Generation of damage cross section for silicon carbide

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1. Introduction

Exact calculation of damage measure, displacement per atom (DPA), is necessary in performance analysis to reflect the irradiation effect on the thermo-mechanical property of materials used in a nuclear reactor. However, there is practically no cross section library for current reactor physics codes which will be used for DPA calculation.

Silicon carbide(SiC) is an important material used in gas-cooled reactor, advanced nuclear fuel, and fusion applications. There are more than 200 polytypes of SiC. However β-SiC, which is produced under 1700°C, is the polytype interesting for a nuclear application.

2. Methods and Results

2.1 DPA cross section

DPA is a microscopic quantity defined as the number of vacancies (or Frenkel pairs) per lattice atom. Ignoring recombination of Frenkel pairs, e.g. by the thermal motion of lattice, the accumulated displacements per atom (DPA) over irradiation is expressed as ;

$$dpa = \int_0^T \int \sigma_{dpa}\left(E_n\right)\phi\left(E_n,t\right)dE_n dt\,.$$

where σ_{dpa} is the DPA cross-section (unit: barn), ϕ is the neutron flux, E_n is the neutron energy, and T is the period of irradiation.

The displacement is mainly caused by knock-on atom by neutron bombardment and its cascade in the lattice. It is important to know the energy of primary knock-on atom(PKA) after the collision with neutron. For elastic scattering, the PKA energy is given by simple kinematics as ;

$$E_{PKA} = 2\left(1-\cos\theta\right)\frac{A}{\left(A+1\right)^2}E_n$$

where A is the mass number of atom and θ is the scattering angle in the center of mass system. The probability density function expressed in PKA energy is

$$p\left(x\right) = \frac{1}{\pi}\left(2+2x-x^2\right)^{-1/2}$$

where x is the ratio of PKA energy with the maximum possible PKA energy.

When we know the number of vacancies produced by the PKA ion with given energy, N_d, we can calculate the DPA cross section as ;

$$\sigma_{dpa}\left(E_n\right) = \int N_d\left(E_{PKA}\right)p\left(E_{PKA}\,|\,E_n\right)\sigma\left(E_n\right)dE_{PKA}$$

The DPA can be estimated by several methods as explained in next sections.

2.2 NRT Model

The standard procedure to compute DPA is well established by Norgett et al.[1] Norgett improved simple model suggested by Kinchin and Pease[2] to consider the energy loss by inelastic scattering by electrons surrounding atom. The number of displaced atom per knock-on atom(PKA) is given as :

$$N_d = \frac{0.8E_{PKA}}{2E_d\left[1+kg\left(\varepsilon\right)\right]}\,,$$

where N_d is the number of vacancies per PKA, E_{PKA} is the kinetic energy of PKA, E_d is the threshold atom displacement energy. The loss factors k and g is given by ;

$$k = 0.1337Z_1^{1/6}\left(Z_1/A_1\right)^{1/2},$$
$$g\left(\varepsilon\right) = \varepsilon + 0.40244\varepsilon^{3/4} + 3.4008\varepsilon^{1/6}$$
$$\varepsilon = \left[A_2E_{PKA}/\left(A_1+A_2\right)\right]\left[a/Z_1Z_2e^2\right]$$
$$a = \left(9\pi^2/128\right)^{1/3}a_0\left[Z_1^{2/3}+Z_2^{2/3}\right]^{-1/2}$$

where a_0 is the Bohr radius, e the electronic charge, Z_1 and A_1 are the charge and mass numbers the projectile and Z_2 and A_2 are those of target atom.

NRT model is widely used in nuclear community to estimate the DPA. However it can be applied only when the target atoms are identical, such as iron.

