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Evaluation of Radiation Damage Distribution in NTD-SiC

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1. Introduction

Silicon carbide (SiC) single crystal has been a substrate material for high power and high frequency electronic devices because of its excellent thermal and electrical properties compared with silicon. And neutron transmutation doping (NTD) of semiconductors is an important method for applications that require high dopant homogeneity, for example in electric power devices [1]. The NTD process takes place when a high purity SiC ingot is irradiated in a thermal neutron flux. In this process, neutrons transfer the energy to SiC by nuclear reaction or nuclear elastic scattering, and damage to the SiC ingot until the irradiation completed. The distribution of displacement damage is determined by energy and spatial distribution of neutron. This displacement damage distribution in SiC ingot should be evaluated in terms of quality management.

In the present study, the neutron flux and the displacement per atom (DPA) distribution in the SiC ingot after HANARO neutron irradiation was calculated using a Monte Carlo code. The value of DPA is a standard for characterizing and comparing the radiation damage induced in crystalline materials by incident particles such as neutrons, charged particles and other radiations. The spatial distribution of displacement damage in the radial and vertical direction was also represented.

2. Methods and Results

2.1 Monte Carlo simulation

For calculating the DPA values, the SRIM (Stopping and Range of Ions in Materials) code [2], which is the major code for radiation damage calculation, was usually used. But SRIM code does not treat nuclear reactions or nuclear elastic scattering, thus it cannot produce PKAs (Primary Knock-on Atoms) created by secondary particles and neutrons. Alternatively, detail DPA distribution of SiC ingot was calculated by using PHITS (Particle and Heavy Ion Transport code System) code. Some researchers have developed a method for calculating DPA values for materials with arbitrary geometries that are being irradiated with neutrons and other particles using the event generator in a Monte Carlo particle transport simulation code PHITS [3, 4, 5, 6]. The PHITS code can simulate electromagnetic cascades using the Electron Gamma Shower version 5 algorithm and calculate DPA values using the recoil energies and the McKinley-Feshbach cross section [6].

In the input condition of the calculation code, neutrons in the NTD2 irradiation hole of HANARO research reactor were considered as a neutron source. Neutron energy spectrum of SiC ingot in the NTD2 irradiation hole was calculated by using MCNP6.1 code. The MCNP equilibrium model (burned core model for 96 operation cycles) was employed for a whole core representation of the HANARO. The starting points of sources were assumed to be uniformly distributed on the surface of a vertical channel with a radius of 9 cm as the NTD2 irradiation hole. Neutrons were set to be released in all direction. A SiC ingot sample for neutron irradiation was modeled as a 6-inch cylindrical SiC with a mass of 1.22×10^4 g. The neutron flux distribution in the SiC ingot was calculated using t-track tally with setting the xyz mesh. And t-dpa tally with xyz mesh was used to calculate the DPA distribution. In the t-dpa tally, there are mainly three parts: transport calculation including nuclear reaction or scattering, coulomb scattering due to PKA, and cascade damage approximation. In the transport calculation, there are mainly two flows to produce the target PKA. One is the Coulomb scattering due to PKA's directly created by the neutron, and the other is that due to PKA's created by the secondary particles [3]. For the secondary particle production, the conservation law on the energy and the momentum is sustained in each event using nuclear reactions for high energy particles and the "Event Generator Mode" for low energy neutrons [4]. The energy of the secondary particles is obtained with PHITS calculations using a nuclear reaction model. The reaction model components of the PHITS code is listed in Table 1. Sufficient particle histories ($NPS=10^8$) were run to reduce the variation of result.

