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Analysis of primary damage in silicon carbide under fusion and fission neutron spectra

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ABSTRACT

Irradiation parameters on primary damage states of SiC are evaluated and compared for the first wall of ITER under deuterium–deuterium (DD) and deuterium–tritium (DT) operation, the high temperature gas-cooled reactor (HTGR) and high flux isotope reactor (HFIR). With the same neutron fluence, the studied fusion spectra produce more damage and much higher gas production than the fission spectra. Due to comparable gas production and similar weighted primary recoil spectra, HFIR is considered suitable to simulate the neutron irradiation in an HTGR. In contrast to the significant differences between the weighted primary recoil spectra of the fission and the fusion spectra, the weighted secondary recoil spectra of HFIR and HTGR match those of DD and DT, indicating that displacement cascades by the fission and the fusion irradiation are similar when the damage distribution among damaged regions by secondary recoils is taken into account.

1. Introduction

Silicon carbide is a promising material for nuclear applications, due to its excellent resistance to high temperatures and corrosion, remarkable mechanical properties, and low neutron capture cross section. SiC has been proposed as a structural material of the first wall in blanket design of ARIES-AT [1], TAURO [2], DREAM [3]. It is also used in TRISO fuels of HTGR [4,5].

Neutron irradiation will inevitably introduce displacement defects and impurities in SiC, which may lead to isotropically volumetric swelling, degradation in thermal conductivity and modification of mechanical properties [5–7]. Most of the neutron irradiations of SiC have been done on fission test reactors [7,8], whose neutron spectra highly differ from those of HTGR and fusion reactors. Differences in neutron spectra will influence the primary damage states, including the generation of displacement damage and transmutation products [9–12], and primary recoil spectra [13], which could affect the long-term evolution of microstructures. It has been noted that with the same cumulative fast ($E > 0.1$ MeV) neutron fluence, comparable displacement damage is produced in the magnetic and inertial confinement fusion (MCF/ICF) systems and HFIR [10], but the gas production in fusion is much larger than that in HFIR [10–12]. The displacement per atom (DPA) unit is generally calculated to quantify the damage production [9,10]. However, the concept of DPA does not contain any information about damage morphology. Different primary recoil energies could lead to different damage morphologies. Therefore, the primary recoil spectrum is an important parameter when comparing different neutron irradiations. For better correlation with damage morphology, the primary recoil spectra are usually weighted with the displacements by recoils, resulting in weighted primary recoils spectra $W(T)$ [14–16] (also referred as the damage function [13] or the cumulative damage production function [17]) which represents the fraction of damage by recoils lower than a given energy. The $W(T)$ calculation has been used as a criteria in the design of neutron moderators of the International Fusion Materials Irradiation Facility (IFMIF) to match the irradiation in the first wall and the breeding blanket of demonstration fusion reactor (DEMO) [18]. Compared to fission test reactors and spallation neutron sources, IFMIF was found more suitable to simulate neutron irradiation of the helium-cooled pebble bed blanket of DEMO, in terms of comparable displacement damage and gas production, and similar $W(T)$ [19]. Due to the similarity in $W(T)$ [13], IFMIF was also found suitable to simulate the neutron irradiation of SiC at the first wall of DEMO with a helium-cooled lithium–lead (HCLL) blanket. It is believed that similar weighted primary recoil spectra should be attained for similar displacement cascades. However, it has been reported that the sub-cascades produced by fusion neutrons resemble the cascades induced by fission neutrons [20,21], suggesting the equivalency of fission and fusion

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irradiation sources in terms of initial damage states [22], which indicates that the sub-structures of cascades should be taken into account for the fission–fusion correlation.

The present study aims to compare the primary damage states in SiC by neutrons with the spectra of the fission test reactor HFIR, prototypical fusion reactors, and an HTGR. Using a Monte Carlo approach, parameters for damage production and gas production and weighted primary recoil spectra have been calculated and compared. To take into account the damage distribution among damaged regions by secondary recoils, weighted secondary recoil spectra are introduced. The study is useful in evaluating the suitability of applying fission test reactors, such as HFIR, to relevant studies of irradiation effects in fusion reactors and HTGRs.

2. Calculation of displacement damage by neutron

2.1. Simulation of neutron interactions

The interactions of neutrons with target atoms involve elastic scattering and a series of non-elastic processes. The elastic scattering produces primary knock-on atoms (PKAs) by knocking atoms off lattice sites, while the non-elastic processes result in PKAs left in an excited state or energetic reaction product. In this study, the PKAs and the reaction products are referred to primary recoils. The production of primary recoils by neutrons is simulated by GEANT4.9.6.p02 [23], a Monte Carlo simulation toolkit for the transportation of particles in matter. Simulations of neutrons by GEANT4 have been validated by TARC experiments [24] and agree well with MCNP [25].

Regarding the GEANT4 simulation setup, a simplified geometry with a 5 mm thick slab of SiC, which is close to the thickness of SiC fusion first wall concepts [1–3], was adopted in this study, and neutrons were incident on the target uniformly and perpendicularly over an area of 1 cm × 1 cm. The material of the slab is defined as SiC with natural Si and C isotopic abundance. In this work, four neutron spectra are considered, including two fusion neutron spectra (the neutron spectra of ITER first wall under DT operation and DD operation [26]), and two fission neutron spectra, the neutron spectrum of an HTGR enriched with 20% ^{235}U [4], and the neutron spectrum at the mid-plane of the peripheral target position of HFIR [16,27]. The neutron spectra of DT, DD, HTGR and HFIR are shown in Fig. 1.

