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Displacement damage cross sections for neutron-irradiated silicon carbide

H.L. Heinisch *, L.R. Greenwood, W.J. Weber, R.E. Williford

Pacific Northwest National Laboratory, P8-15, P.O. Box 999, Richland, WA 99352, USA

Abstract

Displacements per atom (DPA) is a widely used damage unit for displacement damage in nuclear materials. Calculating the DPA for SiC irradiated in a particular facility requires a knowledge of the neutron spectrum as well as specific information about displacement damage in that material. In recent years significant improvements in displacement damage information for SiC have been generated, especially the energy required to displace an atom in an irradiation event and the models used to describe electronic and nuclear stopping. Using this information, numerical solutions for the displacement functions in SiC have been determined from coupled integro-differential equations for displacements in polyatomic materials and applied in calculations of spectral-averaged displacement cross sections for SiC. This procedure has been used to generate spectrally averaged displacement cross sections for SiC in a number of reactors used for radiation damage testing of fusion materials, as well as the ARIES-IV conceptual fusion device.

1. Introduction

Silicon carbide and silicon carbide fiber-reinforced silicon carbide composites hold great promise as structural and component materials in neutron radiation environments. They maintain significant high-temperature strength and stability along with high thermal conductivity in nuclear applications, and they are inherently low-activation materials. In the course of developing and testing SiC materials for nuclear applications, it is very useful to have a standard method for determining and comparing the amount of displacement damage they receive in test irradiations, as well as projecting the effects of displacement damage on their properties in expected applications.

A necessary first step in studying the effects of displacement damage in a material under irradiation is to define a standard measure of the displacement damage it suffers. Displacements per atom (DPA) is a widely used damage unit for displacement damage in nuclear materials. It is especially useful for correlating damage between different neutron radiation environments because it integrates information on the dose and type of irradiation received with a measure of the material's response to it, as opposed to merely counting the number of fast neutrons to which it was exposed. Thus, calculating DPA in irradiated SiC requires specific information about the interactions of neutrons or ions with the atoms of the material as well as quantitative information on the creation of displacement damage in that material by the energetic primary knock-on atoms (PKA). In particular, the amount of displacement damage created depends on the 'damage energy', the amount of energy deposited in the material in an irradiation event that is capable of creating displacement damage, and the 'displacement energy', the amount of damage energy required to displace an atom of the material from its crystal lattice site to a stable interstitial position. At PKA energies where cascades of displacements are produced in high local concentration, considerable recombination of vacancy-interstitial atom pairs occurs in the cascade volume as the residual thermal energy dissipates. Thus DPA is an idealized, calculated quantity, and the number of displacements calculated for an irradiation usually far exceeds the number of stable,

* Corresponding author. Tel.: +1-509 376 3278; fax: +1-509 376 0418.

E-mail address: hl.heinisch@pnl.gov (H.L. Heinisch).

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residual lattice defects actually formed in the material. The actual number of defects in an irradiated material also depends on many other factors, including the temperature, damage rate and condition of the material.

The concept of DPA was originally developed for monatomic metals and it has been extended to alloys by taking simple weighted combinations of monatomic values according to the alloy composition. This is a reasonable procedure, especially when atomic masses of the constituents are similar. In ceramic compounds the displacement damage occurs on the various separate sublattices, and the number of displacements associated with each sublattice depends on the types of the projectile and target atoms. This requires a revised physical model for DPA in ceramic compounds as compared to metals. Also, for compounds of elements having relatively low atomic numbers, such as SiC, the models originally developed for determining damage energy in metals are not appropriate.

The earliest calculations of displacement damage functions and simulations of displacement energies for SiC [1–3] suffered from various deficiencies, and the various efforts to experimentally determine displacement energies show a wide variation in results [4]. Building on these pioneering efforts, Weber and coworkers [5–7] have performed computer simulations of displacement energies in SiC and refined the method for calculating displacement functions for SiC to achieve the best possible representation for DPA in SiC, including consistency with experimental results.

In this paper we briefly review the results of recent computer simulations and damage modeling that have lead to what has been proposed as the standard method for calculating DPA in SiC, then we show the results of calculations using this method in the form of a table of DPA cross sections spectrally averaged over neutron energy spectra for a number of neutron irradiation test facilities and a conceptual fusion reactor.

2. Displacement functions for SiC

The standard method for calculating DPA, originally developed for metals, is the modified Kinchin–Pease method due to Norgett et al. [8], often referred to as the 'NRT' model. Damage energies can be calculated using an analytic expression due to Robinson [9], and the displacement damage function is

$$\begin{aligned} \nu(T) &= 0 \quad T < E_{\mathrm{d}}, \\ &= 1 \quad E_{\mathrm{d}} < T < 2E_{\mathrm{d}}, \\ &= 0.8T/2E_{\mathrm{d}} \quad T > 2E_{\mathrm{d}}, \end{aligned} \tag{1}$$

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. The damage function is integrated over the PKA energy spectrum for a neutron of energy E_{n} and then integrated over the spectrum of neutron energies for a given reactor location. This results in a cross section for DPA averaged over the neutron energy spectrum. The DPA for a given material irradiated in a given neutron spectrum is then the product of the spectrally averaged DPA cross section and the total neutron fluence received by the specimen.

