MODELING OF DISPLACEMENT DAMAGE IN SILICON CARBIDE DETECTORS RESULTING FROM NEUTRON IRRADIATION

DISSERTATION

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Behrooz Khorsandi, M.S.

*****

The Ohio State University
2007

Dissertation Committee:

Dr. Thomas E. Blue, Advisor
Dr. Wolfgang Windl
Dr. Don W. Miller
Dr. Tunc Aldemir
Dr. Richard Denning

Approved by

_________________________
Advisor
Nuclear Engineering Graduate Program
ABSTRACT

There is considerable interest in developing a power monitor system for Generation IV reactors (for instance GT-MHR). A new type of semiconductor radiation detector is under development based on silicon carbide (SiC) technology for these reactors. SiC has been selected as the semiconductor material due to its superior thermal-electrical-neutronic properties.

Compared to Si, SiC is a radiation hard material; however, like Si, the properties of SiC are changed by irradiation by a large fluence of energetic neutrons, as a consequence of displacement damage, and that irradiation decreases the life-time of detectors. Predictions of displacement damage and the concomitant radiation effects are important for deciding where the SiC detectors should be placed. The purpose of this dissertation is to develop computer simulation methods to estimate the number of various defects created in SiC detectors, because of neutron irradiation, and predict at what positions of a reactor, SiC detectors could monitor the neutron flux with high reliability. The simulation modeling includes several well-known – and commercial – codes (MCNP5, TRIM, MARLOWE and VASP), and two kinetic Monte Carlo codes written by the author (MCASIC and DCRSIC). My dissertation will highlight the displacement damage that may happen in SiC detectors located in available positions in the OSURR,
GT-MHR and IRIS. As extra modeling output data, the count rates of SiC for the specified locations are calculated.

A conclusion of this thesis is SiC detectors that are placed in the thermal neutron region of a graphite moderator-reflector reactor have a chance to survive at least one reactor refueling cycle, while their count rates are acceptably high.
Dedicated to My Beloved Mother, Wife

&

All My Instructors Who Have Positively Influenced My Life
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VITA

March 11, 1966

Born- Tehran, Iran

1989

B.S. Materials Engineering
Tehran University

1995

M.S. Materials Engineering
Iran University of Science and Technology

2004

M.S. Nuclear Engineering
The Ohio State University

2004-present

Graduate Research Associate
The Ohio State University

PUBLICATIONS


FIELD OF STUDY

Major Field: Nuclear Engineering
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CHAPTER 1

INTRODUCTION

The purpose of this dissertation is to use computer simulation methods to find locations in the nuclear reactors for SiC neutron power monitors, where high count rate (preferably more than $10^6$ cps) for a long period of time (at least one reactor refueling cycle) is achievable.

There is an appreciable interest in developing neutron-monitoring systems for next generation reactors. This dissertation presents a study regarding the feasibility of using 4H-SiC semiconductor neutron diode detectors in the GT-MHR and IRIS, considering the neutron-induced displacement damage and count rates.

Despite being radiation hard, a 4H-SiC neutron diode detector may not be able to withstand the extreme conditions in the stated reactors. The goal of the study is to introduce simulation methods to identify locations in the GT-MHR and IRIS, where the detector count rate is acceptably high and the detector life-time may be acceptably long. The modeling methods that we have used to determine the count rates and the
displacement damage rates are discussed. Since the GT-MHR and IRIS are still in the design process stage, we modeled the use of SiC in some of OSURR ports so as to be able to compare the simulation results with experimental data when SiC detectors with known design would be available\textsuperscript{1}.

Chapter 2 provides background information. We review the SiC properties and discuss why SiC is the material of interest in several nuclear engineering usages, including neutron power monitors. Then the OSURR, IRIS and GT-MHR are briefly reviewed. The last two reactors are among Generation IV reactors. Then, defects in SiC are studied. To study the displacement damage, we introduce a new term, \textit{PDPA}, which stands for point defects per atom. At the end of Chapter 2, the computers codes that are used in our modeling are introduced.

