INFLUENCE OF PKA DIRECTION, FREE SURFACES, AND PRE-EXISTING DEFECTS ON CASCADE DAMAGE FORMATION—R. E. Stoller and S. G. Guiriec (Oak Ridge National Laboratory)

OBJECTIVE

The objective of this work is characterize primary damage formation in irradiated structural materials, including the impact of all the various irradiation, material, and experimental conditions that may influence defect formation.

SUMMARY

Primary cascade damage production in iron has been extensively investigated by molecular dynamics, and average defect production parameters, such as the total number of stable point defects, in-cascade defect clustering fractions, and in-cascade cluster size distributions have been derived. However, preliminary results indicated several factors could alter "normal" cascade evolution and lead to quite different defect production behavior. Further investigations of three such factors have been carried out: (1) primary knock-on atom (PKA) direction, (2) nearby free surfaces, and (3) pre-existing effects. Results of the investigation confirm these factors can significantly impact cascade damage formation. The effects include enhanced defect survival for PKA directions that lie in close-packed {110} planes, increased point defect clustering and larger defect clusters for cascades initiated near a surface, and reduced defect survival in simulation cells containing defects. The origin and implications of these effects are discussed relative to the interpretation of certain experimental observations and parameters used in other modeling studies.

PROGRESS AND STATUS

Introduction

The use of molecular dynamics (MD) simulations to investigate the evolution of atomic displacement cascades has provided a detailed understanding of primary radiation damage formation in irradiated materials [1-10]. In particular, increased computational capability has enabled this method to be used to obtain a statistically meaningful cascade database for iron [1,5]. Representative values have been derived for several measures of primary damage, including: the number of stable point defects (interstitials and vacancies) created, the number of these stable defects that cluster directly during the cascade event, and the size distribution of these in-cascade defect clusters. For convenience when comparing different materials and cascade conditions, the number of displacements obtained from the standard NRT model [11,12] is often used as a normalizing factor for the number of defects produced and in clusters. This convention is followed in the present work.

Although the iron cascade database in the literature is relatively large, a number of factors have been identified that can cause cascade evolution, and hence defect production, to deviate from the average behavior exhibited in the database. Three of these factors are: PKA direction [3,13], presence of a nearby surface [8,9,14], and pre-existing defects (such as cascade debris) in the simulation cell [15,16]. In some cases, the results just referenced exhibited rather significant differences from the typical MD cascade that is carried out in an atomic simulation cell that contains perfectly crystalline material. However, in other cases the results were either ambiguous, limited in their parameter range, or an insufficient number of simulations were done to establish statistical significance. Since displacement cascades are stochastic events, the quantitative impact of any cascade variable can only be determined by a systematic study with "enough" events to capture inherent statistical variations in their behavior [1,5]. The objective of the current investigation is to establish the degree to which these three factors influence cascade evolution and defect formation by carrying out additional simulations and extending the range of the previous work to higher PKA energies and temperatures. Since the methods and models used have been discussed in detail in previous publications, [1-5,13,14] only a brief description is included here.

