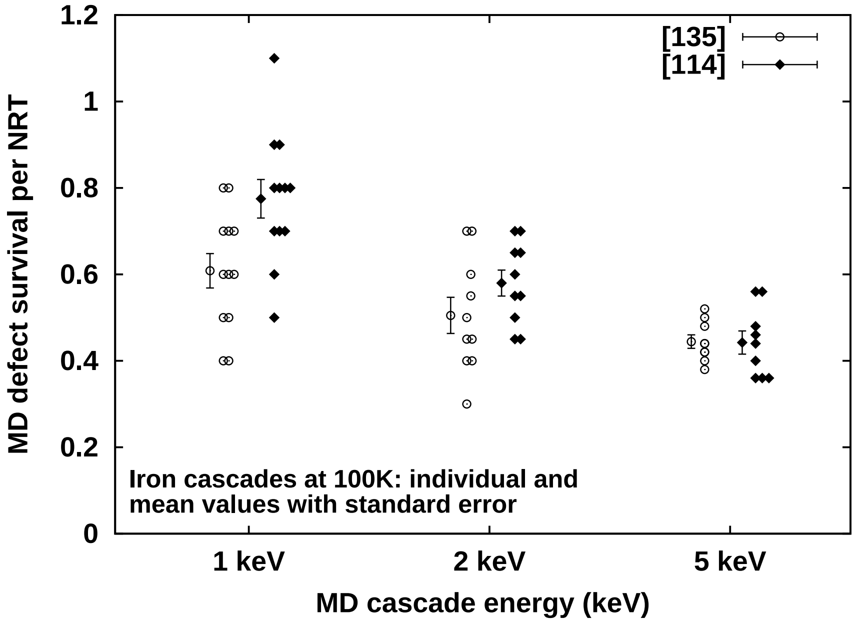

Figure 4. Effect of PKA direction on stable defect formation in iron cascades at 100K for cascade energies of 1, 2, and 5 keV, values normalized using the NRT displacements.

DISCUSSION AND SUMMARY

An unexpected effect of PKA direction was found 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. The two-dimensional nature of cascade development leads to more efficient separation of vacancies and interstitials, thereby reducing in-cascade recombination. Thus, a greater fraction of the radiation-produced interstitials and vacancies survive in cascades with PKA directions such as [114] and [121]. This 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. Interstitial clustering appears to be less sensitive to PKA direction than does total defect survival.

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 [17]. Thus, this effect should also be considered when interpreting the results of experiments intended to measure atomic displacement thresholds.

ACKNOWLEDGEMENTS

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REFERENCES

1. J. B. Gibson, A. N. Goland, M. Milgram, and G. H. Vineyard, Phys. Rev. 120 (1960) 1229.
2. R. S. Averback, T. Diaz de la Rubia, and R. Benedek, Nucl. Inst. and Meth. B33 (1988) 693.
3. T. Diaz de la Rubia and M. W. Guinan, J. Nucl. Mater. 174 (1990) 151.
4 A. J. E. Foreman, W. J. Phythian, and C. A. English, Phil. Mag. A66 (1992) 571.
5. A. F. Calder and D. J. Bacon, J. Nucl. Mater. 207 (1993) 25.
6. D. J. Bacon and T. Diaz de la Rubia, J. Nucl. Mater. 216 (1994) 275.
7. W. J. Phythian, R. E. Stoller, A. J. E. Foreman, A. F. Calder, and D. J. Bacon, J. Nucl. Mater. 223 (1995) 245.
8. R. E. Stoller, “Molecular Dynamics Simulations of High Energy Cascades in Iron,” *Microstructure of Irradiated Materials*, Symp. Proc. Vol. 373, I. M. Robertson, L. E. Rehn, S. J. Zinkle, and W. J. Phythian, Editors, Materials Research Society, Warrandale, PA, 1995, pp. 21-26.
9. R. E. Stoller, J. Nucl. Mater. 233-237 (1996) 999.
10. R. E. Stoller, G. R. Odette, and B. D. Wirth, J. Nucl. Mater. 251 (1997) 49.
11. R. E. Stoller, J. Nucl. Mater. 276 (1999) 22.
12. R.E. Stoller and A. F. Calder, J. Nucl. Mater., 283-287 (2001) 746.
13. R. E. Stoller and L. R. Greenwood, J. Nucl. Mater. 271 & 272 (1999) 57.
14. M. T. Robinson, “The Dependence of Radiation Effects on the Primary Recoil Energy,” *Radiation-Induced Voids in Metals*, Proc. of Int. Conf., J. W. Corbett and L. C. Ianniello, Eds., CONF-710601, U.S. National Technical Information Service, Springfield, VA, 1972, pp.397-428.
15. M. J. Norgett, M. T. Robinson, and I. M. Torrens, Nucl. Eng. and Des. 33 (1975) 50.
16. ASTM E521, Standard Practice for Neutron Radiation Damage Simulation by Charged-Particle Irradiation, Annual Book of ASTM Standards, Vol. 12.02, American Society of Testing and Materials, West Conshohocken, PA.
17. D. J. Bacon, A. F. Calder, J. M. Harder, and S. J. Wooding, J. Nucl. Mater. 205 (1993) 52.