In Chapter 3, the simulation methods that we developed to estimate the displacement damage defects and count rates are discussed. We use MCNP5 to determine the neutron flux and reaction rates in the various positions in the OSURR, IRIS and GT-MHR. TRIM and MARLOWE are used to model the spatial distribution of defects in SiC. Finally, the methodology of using the ab-initio and kinetic Monte Carlo codes, together, to study the effect of temperature on the \textit{PDPA} is introduced.

\textsuperscript{1} The comparison has not been made in the dissertation.
In Chapter 4, we present the $PDPA$ and count rate results for SiC power monitors in the OSURR, IRIS and GT-MHR. The change of $PDPA$ over a reactor refueling cycle for a SiC Schottky diode detector placed in the center of the central reflector of GT-MHR at 500 K is studied.

In Chapter 5, the usefulness of SiC detectors as in-core neutron monitors for graphite moderator-reflector reactors is discussed; their lack of usefulness for LWR is also addressed.

Finally, in Chapter 6 an overall conclusion of the dissertation is presented. Some suggestions to improve the effectiveness of the simulation methods are offered.
CHAPTER 2

BACKGROUND

2.1 Silicon Carbide

2.1.1 SiC Brief History

Silicon carbide (SiC) has a short history. SiC was first observed by Jöns Jacob, a Swedish scientist, while he was attempting to synthesize diamond in 1824 [1]. Later, Edward Goodrich Acheson made SiC around 1893 [2]. Ferdinand Henri Moissan discovered naturally occurring SiC in 1905. In honor of him, the SiC mineral is now called moissanite [1,2].

SiC is a very attractive material in the nuclear engineering field. Excellent neutronic, electronic, chemical and heat transfer properties of SiC have made it useful for a wide variety of applications, e.g., as a coating material for TRISO particles [3], a blanket structural material for fusion power plants [4], and a neutron detection diode for nuclear reactor power monitoring [5]. In this dissertation, the focus is on the last stated
application. However, the displacement damage modeling methodology that is described in the next chapters is also useful for the other stated applications.

For a long time, SiC has been the “high-temperature semiconductor for the future”. The problem with using SiC was the difficulty in the fabrication of high-quality SiC [6,7]. After several decades of research and development on the fabrication processes, SiC was commercialized around 1990 by CREE [6,8,9]. Currently, SiC is one of the state-of-the-art semiconductors; and frequently, conferences such as the International Conferences on Silicon Carbide and Related Materials (ICSCRM) and the European Conferences on Silicon Carbide and Related Materials (ECSCRM) introduce the latest improvements in the field to researchers.

2.1.2 SiC Specifications

2.1.2.1 SiC Polytypes

SiC has significant advantages over silicon (Si) as a radiation detector; however, it is still at an immature stage [10] and a number of graduate student theses have been written on SiC defect creation and properties since 2000 [11-13]. The polytypism of SiC is the main characteristic of SiC that makes it difficult to study. In fact, SiC has more than 170 different crystal polytypes [14,15]. Among those, the most important ones are 3C, 2H, 4H and 6H. The focus of this dissertation is on 4H-SiC.

Each atom in SiC is connected to four atoms of different type, creating tetragonal bonding (Figure 2.1). The bond length of nearest neighbors is approximately 1.89 Å, and the closest distance between two atoms of the same species in the SiC lattice is
approximately 3.08 Å [16]. The difference among SiC polytypes is the stacking order of the unit cell. As shown in Figure 2.2 [16], 3C (β-SiC) is cubic and its stacking order along the [1,15] direction is ABC. On the contrary, α-SiC has hexagonal crystal structure. 2H-SiC is hexagonal with AB stacking order. 4H- and 6H-SiC have stacking orders of ABACA and ABCABCA and hexagonalities of 50 and 33 percent, respectively [1,16]. The crystal structure of 4H-SiC is shown in Figure 2.3. To know more about the polytypism of SiC, we refer the readers to an article written by Bechstedt et al. [17].

Among those four common SiC polytypes, 4H-SiC is the favorite one for our purpose because of its superior properties, described in Section 2.1.2.2.

Figure 2.1: Tetrahedral bonding of a C atom with its four nearest Si neighbors.
Figure 2.2: Stacking sequence of double layers of 3C-, 2H-, 4H-, and 6H-SiC [16].

