TOTAL DPA CROSS SECTIONS FOR SIC AS A FUNCTION OF NEUTRON ENERGY - H. L. Heinisch, L. R. Greenwood, W. J. Weber and R. E. Williford (Pacific Northwest National Laboratory)*

OBJECTIVE

The objective of this work is to calculate total DPA cross sections for SiC as a function of neutron energy using the best available input for stopping powers and displacement threshold energies.

SUMMARY

Total DPA cross sections for SiC as a function of neutron energy have been calculated using the latest and best knowledge about damage production in SiC. We encourage the adoption of these cross sections as the standard to be used for calculating radiation damage production in DPA for all neutron-irradiated SiC samples, including those in past irradiations.

PROGRESS AND STATUS

This is an extended abstract of a paper entitled "Displacement Damage And Transmutation Calculations For Neutron-Irradiated Silicon Carbide" by H. L. Heinisch, L. R. Greenwood, W. J. Weber and R. E. Williford, which has been submitted for publication in the Journal of Nuclear Materials.

Introduction

The standard damage parameter for nuclear materials is displacements per atom (DPA), which incorporates information on the response of the material, i.e. displaced atoms, as well as simply the (fast) neutron fluence to which it was exposed. The concept of DPA was initially developed for monatomic metals, where the definition of DPA is somewhat simpler than in multi-component ceramic materials where the various atom displacement energies are not easily measured. In the past few years significant progress has been made in modeling displacement damage in SiC using molecular dynamics computer simulations to determine displacement threshold energies [1] and employing improved models for stopping powers [2]. This information has been utilized for the calculation of DPA cross sections for SiC as a function of neutron energy [3].

To be most useful, the DPA damage parameter should be defined and calculated the same way by all concerned, and preferably for all past, present and future experiments, models and analyses. To that end, we include here the DPA cross sections as a function of neutron energy for SiC in tabulated form, Table 1. This function, along with neutron flux and energy spectrum information, can be used to calculate the DPA value for SiC in any irradiation.

Displacements per Atom

Displacements per atom is a calculated, hypothetical measure of radiation damage that reflects not only the dose and type of irradiation, but also includes some measure of the material's response to the irradiation. DPA is not a measure of the residual crystal lattice defects actually created in a material, but rather it is a measure of the "damage energy" deposited in the material by the irradiating particles in terms of how many atoms could possibly be permanently displaced from their lattice sites to stable interstitial sites by this damage energy. In each individual radiation damage event, the primary knock-on atom (PKA, an atom that has received kinetic energy through interaction with an irradiating neutron) imparts energy to neighboring atoms, producing a cascade of collisions. Within the affected volume of the collision cascade many atoms are displaced significantly from their lattice sites, creating a near-molten zone in the crystal. But within picoseconds many of the displaced atoms return to vacant sites, healing

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much of the damage. The actual number of lattice defects ("permanently" displaced atoms) remaining after the cascade region cools is usually a small fraction of the atoms initially displaced in the cascade. This fraction is often referred to as the "efficiency" of defect production relative to the calculated DPA value, and it can vary considerably depending on the material and the irradiating conditions, including neutron energies and irradiation temperature. Although it does not reflect the actual residual defects produced in the material, DPA has been found to be an extremely useful damage parameter for correlating the effects of radiation damage in the same material irradiated in different neutron environments, and it is the standard damage parameter for nuclear structural materials.

The original model for displacement damage, developed initially for simple metals, is due to Kinchin and Pease [4], and the standard formulation of it by Norgett et al [5], often referred to as the "NRT" model, is

$$\begin{aligned} \nu(T) &= 0 && T < E_d \\ &= 1 && E_d < T < 2E_d \\ &= 0.8\, T/2E_d && T > 2E_d \end{aligned} \qquad (1)$$

where $\nu(T)$ is the number of displaced atoms produced by a recoil atom of energy E and damage energy T, and E_d is the average threshold displacement energy for an atom in the metal. Damage energies T(E) can be calculated for each recoil energy E using an analytic expression due to Robinson [6]. The threshold displacement energy E_d can be determined experimentally for simple metals, while for more complicated materials, such as polyatomic materials or those with complex crystal structures, where there may be several different displacement energies, the values of E_d are best determined with the aid of computer simulations. The energies required to displace Si and C atoms from their lattice sites to interstitial positions in SiC have been determined using atomic-scale molecular dynamics and first principles calculations [1]. The values of displacement energies averaged over all directions in SiC have been determined to be 20 eV for C and 35 eV for Si, and it is recommended that these values be used universally for calculating DPA in irradiated SiC [7]. There are actually four minimum recoil damage energies required to create displacements in SiC, depending on the projectile/target combinations: 41 eV (C/Si), 35 eV (Si/Si), 24 eV (Si/C) and 20 eV (C/C) [3]. Thus, a C atom must have kinetic energy of at least 41 eV to provide the 35 eV to a Si atom that is necessary to displace it.

