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A SIMPLE METHOD TO CALCULATE THE DISPLACEMENT DAMAGE CROSS SECTION OF SILICON CARBIDE

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We developed a simple method to prepare the displacement damage cross section of SiC using NJOY and SRIM/TRIM. The number of displacements per atom (DPA) dependent on primary knock-on atom (PKA) energy was computed using SRIM/TRIM and it is directly used by NJOY/HEATR to compute the neutron energy dependent DPA cross sections which are required to estimate the accumulated DPA of nuclear material. SiC DPA cross section is published as a table in DeCART 47 energy group structure. Proposed methodology can be easily extended to other materials.

KEYWORDS : Displacement Per Atom (DPA), Cross Section, Silicon Carbide, Compound Material

1. INTRODUCTION

Silicon carbide (SiC) is an important material in advanced nuclear systems such as high temperature gas reactor (HTGR), and advanced nuclear fuel and fusion reactors. In a TRISO fuel particle, β-SiC is used as a coating barrier over a fuel kernel to protect fission product release. Irradiated material property data are important in estimating the safety life time of components in a nuclear reactor and a nuclear fuel. Traditionally, accumulated fast neutron fluence was used as a measure of irradiation. However, it becomes more important to use accumulated DPA as a measure, since an electron or an ion beam is often used in irradiation experiments to reproduce real environmental conditions of the material, to shorten experiment time, and to reduce the experiment cost. Moreover, it is not reasonable to use a fluence measure when the neutron spectrum is significantly different from that of the experiment since the cascade of damage is dependent on incident neutron energy and target material. It is necessary to use the DPA measure when designing a new type of reactor such as HTGR, SFR, and fusion reactor, and when introducing a new material such as SiC.

NJOY[1] is a neutron cross section processing code widely used in generating a multi-group library for neutron transport calculation. NJOY has a module HEATR which can compute the damage energy using Norgett-Robinson-Torrens (NRT) model[2] by tracking the recoil energy in all possible reaction channels such as scattering, capture, inelastic, etc. However, its capability is limited to handling single isotope material which is the generic limitation of NRT model.

For compound materials, a simple method can be applied by taking a weighted average of isotope-wise DPA cross sections. However, this approach is not accurate since the primary recoiled atom can collide with other kinds of atoms having different charge number and mass.

To handle this situation accurately, Parkin and Coulter [3] proposed a set of differential equations on the displacement functions. To solve the set of equations, differential cross sections and displacement trapping probability must be known a priori. A computer code, SPECOMP, was developed by Greenwood [4] using the Parkin and Coulter theory. However, SPECOMP has a limitation on the reaction type, such as (n,t) or (n,α), and the cross section library. Recently Heinisch et al.[5] calculated the DPA cross section of SiC using SPECOMP and SRIM-2000[6,7]. They take weighted average of the four possible cases of the primary knock-on atom (PKA) and the secondary knock-on atom. The results were published in a table of numerical values in 100 group structure.

Parkin and Coulter's method incorporates a complicated process in order to obtain the number of damages for a given PKA energy. For each combination of recoiled atom, target atom, and displaced atom, a set of integro-differential equations on the neutron energy dependent net displacement function is solved with a given differential cross section and electron stopping power. The electron stopping power should be prepared in advance using a code such as TRIM. [7] The equation requires a recoil energy dependent displacement probability and a trapping probability. These are simply approximated by identical particle collision case, which is not true for compound material. Then, the spectral averaged damage is obtained.

TRIM can compute the damage per PKA for a compound material by calculating the electron stopping power using more rigorous treatment on displacement and trapping using isotope-wise threshold displacement energy per each collision through the Monte-Carlo simulation. We can get more accurate results by incorporating the TRIM results in the process of NJOY calculation. The authors propose a simple hybrid method using TRIM and NJOY which can take care of all reactions combined with an up to date cross section library. In this study, the NJOY/HEATR module has been modified to incorporate the TRIM results. For comparison with Heinisch model, the generated DPA cross section for 47 energy group is applied to a neutron transport code, DeCART.[14]

2. LATTICE PARAMETERS

There are more than 250 polytypes of silicon carbide. Among them 3C-SiC, so-called β-SiC, which is formed under 1700oC, is a candidate material for nuclear applications. SiC is a ceramics material and can be modeled as a zinc-blend two-component covalent material.