Table I: The reaction models of the PHITS code [3]

Component		Models
Stopping power		SPAR
Event generator	Particle-induced collisions	JAM
	Heavy-ion induced collisions	JQMD
	Evaporation and fission	GEM
Reaction cross section		Tripathi's

2.2 Distribution of neutron flux and damage

Distributions of neutron flux and DPA/neutron in the SiC ingot were visualized by using ANGEL 4.50 to check the status of simulation. The sum of flux or DPA values in the z-axis was expressed in x-y plane. In the Fig.1 (A), the surface of cylindrical irradiation hole represents the darkest red color, which means the region of higher neutron flux. And the center of the irradiation hole and SiC ingot represents the lightest red color. In the Fig.1 (B), only the inside of the SiC ingot represents the red color because the displacements have been created inside the SiC ingot.

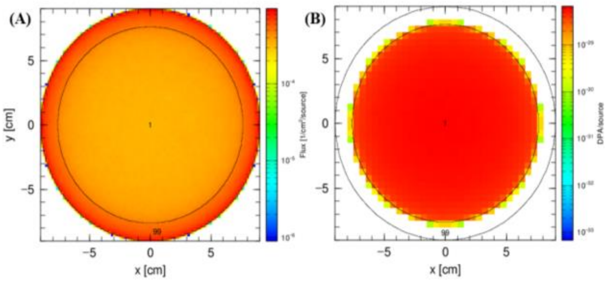

Fig. 1. Distribution of (A) neutron flux and (B) DPA/neutron in the SiC ingot viewed in x-y plane (plotted by ANGEL 4.50).

Ratio of neutron flux to average flux along the radial direction is shown in Fig. 2 to evaluate the distribution of neutron flux in the SiC ingot. The neutron flux is the highest on the surface of the SiC ingot and the lowest inside the SiC ingot. The ratio of neutron flux to average flux on the surface of the SiC ingot is 1.32, the ratio of neutron flux to average flux on the inner center of the SiC ingot is 0.92.

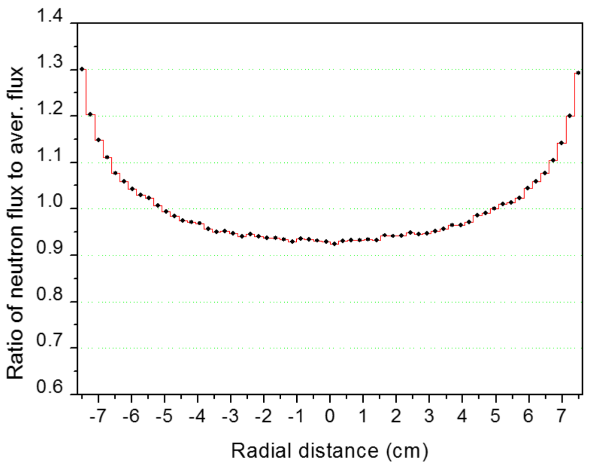

Fig. 2. Ratio of neutron flux to average flux along the radial direction.

Ratio of DPA to average DPA along the radial direction is also shown in Fig. 3. Interestingly, DPA is the highest on the center of the SiC ingot and the lowest on the surface of SiC ingot contrary to the distribution of neutron flux. The ratio of DPA to average DPA on the surface of the SiC ingot is 0.62, the ratio of DPA to average DPA on the inner center of the SiC ingot is 1.11.

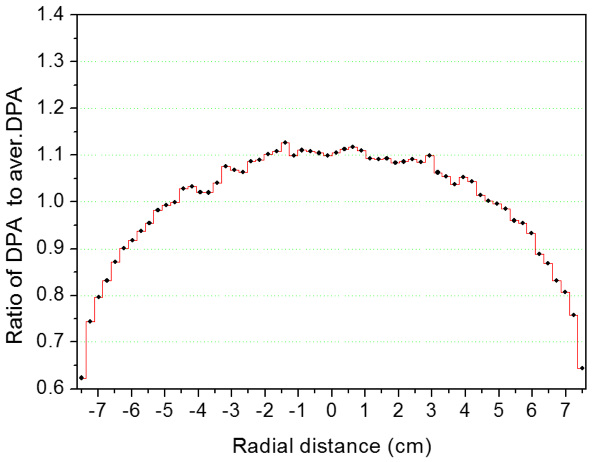

Fig. 3. Ratio of DPA to average DPA along the radial direction.