Figure 2.3: 4H-SiC crystal structure from different views [18]. The blue and orange colors represent C and Si atoms, respectively.
2.1.2.2 SiC Properties

Pure $\alpha$-SiC is an intrinsic semiconductor with a bandgap of 3.23 eV for 4H-SiC [19]. Because of this high bandgap and low leakage current, compared to Si, SiC is attractive for power monitoring of nuclear reactors at high temperatures. Table 2.1 shows some of the SiC properties compared to other common semiconductors.

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<th>4H-SiC</th>
<th>6H-SiC</th>
<th>3C-SiC</th>
<th>Si</th>
<th>GaAs</th>
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</table>

Table 2.1: Some important properties for different SiC polytypes and some other common semiconductors. The properties are measured at room temperature. The numbers in brackets cite the references.
In addition to the stated positive properties, Si and C neutron absorption cross sections are small. Therefore, the damage caused by (n,\(\gamma\)) reactions in the SiC lattice is small compared to damage caused by fast neutrons. This property helps SiC to endure the thermal neutron flux for a longer period of time compared to the fast neutron flux, where SiC diodes fail rapidly to effectively detect fast neutron projectiles.

Chemically, SiC is a stable material and does not react with the other materials in nuclear reactors. The main concerns in this regard are Schottky and ohmic contact materials which may diffuse into the SiC lattice at high temperatures (above 500 °C [22]) and degrade the detector properties.

In spite of their stated strengths, SiC crystals suffer from micropipes and some other defects [23]. Because of these defects, SiC detectors may not detect particles as well as they should. Recently, Toyota claimed that it has manufactured SiC wafers with very low defect densities [24,25]. This topic is out of the scope of this dissertation.

2.1.2.3 Fermi Energy

As it is stated in Section 2.3, neutron irradiation in nuclear reactors creates defects in SiC detectors. These defects may diffuse and/or evolve in a high-temperature environment. In order to study the diffusion and possible evolution of defects, we need to understand the Fermi energy concept.
The Fermi energy ($E_F$) is the thermodynamic average of the increase in ground state energy, when one electron is added to the system. It is equivalent to the electron chemical potential of the system [26]. The Fermi Energy for intrinsic semiconductors, $E_{Fi}$, can be calculated using Eq. 2.1:

$$E_{Fi} = E_v + \frac{E_g}{2} - \frac{1}{2} k_B T \ln\left(\frac{m_e^*}{m_h^*}\right)$$  \hspace{1cm} (2.1)

where $E_v$ is the valence band edge and $E_g$ is the bandgap energy [27]. $m_e^*$ and $m_h^*$ are the effective electron and hole masses, respectively. The average effective mass of an electron is 0.36 $m_0$ in 4H-SiC (0.29 $m_0$ longitudinal and 0.42 $m_0$ transverse) [19], and the effective mass of a hole is approximately 1.0 $m_0$ [19], where $m_0$ is the mass of an electron.

At special cases, where $m_e^* = m_h^*$ or at zero temperature:

$$E_{Fi} = E_v + \frac{E_g}{2}$$  \hspace{1cm} (2.2)

The Fermi energy for $n$-type semiconductors, $E_{Fn}$, can be calculated using Eq. 2.3 [27]:

$$E_{Fn} = E_{Fi} + k_B T \ln\left(\frac{N_d}{n_i}\right)$$  \hspace{1cm} (2.3)
where \( N_d \) is the donor concentration, \( n_i \) is the intrinsic carrier concentration, which is given by the formula:

\[
    n_i^2 = 2 \left( \frac{2\pi k_B T}{h^2} \right)^{3/2} \left( m_e^* m_h^* \right)^{3/4} \exp(-\frac{E_g}{2k_B T})
\]

where \( h \) and \( k_B \) are Plank and Boltzmann constants, respectively [27].

Usually, one is interested in knowing the Fermi level, \( \mu_F \), (to calculate defect formation energies as is discussed in Section 2.1.2.3), where:

\[
    \mu_F = E_{F_n} - E_V
\]

2.1.3 SiC Diode Design

Per the design of Westinghouse Electric Company [28], the \( n \)-type SiC neutron detector is based on a Schottky diode that detects tritons that are emitted from a LiF radiator layer that is comprised of 90\% enriched \(^6\)Li. This enriched LiF layer plays an essential role in the functioning of the SiC neutron detector, since the tritons create a peak in the detector’s pulse height spectra, within the continuum of events that are the results of energy deposition by neutron induced Si and C recoil nuclei.

