SUBCASCADE FORMATION IN DISPLACEMENT CASCADE SIMULATIONS: IMPLICATIONS FOR FUSION REACTOR MATERIALS[1] — Roger E. Stoller (Oak Ridge National Laboratory)[2] and Lawrence R. Greenwood (Pacific Northwest National Laboratory)

Extended Abstract

Primary radiation damage formation in iron has been investigated by the method of molecular dynamics (MD) for cascade energies up to 40 keV. The initial energy EMD given to the simulated PKA is approximately equivalent to the damage energy in the standard secondary displacement model by Norgett, Robinson, and Torrens (NRT); hence, EMD is less than the corresponding PKA energy. Using the values of EMD in Table 1, the corresponding EPKA and the NRT defects in iron have been calculated using the procedure described in Ref. 1 with the recommended 40 eV displacement threshold [2]. These values are also listed in Table 1. Note that the difference between the EMD and the PKA energy increases as the PKA energy increases and that the highest simulated PKA energy of 61.3 keV is the average for a collision with a 1.77 MeV neutron. Thus, these simulations have reached well into the fast neutron energy regime. For purposes of comparison, the parameters for the maximum DT neutron energy of 14.1 MeV are also included in Table 1. Although the primary damage parameters derived from the MD cascades exhibited a strong dependence on cascade energy up to 10 keV, this dependence was diminished and slightly reversed between 20 and 40 keV, apparently due to the formation of well-defined subcascades in this energy region. Such an explanation is only qualitative at this time, and additional analysis of the high energy cascades is underway in an attempt to obtain a quantitative measure of the relationship between cascade morphology and defect survival.

The results of the MD simulations have been used in the SPECOMP code to obtain effective, energy-dependent cross sections for two measures of primary damage production: (1) the number of surviving point defects expressed as a fraction of the those predicted by the NRT model, and (2) the fraction of the surviving interstitials contained in clusters. PKA spectra for iron were obtained from the SPECTER code and used to weight the MD-based damage production cross sections in order to obtain spectrum-averaged values for various irradiation environments. The primary results of these calculations are summarized in Fig. 1, where the PKA-spectrum-averaged defect survival fraction is shown in Fig. 1a, and the interstitial clustering fraction in Fig. 1b. Both average cross sections have been divided by the NRT dpa cross section. To provide a broad comparison, results are listed for: the ITER first wall, HFIR PTP and RB* positions, FFTF midcore and below core locations, and the 1/4-thickness position in a commercial reactor pressure vessel.

The average defect survival fraction decreases as the average PKA energy increases. Thus, the lowest defect survival is obtained in the ITER first wall which has the highest average PKA energy as result of the 14.1 MeV neutron source term. However, the differences between the various environments are small. This similarity arises for two reasons. First, the differences between the various fission and fusion PKA spectra are relatively modest in the region below about 10 keV where the energy dependence of the defect survival fraction is strongest. Then, when the PKA spectra become more different at higher energies, the defect survival fraction becomes nearly