Ratio of neutron flux to average flux along the vertical direction is shown in Fig. 4. Except for the upper and lower surface, neutrons are uniformly distributed along the vertical direction. Ratio of DPA to average DPA along the vertical direction is also shown in Fig. 5. Similar to the radial distribution of DPA in Fig.3, DPA is the highest on the center of the SiC ingot and the lowest on the surface of SiC ingot. The ratio of DPA to average DPA on the surface of the SiC ingot is 0.58, the ratio of DPA to average DPA on the inner center of the SiC ingot is 1.11

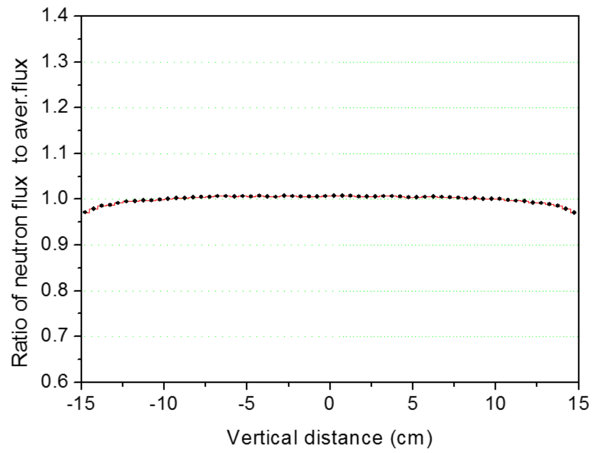

Fig. 4. Ratio of neutron flux to average flux along the vertical direction.

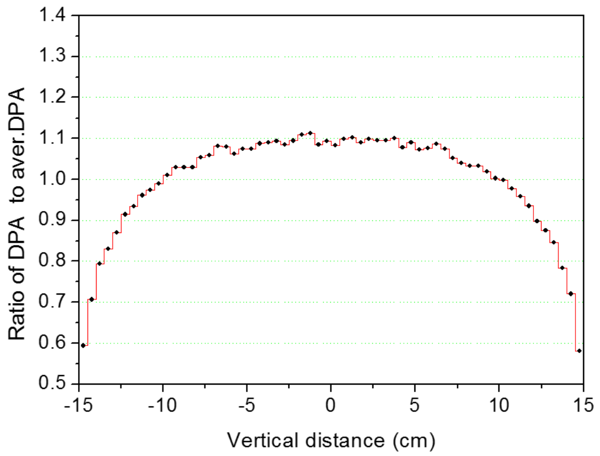

Fig. 5. Ratio of DPA to average DPA along the vertical direction.

The results of this study indicate that the DPA is the highest on the center of the SiC ingot contrary to the distribution of neutron flux. Thermal neutrons transfer their energy by neutron capture reaction instead of nuclear elastic scattering. The minimum kinetic neutron energy needed to transfer enough energy for displacements by elastic scattering is about 185 eV [7]. But gamma rays emitted from neutron capture reaction result in a recoil energy of about 1 keV. This is much higher than the displacement threshold energy, therefore this part of displacement damage can't be neglected. The gamma rays on the surface escape easily from the SiC ingot without delivering all of their energy. But the gamma rays in the center can transfer their all energy to SiC ingot, the charge compensation effect occur as well. These increase the DPA in the center of SiC ingot.

3. Conclusions

In conclusion, we have represented the neutron flux and the displacement per atom (DPA) distribution in the SiC ingot after HANARO neutron irradiation. The spatial distribution of displacement damage in the radial and vertical direction is represented by ratio of DPA to average DPA. DPA is the highest on the center of the SiC ingot contrary to the distribution of neutron flux. These results will be a base data for controlling the defect of NTD-SiC.

Acknowledgements

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