2.1. Displacement energies

Atomic-scale molecular dynamics and first principles calculations have been employed to determine displacement energies of Si and C atoms in SiC [6]. Displacement energies are directionally dependent, and the displacement energies are different for Si and C atoms. Simple geometrical averages give too much weight to the higher energy displacement directions, so additional information on displacements has been obtained from simulations of low energy displacement cascades in which many atoms are displaced at the same time in various directions selected 'naturally' by the collisions within the cascade event. Based on both single displacements and cascade simulations, as well as consistency with experimental values, 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. It is recommended that these values be used universally for calculating DPA in irradiated SiC [7].

2.2. Polyatomic materials

For compounds such as SiC the displacement damage occurs on each sublattice and is a result of collisions between like and unlike atoms. Thus there are four possible combinations of projectile and target atoms: Si/Si (Si PKA and Si displacement), Si/C, C/Si and C/C. The maximum (damage) energy transferred in a collision depends on the atomic masses through the factor $\Lambda_{12} = 4M_1M_2/(M_1 + M_2)^2$. Thus, the minimum damage energy needed by a Si recoil atom to create a C displacement is $E_{\mathrm{d}}(C)/\Lambda_{\mathrm{SiC}}$. There are actually four minimum recoil damage energies required to create displacements in SiC, depending on the projectile/target combinations. Given the masses of Si and C, the two displacement energies 35 and 20 eV for Si and C, respectively, and $\Lambda_{\mathrm{SiC}} = 0.84$, a displacement can be achieved with minimum recoil damage energies of 41 eV (C/Si), 35 eV (Si/Si), 24 eV (Si/C) and 20 eV (C/C).

Parkin and Coulter [10–12] devised 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, that are described in terms of coupled integro-differential equations. In the present work nu-

merical solutions for the displacement functions in SiC have been determined from these coupled integro-differential equations and the displacement energies discussed above. Atomic scattering cross sections based on the Ziegler, Biersack, and Littmark (ZBL) universal screening potential [13] 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 [14]. The use of these representations of the scattering and stopping powers in the calculation of displacement functions for SiC is demonstrated and discussed in [5]. The results of these displacement function calculations for the Si on C combination are illustrated in Fig. 1.

The low energy behavior of the calculated displacement function in Fig. 1 is different from the NRT model in that it decrease smoothly to values <1 at damage energies less than the displacement threshold energies. To maintain consistency with the concepts of the NRT model, we have modified the calculated displacement functions to have the step function behavior similar to Eq. (1). In SiC electronic energy losses are significant at small PKA energies, unlike in metals. Thus, in SiC the damage energy is noticeably smaller than the recoil energy even at small recoil energies. This fact was taken into account in determining the energies at which the step functions were introduced. The modified displacement function for Si on C is also shown for comparison in Fig. 1. The modified displacement functions for the four combinations of projectile and target are shown in Fig. 2. Since this modification affects only the low energy end of the displacement function, the DPA cross sections calculated with the two versions of the displacement functions exhibit negligible differences for any of the neutron spectra we have used.

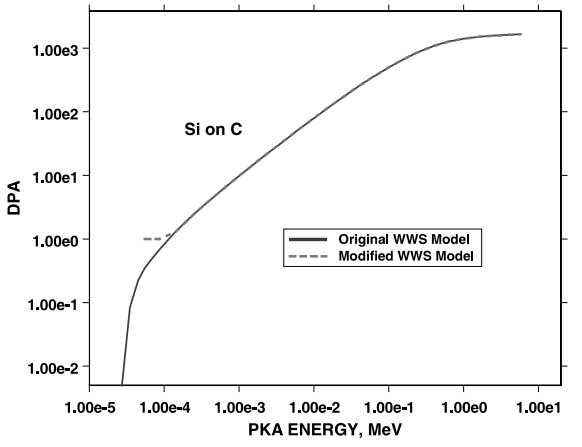

Fig. 1. Displacement functions for Si projectiles on C targets. The solid line is the original model of Weber et al. [5], and the dashed line shows the modification for the Kinchin–Pease type behavior at energies at the displacement threshold used in the present work.