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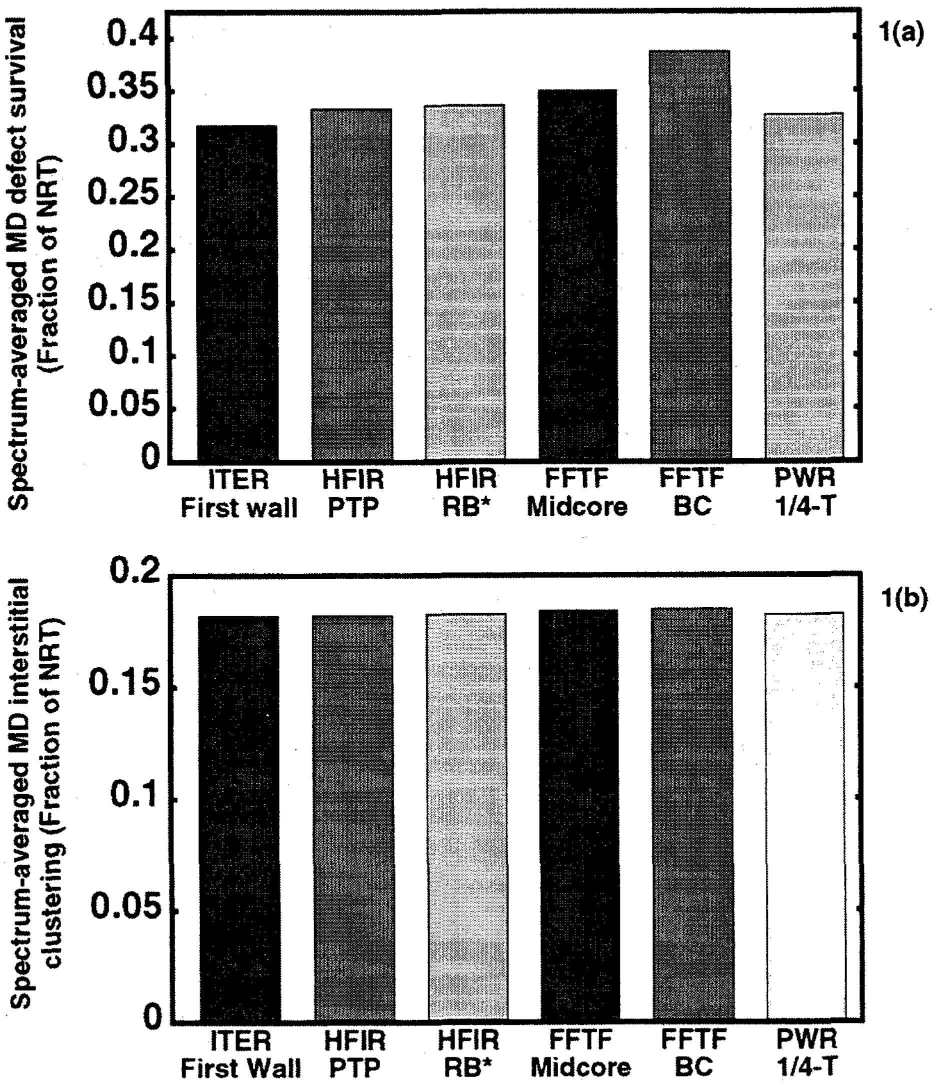

Figure 1. Comparison of spectrally-averaged damage production cross sections (per NRT dpa) for various irradiation environments; point defect survival ratio is shown in (a) and the interstitial clustering fraction is shown in (b).

independent of energy. The average interstitial clustering fraction shown in Fig. 1b is almost independent of the initial neutron energy spectrum.

The spectrum-averaged primary damage parameters shown in Fig. 1 are only weakly dependent on the initial neutron energy spectrum. This result appears unlikely to change significantly if higher energy cascades are included in the analysis. In particular, the extensive subcascade formation observed at 40 keV suggests that the results reported here should be relevant to high-energy neutron sources such as ITER. This conclusion implies that the displacement damage component of radiation damage produced in a DT fusion reactor should be well simulated by irradiation in a fission reactor neutron spectrum, and that differences in nuclear transmutation production may be the primary source of uncertainty in the prediction of material performance at high doses in DT fusion reactors.

Table 1. Typical MD cascade parameters and required atom block sizes

Neutron Energy (MeV)	Average PKA Energy (keV)	Corresponding EMD (keV)	NRT Displacements	Atoms in Simulation
0.00335	0.116	0.1	1	3,456
0.00682	0.236	0.2	2	6,750
0.0175	0.605	0.5	5	6,750
0.0358	1.24	1.0	10	54,000
0.0734	2.54	2.0	20	54,000
0.191	6.6	5.0	50	128,000
0.397	13.7	10.0	100	250,000
0.832	28.8	20.0	200	250,000
1.77	61.3	40.0	400	1,024,000
14.1	487.	220.4	2204	(1)

(1) no simulations done, displacement parameters included for comparison only

References

1. M. J. Norgett, M. T. Robinson, and I. M. Torrens, Nucl. Eng. and Des. 33 (1975) 50-54.
2. 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, Philadelphia.