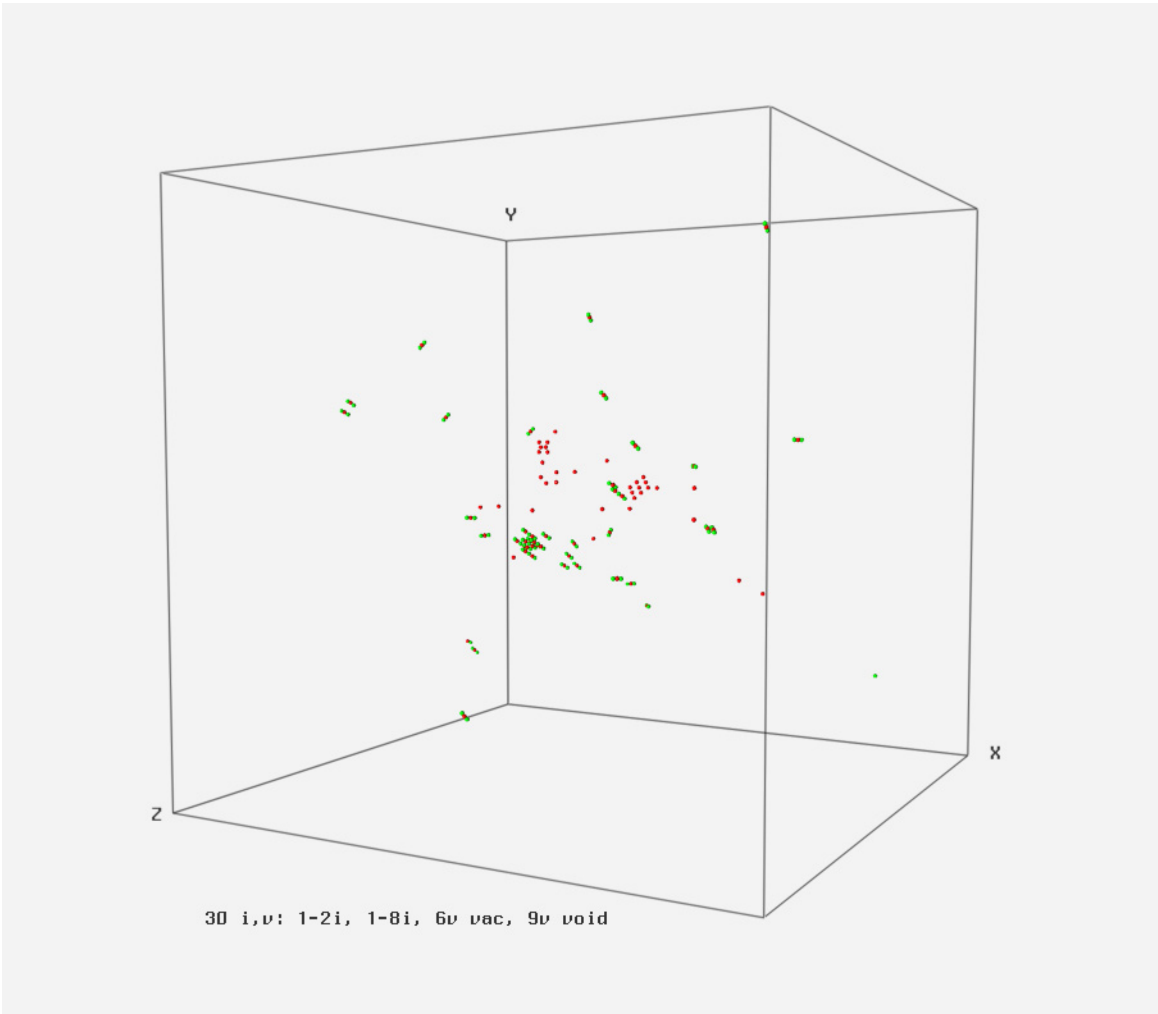

Fig. 4. Second pre-existing defect configuration for 10 keV displacement cascades (see text).

Although the approach in this investigation of pre-existing damage effects was slightly different, the results are generally consistent with the previous studies by English, et al. [15] and Gao, et al. [16]. In both cases, the authors observed substantial reductions in defect production when a cascade was initiated in material containing defects. The reductions in defect production observed in this study (Fig. 5 and Table 1) are somewhat smaller. This difference may partially be due to the higher cascade energy employed here (10 keV vs. 0.4 to 5 keV); but the statistical nature of cascade damage production is also a factor. A number of cascades were carried out in the work of Gao, et al., and the results were analyzed as a function of the distance between the center of mass (COM) of the new cascade and that of the pre-existing damage. A good correlation was found between this spacing and the number of defects produced, and their results provide a trend based on individual cascades as a function of COM distance. In the work reported here, the distance between the cascade origin and the pre-existing damage was nearly the same for all of the simulations. However, the morphology developed in each of the 8 cascades was quite different, so the COM spacings also varied. The average behavior for a fixed initial separation can not be directly compared to the earlier results. Because of the reduced defect survival observed in defective material, these results and the earlier work suggest that the possibility of developing a fluence-dependent cascade survival efficiency for use in kinetic radiation damage models should be investigated.