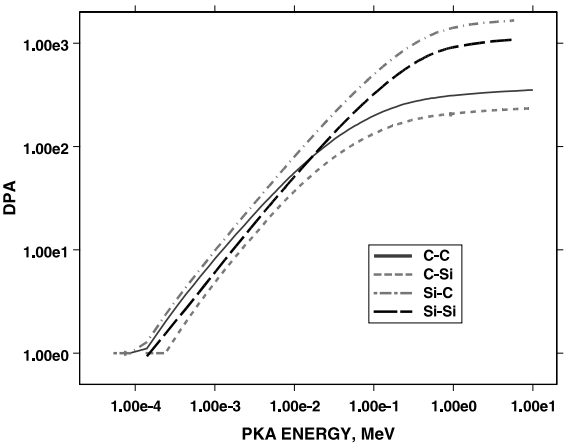

Fig. 2. Displacement functions (modified model) for SiC for each of the four sets of projectile-target combinations.

3. DPA cross sections

A method for calculating spectral-averaged displacement cross sections for SiC was developed using the SPECOMP code [15]. First the numerically determined displacement functions (modified at low energies) for SiC are integrated over the spectrum of recoil atom energies for a given neutron energy to obtain the DPA cross section as a function of neutron energy, shown in Fig. 3. The recoil energy spectra were determined using the latest version of ENDF/B-VI nuclear cross section

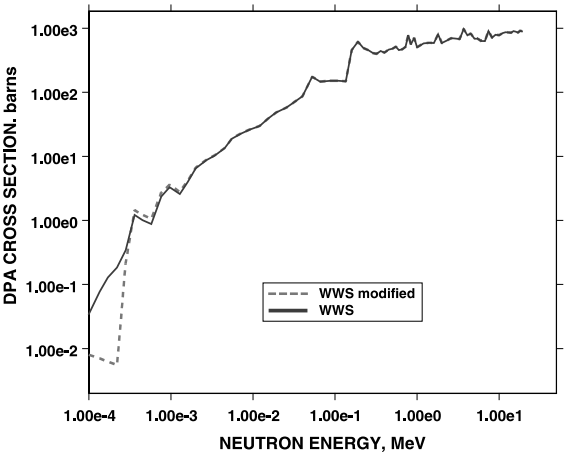

Fig. 3. DPA cross sections for SiC as a function of neutron energy. The results for the unmodified model are shown for comparison.

Table 1
Spectrally averaged total DPA cross sections, σ_{DPA}, in barns for SiC in several fission test reactors and a conceptual fusion reactor design incorporating SiC

Reactor	Position	σ_{DPA}, barns	
		Fe	SiC
HFIR	PTP mid	191	158
ATR	Midplane	302	260
HFR	C5	300	263
FFTF-MOTA	Midplane	267	324
EBR-2	Midplane	390	423
ARIES-IV	First wall	762	348

Values for pure Fe are shown for comparison to typical metals.

data for Si and C [16]. The spectrally averaged displacement cross section for a specific neutron field is then obtained by integrating over the spectrum of neutron energies. The experimenter or data analyst can determine the DPA for a particular irradiation by multiplying the total neutron fluence received times the spectral averaged displacement cross section for that reactor position.

Spectrally averaged DPA cross sections have been calculated for the neutron spectra of several previous and existing fission test reactors as well as the first wall of ARIES-IV, a conceptual gas-cooled fusion reactor. Table 1 contains the DPA cross sections for SiC in barns for these reactor positions. Also included in the table are DPA cross sections for Fe for the purpose of illustrating that the neutron energy dependence of the DPA for SiC is quite different from that of Fe. Thus, it is not advisable to try estimating the DPA for one material from the DPA calculated for another material in the same reactor position.

Table 2 contains values of the DPA rates to be expected in the reactor positions of Table 1. These were obtained by multiplying the DPA cross sections by the total neutron fluences in one effective full power year for each reactor. The DPA rates for SiC also show a different dependence on the neutron energy spectral characteristics of the various reactors than Fe does.

Table 2
Displacement damage rates in DPA per effective full power year (DPA/efpy) for SiC in several fission test reactors and a conceptual fusion reactor design incorporating SiC

Reactor	Position	DPA/efpy	
		Fe	SiC
HFR	C5	12	11
ATR	Midplane	14	12
EBR-2	Midplane	25	27
HFIR	PTP mid	33	28
FFTF-MOTA	Midplane	43	53
ARIES-IV	First wall	61	28

Values for pure Fe are shown for comparison to typical metals.

It is interesting to note that the DPA rates expected for SiC in ARIES-IV are easily matched in HFIR PTP. However, it should also be noted that the helium generation rates are significantly higher in a fusion reactor than in HFIR (6400 appm/efpy for ARIES-IV versus 200 appm/efpy in HFIR PTP).

4. Conclusions

A method for calculating spectrally averaged DPA cross sections for SiC under neutron irradiation has been developed using the best achievable displacement functions and displacement energies. It is highly recommended that DPA values calculated by this method become the standard for reporting radiation doses for all past, present and future reactor irradiations of SiC. The authors will continue work on making DPA cross sections for SiC, or the ability to calculate them, widely available.

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