In SiC lattice, PKA can be Si atom or C atom. The collided atom can be Si or C. There are many combination of collision cascade. Heinisch et al. proposed simple weighting of the four cases with adjusted threshold displacement energies: 41 eV(C/Si), 35 eV(Si/Si), 24 eV(Si/C), and 20 eV (C/C).[3]

2.3 Molecular dynamics(MD) simulation

There are several computer codes which can simulate the cascade of ions in a solid lattice. One of the most

popular and reliable software is SRIM/TRIM developed by Ziggler.[4] SRIM requires three important lattice parameters to do simulation, displacement energy, lattice binding energy, and surface binding energy. Those parameters are usually determined by unit cell MD calculation for the crystal structure corresponding to the polytype. The displacement energy is the most important parameter to determine number of vacancies. Lucas et al. performed the MD simulation for β-SiC.[5] We adopt their recommended values; 19 eV(C) and 38 eV(Si). The lattice binding energies are calculated from eigenvalue problem in a unit cell. We adopt the data obtained by Huang and Ghoniem; 2.63 eV(C) and 3.25 eV(C). The surface binding energy is derived from the heat of sublimation for each solid element; 7.4 eV(C) and 4.7 eV(Si).

2.4 Recommended procedure

Figure 1 compares the results of displaced atom per carbon PKA(N_d) on β-SiC lattice. The results by NRT and SRIM/TRIM are similar for low PKA energy which corresponds to neutron energy below 1 MeV. NRT model over-estimates about 7.7% at 200 keV PKA energy. This corresponds to the neutron energy of 3 MeV. Considering that the most probable energy of fission neutron is about 1 MeV, there is no practical difference in NRT and TRIM model calculations.

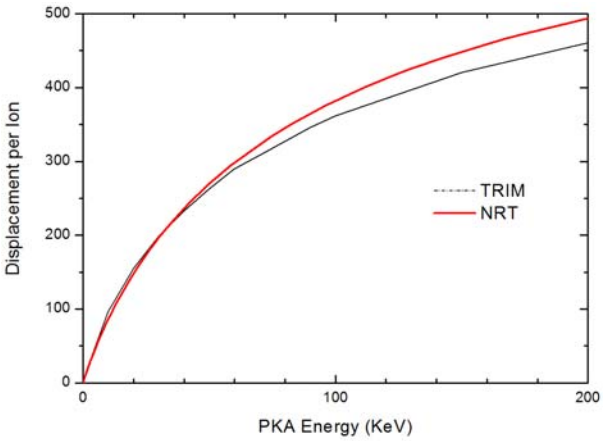

Fig. 1. Displacement per atom for C ion on β-SiC lattice.

Considering the fact; that NRT model is widely used, and that NRT gives conservative (higher) value, we recommend the NRT model with proper modification in the threshold displacement energy depending on sub-cascade.

NJOY/HEATR module was used to obtain PKA energy multiplied by cross section from the ENDF/B-VII.[7] The 190 group structure used in HELIOS is adopted in this work. We used the average PKA energy to avoid the complication and the integration in this work.

$$\sigma_{dpa}\left(E_n\right)=\frac{1}{2}\sum_{k=\mathrm{C,Si}} N_d^{(k)}\left(\bar{E}_{PKA}\right)\left(E\sigma\right)_{MT=444}^{(k)}$$

where $\bar{E}_{PKA}=\dfrac{A}{\left(A+1\right)^2}E_n$

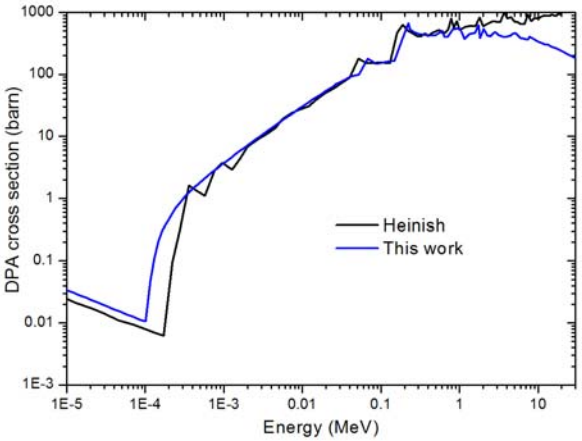

Fig. 2. DPA cross section of β-SiC.

Figure 2 compares the DPA cross section generated in this work with that of Heinish et al.[8]

3. Conclusion

A HELIOS compatible 190 group DPA cross section set for β-SiC is generated in this work.

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