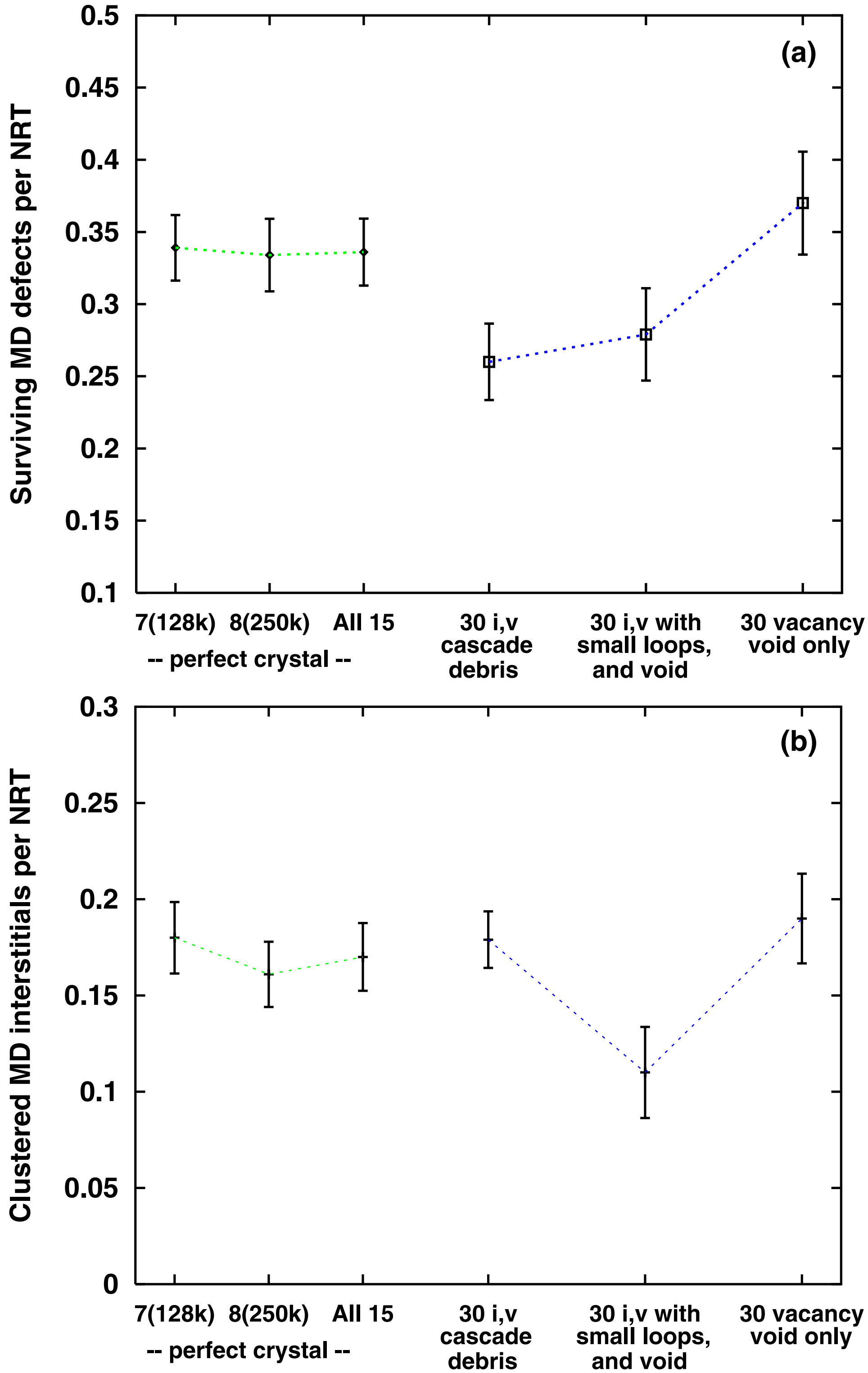

Fig. 5. Comparison of defect formation parameters in perfect and defective simulation cells: (a) total point survival and (b) interstitial clustering.

Acknowledgements

Research support for S. G. Guiriec was provided at ORNL during an internship for the Master of Engineering, Institut Supérieur des Matériaux du Mans (ISMANS), Le Mans, France.

References

[1] R. E. Stoller and A. F. Calder, *J. Nucl. Mater.* 283-287 (2000) 746-752.

[2] W. J. Phythian, R. E. Stoller, A. J. E. Foreman, A. F. Calder, and D. J. Bacon, *J. Nucl. Mater.* 223 (1995) 245.

[3] A. F. Calder and D. J. Bacon, *J. Nucl. Mater.* 207 (1993) 25-45.

[4] R. E. Stoller, G. R. Odette, and B. D. Wirth, *J. Nucl. Mater.* 251 (1997) 49-69.

[5] R. E. Stoller, *J. Nucl. Mater.* 276 (2000) 22-32.

[6] D. J. Bacon, F. Gao, and Yu. N. Osetsky, *J. Nucl. Mater.* 276 (2000) 1-12.

[7] M. J. Caturla, N. Soneda, E. Alonso, B. D. Wirth, T. Diaz de la Rubia, and J. M. Perlado, *J. Nucl. Mater.* 276 (2000) 13-21.

[8] K. Nordlund and R. S. Averback, *J. Nucl. Mater.* 276 (2000) 194-201.

[9] M. Ghaly and R. S. Averback, *Phys. Rev. Let.* 72 (1994) 364.

[10] K. Nordlund, J. Keinonen, M. Ghaly and R. S. Averback, *Nature* 398 (1999) 48.

[11] M. J. Norgett, M. T. Robinson, and I. M. Torrens, *Nucl. Engr. and Design* 33 (1975) 50-54.

[12] 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.

[13] R. E. Stoller, "The Influence of PKA Direction on Displacement Cascade Evolution," *Microstructural Processes in Irradiated Materials*, Vol. 650, G. E. Lucas, L. L. Snead, M. A. Kirk, and R. G. Elliman, Editors, Materials Research Society, Pittsburgh, PA, 2001, pp. 3.5.1-3.5.6.

[14] R. E. Stoller, *J. Nucl. Mater.* 307-311 (2002) 935-940.

[15] A. J. E. Foreman, W. J. Phythian, and C. A. English, private communication, unpublished.

[16] F. Gao, D. J. Bacon, A. F. Calder, P. E. J. Flewitt, and T. A. Lewis, *J. Nucl. Mater.* 276 (1996) 47-56.

[17] M. W. Finnis, "MOLDY6-A Molecular Dynamics Program for Simulation of Pure Metals," AERE R-13182, UKAEA Harwell Laboratory, Harwell, UK, 1988.

[18] M. W. Finnis and J. E. Sinclair, *Phil. Mag. A* 50 (1984) 45-55, and Erratum, *Phil. Mag. A* 53 (1986) 161.