Figure 2.4 presents the design of a Schottky diode neutron detector. As can be seen, the neutrons interact with \(^6\)Li atoms producing \(^4\)He (\( \alpha \)) and 2.73-MeV \(^3\)H (triton) particles. The tritons pass through an Al layer and deposit a fraction of their energy as ionization in the depleted region (depleted region) of the detector. \( \alpha \) particles, which also
produce damage in the depleted SiC layer, are shielded by an aluminum layer. Computational analyses made by using the TRIM code have shown that an 8-μm aluminum layer between the $^6$LiF and SiC layers stops all $\alpha$ particles. Stopping $\alpha$ particles from producing radiation damage in the SiC depleted region prolongs the detector lifetime.

Figure 2.4: Schottky diode concept. Picture is not drawn to scale.

In our analysis, it is assumed that the detector is configured as shown from a lateral perspective in Figure 2.4, and that the detector, when viewed from the top, is circular with a diameter of 500 μm. In addition, we assumed that $N_d$ for the SiC depleted region is $2.2 \times 10^{15}$ cm$^{-3}$. Based on this $N_d$, $\mu_F$ for the depleted region is 2.65 eV.
2.2 Studied Reactors

In this dissertation, we have highlighted two commercial reactors (IRIS and GT-MHR) and the Ohio State University research reactor (OSURR). We studied the neutron spectrum at various locations in those reactors. It should be noted that both IRIS and GT-MHR are in the design process stage and have not yet been built. However, the computer modeling methods that are described in this dissertation can be used to estimate the neutron and triton count rates, and displacement damage rates for semiconductor detectors placed in various nuclear reactors.

2.2.1 OSURR

Having been operational since March 1961, the Ohio State University research reactor (OSURR) is an open-pool light-water reactor (Figure 2.5). The maximum nominal thermal power is 500 kW. The reactor fuel is 19.5% enriched U$_3$Si$_2$ with Al cladding. The cooling system works by natural convective flow.
The OSURR has several neutron irradiation facilities. We are interested in three of them in this dissertation:

1) The auxiliary irradiation facility (AIF) is a 6.35-cm (2.5-in) inner-diameter tube that extends from the top of the reactor pool down into a position in the core grid along the south edge of the core. It has a $1.2 \times 10^{13}$ cm$^{-2}$s$^{-1}$ maximum total flux and $5.2 \times 10^{12}$ cm$^{-2}$s$^{-1}$ maximum thermal flux. Figure 2.6 shows a schematic of OSURR-AIF modeled by MCNP5.
2) Beam port 1 (BP1) is a 15.24-cm (6-in) inner-diameter porthole that penetrates the north wall of the reactor pool. BP1 intersects the core perpendicularly on its North face in the core’s North-South centerline plane. BP1 has a $7.8 \times 10^{12} \text{ cm}^2 \text{s}^{-1}$ maximum total flux and a $4.5 \times 10^{12} \text{ cm}^2 \text{s}^{-1}$ maximum thermal flux [29]. Figure 2.7 shows a schematic of OSURR-BP1 modeled by MCNP5.
3) The thermal column (TC) irradiation facility is situated on the West boundary of the thermal column extension that is in the west wall of the reactor pool. It offers a very thermalized neutron field in an approximately a 10.16 cm (4-inch) diameter by 10.16 cm axial length cylindrical volume for experimentation. MCNP modeling and Au wire tests indicate that the thermal neutron flux is approximately $1.4 \times 10^9$ at the nominal full power. Figure 2.8 shows a schematic of OSURR-TC modeled by MCNP.
2.2.2 IRIS Design

The IRIS is a modular, integral, pressurized water reactor whose design addresses the requirements set forth by the DOE Generation IV reactor program [30]. Its integral layout features all primary circuit components placed within the pressure vessel, including the steam generators, coolant pumps, and pressurizer [31,32]. As a consequence of the integrated in-vessel design of the IRIS steam generators, a wide inner annulus exists in the downcomer region surrounding the core (Figure 2.9). High neutron attenuation in this region results in a relatively low ex-vessel neutron flux (on the order of $1 \times 10^5$ – $1 \times 10^8$ times lower than that of conventional light water reactors [33-35]).
For neutron monitoring purposes, a scale-up of existing neutron detection technology, in particular for source and intermediate range monitoring, would be detrimental to the cost competitiveness goals of the IRIS. Thus, alternative detector technologies for use in vessel are being investigated for their potential application to the IRIS design, and subsequent studies on the means of introducing these detectors in the IRIS pressure vessel have also been initiated [36].

