

## ANALYSIS AND RECOMMENDATIONS FOR DPA CALCULATIONS IN SiC - H.L. Heinisch (Pacific Northwest National Laboratory)\*

### OBJECTIVE

The objective of this work is to recommend a procedure for calculating the radiation dose parameter displacements per atom (DPA) for SiC that will be accepted for use throughout the international fusion materials community.

### SUMMARY

Recent modeling results, coupled with the implications of available experimental results, provide sufficient information to achieve consensus on the values of threshold displacement energies to use in DPA calculations. The values recommended here, 20 eV for C and 35 eV for Si, will be presented for adoption by the international fusion materials community at the next IEA SiC/SiC workshop.

### PROGRESS AND STATUS

Displacements per atom (DPA) has become the standard unit for irradiation doses in structural materials, especially under neutron irradiation, because DPA represents, in a simple way, not only the amount of radiation received, but also the response of the material to the irradiation. Damage-based dose parameters are required because radiation damage in structural materials is studied using a variety of irradiation sources, which differ in their ability to produce damage depending on the mass and energy of the irradiating particles. Furthermore, results of these studies must be extrapolated to fusion irradiation environments that do not yet exist. DPA is a calculated dose parameter that takes into account the energy lost to the material by the irradiating particles in the form of energy that is available to cause displacement damage. The "damage energy" is converted into "displacements" in terms of the threshold displacement energy for the material.

DPA is not generally a measure of the number of stable defects created or remaining in the material at any time. This is especially true in the case of cascade-producing irradiation, where a high percentage of displaced atoms recombine immediately within the cascade volume. The calculated DPA value has, however, become a standard against which to compare the numbers of stable defects actually produced in cascade-producing irradiations. Thus, the concept of DPA is important not only as a measure of radiation dose received, but also in assessing the efficiency of defect production as a function of cascade energy and irradiating particle type.

DPA is calculated using the measured fluence of irradiating particles, the energy spectrum of the irradiating particles, the recoil atom energy spectrum for each irradiating particle, the damage energy of each recoil (the kinetic energy of the recoil less the energy lost to electronic stopping), and the model for displacements as a function of recoil damage energy. The displacement model is usually taken to be the NRT model [1], in which the number of displacements produced by a recoil atom with energy  $E_r$ , having damage energy  $T_{dam}$  is

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\* Pacific Northwest National Laboratory (PNNL) is operated for the U.S. Department of Energy by Battelle Memorial Institute under contract DE-AC06-76RLO-1830.

$$n(E_r) = \frac{0.8T_{dam}}{2E_d},$$

where  $E_d$  is the threshold displacement energy, and  $T_{dam} > 2 E_d$ .

The concept of DPA was first developed for metals, and originally formulated within the context of pure metals. In alloys, DPA values are commonly determined as the compositionally weighted sum of DPA calculated for the individual elements in their pure metals. In SiC and other non-metallically bonded compounds, the separate elements have displacement energies unique to the compound and often significantly different from each other. Calculation of DPA for SiC is straightforward once the threshold displacement energies are known for Si and C in SiC.

The threshold displacement energy is an experimentally measurable quantity (usually by determining the threshold electron energy for measurable displacements), but in multicomponent systems it is often difficult to measure the displacement energy of each component separately, except for the component with the lowest displacement threshold. Such is the case with SiC, where the reported measurements of especially the Si displacement threshold vary widely [2]. Computer simulations indicate that the displacement energy varies significantly with crystallographic direction, which may account for some of the variation in measured values. (The two-step electron-C-Si collision process can also lead to erroneously small electron energy thresholds for Si displacements [2].)

Since  $E_d$  is essentially a scaling parameter in the DPA calculation, why is it important to use the correct, measured displacement threshold energies, as long as everyone agrees to use the same values? For simply the purpose of damage correlation, it probably does not matter what values are used as long as they are used universally. On the other hand, our understanding of the radiation-induced defect structure and microstructural changes will be greatly enhanced if we use as a reference the DPA values that correctly reflect the relative numbers of each type of displacement. Furthermore, the displacement energies will eventually be measured precisely, so it is important for any values chosen as standards for DPA calculations to be as realistic as possible to avoid significant reevaluation or possible confusion in the future.

A comprehensive review of experimental measurements and results of molecular dynamics (MD) simulations of displacement energies in SiC is given in Ref. 2. Since the publication of Ref. 2, more MD simulations were done in a few selected directions by R. Devanathan, T. Diaz de la Rubia and W.J. Weber (under DOE/OBES and DOE/OFES sponsorship) using an improved interatomic potential, as reported in Ref. 3. Even more recently, Devanathan and Weber (under DOE/OBES) have extended their MD calculations to include many more directions. Also, MD simulations of the threshold displacement energies in alpha-SiC have been initiated by H. Serizawa, R. Devanathan, W.J. Weber and H.L. Heinisch. Publications on the most recent simulations in both alpha- and beta-SiC are under preparation. Based on these additional MD simulations, it now appears that sufficient information exists for promoting a consensus on the values of threshold displacement energies to use in DPA calculations. The values recommended here are 20 eV for C and 35 eV for Si, Pending publication of the most

recent MD results, a recommendation will be circulated within the fusion SiC community that these threshold displacement energy values be adopted for DPA calculations.

#### REFERENCES

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2. S.J. Zinkle and C. Kinoshita, *J. Nucl. Mater.* 251 (1997) 200.
3. R. Devanathan, T. Diaz de la Rubia and W.J. Weber, *J. Nucl. Mater.*, 253 (1998) 47.