Significant differences exist among these computed spectra. Due to the D–T reaction, a prominent peak at 14.1 MeV exists for the DT spectra. As the D–D reaction is generally accompanied by the D–T reaction, two peaks at 2.45 MeV and 14.1 MeV can be found in the DD spectra. The spectra of HTGR and HFIR are much softer than the fusion spectra, with less remarkable peaks at about 2 MeV. For HFIR, a peak at the thermal region can also be observed. The spectrally averaged energies of neutron are much higher in DD (1.69 MeV) and DT (2.57 MeV) spectra, compared to HTGR (0.76 MeV) and HFIR (0.43 MeV) spectra.

Since neutron energies of the studied spectra are lower than 20 MeV, High Precision Neutron Elastic processes (G4NeutronHPElastic), High Precision Neutron Inelastic processes (G4NeutronInelastic), High Precision Neutron Capture processes (G4NeutronHPCapture) and High Precision Neutron Fission processes (G4NeutronHPFission) were used to treat the neutron elastic scattering, inelastic scattering, capture, and fission with the G4NDL 4.2 neutron data library, with most of the data from ENDF/B-VII neutron evaluated libraries. The type, energy, position and direction of primary recoils by neutrons can be obtained from GEANT4 simulations using the above setup.

2.2. Calculation of displacement damage by recoils

The primary recoils are produced by neutrons slowing down in the target by inelastic scattering with electron and screened

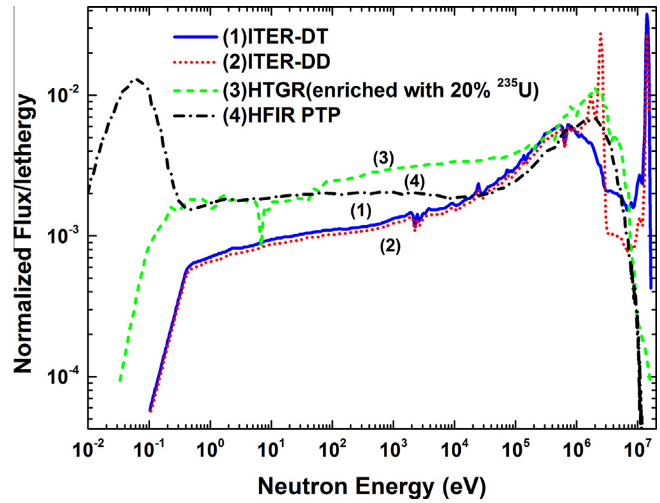

Fig. 1. Neutron spectra of: (1) the first wall of ITER under DT operation from Ref. [26]; (2) the first wall of ITER under DD operation from Ref. [26]; (3) the HTGR enriched with 20% ^{235}U from Ref. [4]; (4) the mid-plane of the peripheral target position of HFIR from Refs. [16,27].

columbic scattering with target nuclei, with the latter process producing displacement cascades. The total displacement function of SiC has been generally calculated by solving the integro-differential equations presented by Parkin and Coulter [28–30]. However, details of recoil cascades cannot be obtained by that approach. Based on the binary collision approximation (BCA), SRIM [31] is a well accepted tool suitable for the calculation of displacement damage by ions with energies up to 1 GeV. With the Ziegler, Biersack, and Littmark (ZBL) universal screening potential, SRIM provides a rigorous treatment of the elastic scattering. Compared to the approach that numerically solves the integro-differential equations, SRIM provides more details of recoil production with the Monte Carlo approach. In this study, the displacement damage by primary recoils is calculated by SRIM-2013. Recently, Stoller et al. [32] recommended the use of "Ion Distribution and Quick Calculation of Damage" ("K–P" mode) when performing damage calculations with SRIM. They also suggested that calculating the number of displacements should be based on the damage energy instead of integrating the VACANCY.txt file produced by SRIM, which provides the total number of vacancies. In addition, the "K–P" mode can underestimate the total ionization energy loss, as only the incident ions and their primary recoils are considered. In this work, the following procedure, which was also depicted in Ref. [32], is adopted to calculate the damage by recoils:

(1) Set the lattice binding energy of Si and C set to be 0, and set the threshold energy for displacement of Si and C atom to be 35 eV and 20 eV respectively [33] and do the calculation with the "Detailed Calculation with full Damage Cascade" mode.
(2) Calculate the total ionization energy loss (E_i) in the IONZ.txt or the COLLISON.txt files produced by SRIM [34], and obtain the damage energy with $E_{dam} = E_{tot} - E_i$, where the E_{tot} is the incident energy of the recoil.
(3) Obtain the number of displaced atoms by the standard NRT calculation [35]:

$$N_d = 0.8E_{dam}/2E_d \quad (1)$$

For SiC, the threshold energy for displacement E_d is assumed to be 25 eV [36].

Neutron interactions with SiC were simulated with GEANT4, by which the production of helium and hydrogen were obtained