Figure 2.9: IRIS vessel layout [37].
2.2.3 GT-MHR Design

The GT-MHR module arrangement is shown in Figure 2.10. The primary components for each module are the reactor vessel and the power conversion vessel, which are connected by a cross-vessel. The vessel systems are located inside an underground silo that is 23.9 m in diameter by 42.7 m deep, which serves as the containment structure. The reactor vessel is made of high strength alloy steel and is approximately 7.58 m in diameter and about 31.2 m high [38]. It contains the reactor core, core supports, internal structure, reactivity control assemblies, and hot duct.

The reactor core consists of hexagonal fuel and reflector elements, plenum elements, and reactivity control material, all located inside a reactor pressure vessel. The core is designed to provide 600 MW_{th} at a power density of 6.6 MW/m^3. The active core consists of an assembly of hexagonal graphite fuel elements (blocks) containing blind holes for fuel compacts and full-length channels for helium coolant flow. The active fuel region of the core consists of 102 fuel columns by 10 blocks high, arranged in three annular rings.
The core is cooled by helium, which flows through the outer annulus within the cross-vessel, up the core inlet riser channels located between the core barrel and reactor vessel, and finally down through the core. The helium that is flowing into the reactor vessel is the working fluid in the power conversion system as well. The GT-MHR
operates at elevated temperature with helium inlet temperatures of 491 °C (764 K) and outlet temperatures of 850 °C (1123 K) [39-40].

2.3 Displacement Damage

Semiconductor electrical properties degrade in a neutron irradiation environment due to interactions between neutrons and semiconductor atoms, creating displacement damage defects. Displacement damage may influence the generation and recombination of electron-hole pairs, free carrier mobility, resistivity, compensation of donors or acceptors, and carrier tunneling [26,41]. In this section, displacement damage is briefly reviewed.

2.3.1 Modeling Literature Review

In studies of displacement damage, one attempts to estimate the number and configuration of displacements created by projectile particles [42]. The study of displacement damage does not deal specifically with the effects of radiation, the impact of time or temperature, or the recovery of defects. These are considerations in the study of radiation effects; however, the accurate prediction of displacement damage is the first step in the accurate prediction of radiation effects.

In a classic paper, Kinchin and Pease introduced a simple model to estimate the number of displacements per PKA (Primary Knock-on Atom) [43]. Later, Norgett et al. proposed a method to approximate the number of Frenkel pairs that are created by energetic particles more accurately [44]. Because of the importance of these analytic
formulations, later in this dissertation, predictions of displacement damage that we have obtained using detailed Monte Carlo (MC) modeling are compared with predictions of displacement damage made using these simple models. Coulter and Parkin formulated the displacement damage methodology for polyatomic materials [45,46].

Most modeling of neutron induced displacement damage, until recent times, has been focused on structural materials, especially iron. Notable among the papers that are not focused on iron, is the paper by Lee and Farnum [47] that used SPECTER [48] and TRIM [49] to estimate the number of vacancies per neutron in alumina. The methods that we have used in this dissertation are similar to the methods that Lee and Farnum have used in that both we and they have predicted PKA source distributions with a computer code and used the resultant PKA source distributions as input to TRIM. However, our methods are different in that our calculations of the PKA source have been generated using the Monte Carlo code MCNP5 [50] with cross sections that are continuous in energy, whereas their PKA source has been generated by using SPECTER. As an additional point of reference, Weber et al. at PNNL have estimated the number of displacements per PKA [51] for SiC as a function of the PKA energy to calculate the efficiency of damage production in SiC.