Treating polyatomic materials introduces other complications to the formulation of damage functions due to the interactions among sublattices. Thus, in the present work displacement functions for polyatomic materials, $\nu_{ij}(E)$, for the average number of atoms of type j initiated by a PKA of type i and energy E, were obtained by numerical solutions of the coupled integro-differential equations for $\nu_{ij}(E)$ devised by Parkin and Coulter [8-10] and using the displacement energies discussed above. Atomic scattering cross sections based on the Ziegler, Biersack, and Littmark (ZBL) universal screening potential [11] were used in the calculation of the displacement functions, and the electronic stopping powers used in the calculations were generated from the SRIM 2000 electronic stopping power database [12]. The use of these representations of the scattering and stopping powers in the calculation of displacement functions for SiC is demonstrated and discussed in Reference [2].

The damage functions $\nu_{ij}(T)$ are integrated over the PKA damage energy spectrum for a neutron of energy E_n in the material, to yield the Si, C and total (Si + C) displacement cross sections for neutrons of energy E_n. This has been done for SiC using the SPECOMP code [13], and the results for total DPA cross sections are tabulated in Table 1 and shown graphically in Figure 1 as a function of E_n.

Spectrally Averaged DPA Cross Sections

When the displacement function is integrated over the flux spectrum of neutron energies for a given reactor location, the result is a cross section for total DPA in SiC averaged over the neutron energy spectrum. The total DPA obtained by a SiC specimen in a specific irradiation is then the product of the spectrally averaged DPA cross section for SiC and the total neutron fluence received by the specimen.

Table 1. Total DPA cross sections in barns for SiC as a function of neutron energy in MeV.

E,MeV	σ_d, b
1.00E-10	4.14E+00
1.00E-09	1.31E+00
1.00E-08	6.84E-01
2.30E-08	4.58E-01
5.00E-08	3.44E-01
7.60E-08	2.80E-01
1.15E-07	2.30E-01
1.70E-07	1.88E-01
2.55E-07	1.54E-01
3.80E-07	1.27E-01
5.50E-07	1.04E-01
8.40E-07	8.43E-02
1.28E-06	6.86E-02
1.90E-06	5.66E-02
2.80E-06	4.61E-02
4.25E-06	3.75E-02
6.30E-06	3.11E-02
9.20E-06	2.57E-02
1.35E-05	2.10E-02
2.10E-05	1.72E-02
3.00E-05	1.42E-02
4.50E-05	1.15E-02
6.90E-05	9.46E-03
1.00E-04	8.02E-03
1.35E-04	7.03E-03
1.70E-04	6.25E-03
2.20E-04	9.53E-02
2.80E-04	3.56E-01
3.60E-04	1.60E+00
4.50E-04	1.34E+00
5.75E-04	1.15E+00
7.60E-04	2.86E+00
9.60E-04	3.74E+00
1.28E-03	2.91E+00
1.60E-03	4.32E+00
2.00E-03	6.89E+00
2.70E-03	9.07E+00
3.40E-03	1.06E+01
4.50E-03	1.38E+01
5.50E-03	1.95E+01
7.20E-03	2.36E+01
9.20E-03	2.69E+01
1.20E-02	3.06E+01
1.50E-02	3.91E+01
1.90E-02	4.91E+01
2.55E-02	5.90E+01
3.20E-02	7.26E+01
4.00E-02	8.86E+01
5.25E-02	1.79E+02
6.60E-02	1.51E+02
8.80E-02	1.54E+02
1.10E-01	1.54E+02
1.35E-01	1.51E+02
1.60E-01	4.67E+02
1.90E-01	6.32E+02
2.20E-01	5.04E+02
2.55E-01	4.62E+02
2.90E-01	4.16E+02
3.20E-01	4.08E+02
3.60E-01	4.53E+02
4.00E-01	4.25E+02
4.50E-01	4.75E+02
5.00E-01	4.89E+02
5.50E-01	5.28E+02
6.00E-01	4.67E+02
6.60E-01	4.78E+02
7.20E-01	5.20E+02
7.80E-01	8.01E+02
8.40E-01	5.75E+02
9.20E-01	7.22E+02
1.00E+00	5.19E+02
1.20E+00	5.95E+02
1.40E+00	6.08E+02
1.60E+00	6.03E+02
1.80E+00	8.27E+02
2.00E+00	6.02E+02
2.30E+00	6.60E+02
2.60E+00	7.15E+02
2.90E+00	7.09E+02
3.30E+00	6.92E+02
3.70E+00	9.96E+02
4.10E+00	7.96E+02
4.50E+00	8.46E+02
5.00E+00	7.04E+02
5.50E+00	7.01E+02
6.00E+00	6.49E+02
6.70E+00	6.42E+02
7.40E+00	9.25E+02
8.20E+00	7.31E+02
9.00E+00	8.08E+02
1.00E+01	7.99E+02
1.10E+01	8.57E+02
1.20E+01	8.86E+02
1.30E+01	8.79E+02
1.40E+01	8.70E+02
1.50E+01	9.21E+02
1.60E+01	9.05E+02
1.70E+01	8.72E+02
1.80E+01	9.36E+02
1.90E+01	9.20E+02
2.00E+01	