The collision cascade of recoiled nuclides is characterized by threshold displacement energy, lattice binding energy and surface binding energy. Among them, threshold displacement energy that causes Frenkel pairs is the most important parameter in estimating the displacement damage. This parameter is dependent on the lattice structure and can be obtained by an irradiation experiment, or predicted by molecular dynamics simulations. Many experimental results were published on SiC, however, reported values vary widely, 20-50 eV for C defect and 35-110 eV for Si defect . Zinkle and Kinoshita [8] recently recommended 20 eV for C and 40 eV for Si.

There are many studies to predict threshold displacement energy using molecular dynamics simulations. Devanathan et al.[9] obtained 20 eV for C displacement and 35 eV for Si displacement. Heinish et al. adopted these values. [5] Recently, Lucas and Pizzagalli [10] pointed out that the different empirical potentials used in the previous studies may result in poor prediction of Frenkel pairs production for covalent materials. They made a more fundamental approach to produce the inter-atomic potential using electron the density functional theory (DFT) [11]. They obtained the lattice averaged threshold displacement energy as 19 eV for C sublattice and 38 eV for Si sublattice. Those values are largely different from that of single element material, 31 eV for graphite and 25 eV for silicon.[1] The difference comes from the difference in lattice structure. The result of Lucas and Pizzagalli was adopted in this study, 19eV and 38eV as the threshold displacement energy for C and Si, respectively.

Lattice binding energy is required for SRIM/TRIM simulation. This value, the vacancy formation energy, can be predicted using another molecular dynamics calculation. This study adopted Huang and Ghoneim's result [12]; 2.63eV and 3.25eV for C and Si, respectively.

Surface binding energy, which is less important in the DPA estimation, can be derived from heat of vaporization for each element. This study adopted 7.4 eV and 4.7eV for C and Si, respectively.

3. NRT MODEL IN NJOY

The NRT model in the NJOY/HEATR module deviates from the original NRT model in the low energy cutoff and also deviates from the modified NRT model which multiplies the efficiency factor (0.8) to the number of vacancies. This factor can be taken into account when deriving the DPA cross section from the NJOY produced damage production cross section ($E\sigma$) (MT=444). NJOY sums up the cross section multiplied by damage energies, which is the damage production cross section representing the effective kinetic energy of recoiled atom for possible reaction types (k) at a given incident neutron energy (E_n).

$$\left(E\sigma\right)_{DPA} = \sum_k E_{d,k}\sigma_k\left(E_n\right)$$

For a specific reaction, the damage function is calculated using the following formulae.

$$\mathrm{df} = 0 \quad \text{when} \quad E_{PKA} < E_d ,$$

$$\mathrm{df} = \frac{E_{PKA}}{1 + F_L g\left(\varepsilon\right)} \quad \text{when} \quad E_{PKA} \geq E_d ,$$

where, E_{PKA} is the kinetic energy of the PKA, E_d is the threshold displacement energy,

$$F_L = \frac{0.0793 Z_R^{2/3} Z_L^{1/2} \left(A_R + A_L\right)^{3/2}}{\left(Z_R^{2/3} + Z_L^{2/3}\right)^{3/4} A_R^{3/2} A_L^{1/2}},$$

$$g\left(\varepsilon\right) = 3.4008\varepsilon^{1/6} + 0.40244\varepsilon^{3/4} + \varepsilon ,$$

$$\text{and} \quad \varepsilon = \frac{E_{PKA}}{30.724 Z_R Z_L \left(Z_R^{2/3} + Z_L^{2/3}\right)^{1/2}} \frac{A_L}{A_R + A_L} .$$

Z_L and A_L are the charge number and atomic mass of lattice atom, Z_R and A_R are those of recoiled atom.

The number of displacement per atom, N_d, is calculated as

$$N_d = \frac{1}{2E_d}\mathrm{df} .$$

The NRT model can effectively handle the electron energy loss of the recoil atom for single element material. A simple method may be devised for SiC by considering four cases of collision cascade as proposed by Heinish et al.[5] These are C-C (PKA C collides with C), C-Si (PKA C collides with Si), Si-Si (PKA Si collides with Si), and Si-C (PKA Si collides with C). The effective displacement energy of chains can be derived from the maximum energy