2.3.2 Displacement Damage

The energy transferred from an energetic neutron with energy $E_n$ to a Primary Knock-on Atom (PKA) in the target, in an elastic collision is [42]:

22
\[ T = \frac{1}{2} \Lambda E (1 - \cos \theta) \]

where \( T \) is the kinetic energy of the PKA, \( E \) is the projectile energy (i.e. \( E_n \) if the projectile is a neutron) and \( \theta \) is the projectile scattering angle. \( \Lambda \) is:

\[
\Lambda = \frac{4m_1 m_2}{(m_1 + m_2)^2}
\]

where \( m_1 \) is the mass of the projectile (i.e. neutron in this case and equal to 1.00), and \( m_2 \) is the atomic mass of the target atom. \( \Lambda E_n \) is the maximum energy that can be transferred from a projectile to the struck atom in an elastic-binary collision (the transferred energy is maximum when \( \cos(\theta) = -1 \) (i.e. head-on collision)). This means that in an elastic collision between a neutron with energy \( E_n \) and a \( ^{12}\text{C} \) atom, the maximum transferred energy to \( ^{12}\text{C} \) is \( 0.284E_n \).

If instead of elastic scattering, an inelastic scattering occurs, the transferred kinetic energy to the PKA is:

\[
T = \frac{1}{2} \Lambda E_n [1 - \frac{1}{2} \frac{E_n^{th}}{E_n} - (1 - \frac{E_n^{th}}{E_n})^{1/2} \cos \theta]
\]

where \( E_n^{th} \) is the threshold neutron energy which is equal to:

\[
E_n^{th} = \frac{m_2 + 1}{m_2} E^* 
\]
where $E^*$ is the excitation energy of the struck nucleus. The lowest (first) excitation energy for $^{12}C$ exists at $E_n^{1th} = 4.82 MeV$ [52]. Therefore, if a neutron with energy $E_n = 5 MeV$ hits a $^{12}C$ atom, and an elastic collision occurs, the maximum C-PKA kinetic energy will be 1.42 MeV. But if an inelastic collision occurs, with excitation of the lowest energy level (hereafter called first inelastic collision), the maximum C-PKA kinetic energy will be 503 keV. Hence, for the $E_n$ and $\cos \theta$, the elastic collision is more destructive than an inelastic scattering event.

The maximum energy that can be transferred in an elastic collision from a neutron to a $^{28}Si$-PKA is 0.133$E_n$. The first excitation energy for $^{28}Si$ occurs at $E_n^{1th} = 1.39 MeV$ [52]. Therefore, if a neutron with energy $E_n = 5 MeV$ hits a $^{28}Si$ atom, the maximum Si-PKA kinetic energy will be 665 keV. But if a first inelastic collision occurs, the maximum Si-PKA kinetic energy will be 569 keV.

### 2.3.2.1 $E_d$ Values

Displacement damage theories are based on the assumption that a target atom must receive a minimum amount of kinetic energy ($E_d$) in a collision in order to be removed from its original position. The $E_d$ values are set equal to 20 eV and 35 eV for C and Si, respectively, to be consistent with Gao et al. [53]. It should be noticed that some other researchers have used other values for $E_d$ [54,55] that might be very different from the values that we used.
The minimum energy that a projectile should have to be able to displace a target atom is $E_d / \Lambda$. Based on Eq. 2.6, a projectile may transfer all its energy to the struck atom, if the projectile and the struck atom have the same masses. Therefore, a 20-eV C-projectile may displace a C atom, and a 35-eV Si projectile may displace a Si atom. But the C-projectile energy should at least be 41.7 eV to displace a Si atom in a head-on binary collision, and the Si-projectile energy should at least be 23.8 eV to displace a C atom in a head-on binary collision. Hence, when the dominant PKAs are C atoms, the dominant defects are C-based defects. This situation happens, particularly, at low neutron energies, where the scattering cross section for C is higher than the scattering cross section for Si.