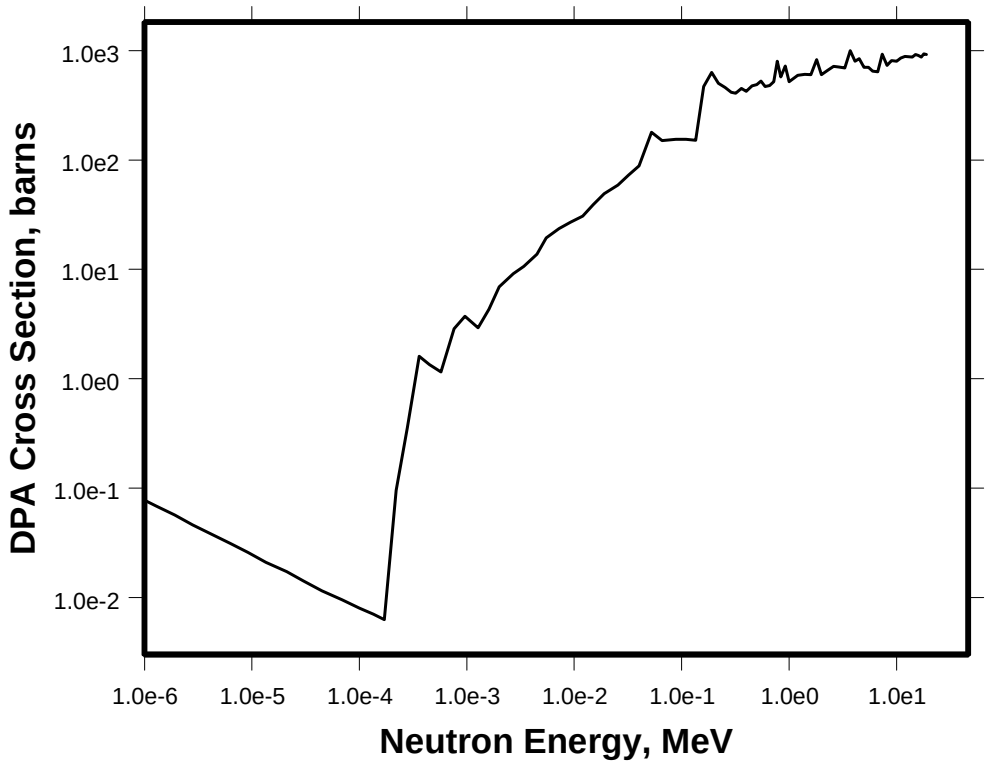

Figure 1. Total DPA cross sections in barns for SiC as a function of neutron energy in MeV.

Conclusions

The DPA cross sections in Table 1 represent the latest and best knowledge about damage production in SiC. We encourage the adoption of these cross sections as the standard to be used for calculating radiation damage production in DPA for all neutron-irradiated SiC samples, including those in past irradiations if possible.

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REFERENCES

[1] R. Devanathan and W. J. Weber, J. Nucl. Mater. 278 (2000) 258.

[2] W. J. Weber, R. E. Williford and K. E. Sickafus, J. Nucl. Mater. 244 (1997) 205.

[3] H. Heinisch, L. R. Greenwood, W. J. Weber and R. E. Williford, J. Nucl. Mater. 307-311 (2002) 895.

[4] G. H. Kinchin and R. S. Pease, Rep. Prog. Phys. 18 (1955) 1.

[5] M. J. Norgett, M. T. Robinson and I. M. Torrens, Nucl. Eng. Design 33 (1975) 50.

[6] M. T. Robinson, Nuclear Fusion Reactors, Proc. British Nuclear Energy Soc., UKAEA, London, (1970) 364.

[7] R. Devanathan, W. J. Weber, and F. Gao, J. Appl Phys. 90 (2001) 2303.

[8] D. M. Parkin and C. A. Coulter, J. Nucl. Mater.101 (1981) 261.

[9] D. M. Parkin and C. A. Coulter, J. Nucl. Mater.103-104 (1981) 1315.

[10] D. M. Parkin and C. A. Coulter, J. Nucl. Mater.117 (1983) 340.

[11] J. F. Zeigler, J. P. Biersack and U. Littmark, The Stopping and Range of Ions in Solids (Pergamon Press, New York, 1985).

[12] J. F. Zeigler, SRIM-2000, code and manuals available on the Internet at http://www.srim.org, (2001).

[13] L. R. Greenwood, Reactor Dosimetry: Methods, Applications, and Standardization, ASTM STP 1001(1989) 598.