2.3.2.2 Number of Displacements

As it was stated previously, target atoms which receive $E_d$ in a collision will be displaced. For PKA energies that are much larger than $E_d$, the number of displaced atoms that are produced by the PKA is proportional to the PKA energy. Based on the Nogrett-Robinson-Torrens (NRT) model and the Linhard method, the following equations can be used to approximate the number of displacements that are produced per PKA ($n(T)$) [42,57,58], for large $T$ values:

$$n(T) = \xi(T)\left(\frac{\kappa T}{2E_d}\right)$$ 2.10
where $\kappa$ is the damage efficiency and is equal to 0.8, independent of the PKA energy, and $\xi(T)$ accounts for the effects of inelastic energy loss by the PKA. $\xi(T)$ can be determined using

$$\xi(T) = \frac{1}{1 + k \ g(\varepsilon)}$$  \hspace{1cm} 2.11$$

where

$$k = \frac{0.13372 \ Z^3}{A^2}$$  \hspace{1cm} 2.12$$

and

$$g(\varepsilon) = 3.48008 \varepsilon^6 + 0.40244 \varepsilon^4 + \varepsilon$$  \hspace{1cm} 2.13$$

where

$$\varepsilon = \frac{T}{86.931Z^3}$$  \hspace{1cm} 2.14$$

where the unit of $\varepsilon$ is eV. In the above equations, $Z$ and $A$ are the atomic number and the atomic mass of the target atom, respectively [58].
In Section 4.2.1, we have compared our displacement damage modeling results with the number of defects estimated by the NRT model.

2.4 Defects and Their Properties in 4H-SiC

Displacement damage defects restrict the use of semiconductors as neutron power monitors in nuclear reactors. The greater the displacement damage defects formation rate in a semiconductor, the less chance it has to survive an appropriate time period, e.g. at least one reactor refueling cycle for semiconductors placed in nuclear reactors.

In a pure SiC crystal, either point defects or defect cascades may form. In this section, first some basic data on isolated SiC point defects are presented. Then, defect clusters are discussed. It should be noted that impurities represent other kinds of defects in SiC that are not discussed in this dissertation. The author refers the readers to Refs. [59,60] for those.

2.4.1 Point Defects

Three kinds of point defects can form in SiC, which are vacancies, interstitials and antisites. A vacancy is an unoccupied site for an atom or ion in a crystal [61], as shown in Figure 2.11. In 4H-SiC, both Si and C-vacancies may form in different charged states (charge states of the atoms surrounding the unoccupied site) depending on whether the SiC is $n$-type or $p$-type.
A crystal lattice can be modeled by spherical atoms or ions between which there is empty space. An atom or ion fitting into this space would be described as an interstitial atom or ion \([\text{SI}]\) (Figure 2.12). An interstitial might be an impurity or self-interstitial, i.e. a C or Si interstitial in the SiC crystal. In this dissertation, only self-interstitial defects are discussed. Like vacancies, interstitials may exist with different charge states.

An antisite is a defect where, for a binary compound, a crystal site is occupied by the wrong species\(^2\) (Figure 2.13). For instance, if in SiC, a C lattice site is occupied by a Si atom, then this is called a Si antisite, and if in SiC, a Si lattice site is occupied by a C atom, then this is called a C antisite.

---

\(^2\) It should be noted that if a crystal site is occupied by the right species, but another atom, there is replacement. For instance, if in SiC, a C lattice site is occupied by another C atom rather than the original one, this is called C replacement. A replacement is not a defect.
In pure 4H-SiC, six different point defects may be produced. These are: C interstitial (I_C), Si interstitial (I_{Si}), C vacancy (V_C), Si vacancy (V_{Si}), Si antisite (Si_C), and C antisite (C_{Si}). These defects may diffuse in SiC. We are concerned about the diffusion properties of defects, particularly defect formation energies and diffusion coefficients. The diffusion properties of SiC point defects are presently under study by several research groups [63,64]. The focus of most researchers has been on the 3C-SiC polytype, due to its simple crystalline lattice. Because of the similarities between 3C- and 4H-SiC, most of the 3C-SiC data can be used without any significant change for 4H-SiC [65]. The only important exception might be V_{Si} which is not stable in 3C-SiC and decomposes to a V_C and a C_{Si} [69]. However, V_{Si} is a stable defect in our n-type 4H-SiC. For our work, we used the point defect properties from literature, admittedly with some uncertainty, as follows:

1) Defect formation energy: The defect formation energy determines whether a defect is stable or not. The formation energy of a defect in a SiC crystal is a function of the type of the defect, crystal stoichiometry, doping element and doping concentration.
Defect formation energies of different defects in 3C- and 4H-SiC have been extensively studied [69-73].

In this dissertation, we used the defect formation energies to determine for what charge state the $n$-type 4H-SiC defects are stable. Based on data presented in Ref. [75], we chose those defects that have the lowest formation energies, i.e. the neutral $V_C$ ($V_C^{0}$), $2^-$ $V_{Si}$ ($V_{Si}^{2-}$), $1^-$ $I_{C}$ ($I_{C}^{1-}$), and neutral $I_{Si}$ ($I_{Si}^{0}$) as stable defects in our calculations.

2) Diffusion coefficient: The Diffusion coefficients for C and Si atoms and defects in SiC vary significantly in the literature. Using the self-diffusion isotope technique, Hong et al. [76,77] found $D_C^* = (8.62 \pm 2.01) \times 10^5 \times \exp(-\frac{7.41 \pm 0.05}{k_B T}) \text{ cm}^2 \text{s}^{-1}$ for pure $\alpha$-SiC, $D_C^* = (3.32 \pm 1.43) \times 10^7 \times \exp(-\frac{8.20 \pm 0.08}{k_B T}) \text{ cm}^2 \text{s}^{-1}$ for N (nitrogen)-doped $\alpha$-SiC, $D_{Si}^* = (5.01 \pm 1.71) \times 10^2 \times \exp(-\frac{7.22 \pm 0.07}{k_B T}) \text{ cm}^2 \text{s}^{-1}$ for pure $\alpha$-SiC, and $D_{Si}^* = (1.54 \pm 0.78) \times 10^5 \times \exp(-\frac{8.18 \pm 0.10}{k_B T}) \text{ cm}^2 \text{s}^{-1}$ for N-doped $\alpha$-SiC. Linnarsson et al. [78] found $D_C^* = 8.4 \times 10^2 \times \exp(-\frac{8.50}{k_B T}) \text{ cm}^2 \text{s}^{-1}$ for 4H-SiC. K. Ruschenschmidt et al. [79]

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3 There are different methods to calculate defect formation energies. We refer the readers to Ref. 74.

4 It should be noticed that C and Si atoms diffuse (self-diffusion) through defects in the SiC.
measured $D^* = (4.8^{+573}_{-47}) \exp(-\frac{+7.6 \pm 1.0}{k_B T})$ cm$^2$/s for both Si and C self-diffusion in 4H-SiC. Using ab initio techniques, Bockstedte et al. [75] determined $Q$ (recall that $D = D_0 \exp(-\frac{Q}{k_B T})$ where $D_0$ is the diffusion prefactor) for point defects in 3C-SiC. Based on their calculations, for $\mu_C = 2.65$ eV and $\Delta \mu = -0.3$ eV ($\Delta \mu$ is the chemical potential difference and varies between the negative heat of formation of the corresponding polytype ($-H_f,\text{SiC} = -0.61 eV$) for C-rich SiC and 0 for Si-rich SiC) for stoichiometric SiC, $Q$ is 7.6 eV for $V_C^0$, 6.24 eV for $I_C^{1-}$, 7.68 eV for $V_{Si}^{2-}$ and 10.2 eV for $I_{Si}^0$ [75] 

As it can be seen, different researchers determined different $Q$ values for C and Si defects in SiC. For the sake of consistency, we used the $Q$ values provided by Bockstedte et al. [75] in this dissertation.

Data given by Gao et al. [80] were used for the diffusion prefactors, $D_0$, for point defects in SiC. Using a classic Molecular Dynamic (MD) code, they determined $D_0$ for $I_C$ and $I_{Si}$ to be $1.23 \times 10^{-3}$ cm$^2$/s and $3.30 \times 10^{-3}$ cm$^2$/s, respectively. Due to the lack of available data, the same values were used for $D_0$ for $V_C$ and $V_{Si}$, respectively.

5 A variety of vacancies and interstitials in 3C- and 4H-SiC may happen, depending on the position of the defects. We have chosen those types of defects that are more stable in our case.
It was assumed that diffusion coefficients for antisites are zero. In other words, we assumed that antisites are immobile.

2.4.2 Defect Clusters

As shown by Weber et al. [63], approximately 25% of interstitials created by isolated 10 and 50 keV Si-PKAs in 3C-SiC form clusters with 2 or more interstitials. This example shows the importance of defect clusters. In fact, defect clusters may dominate annealing at different annealing temperature stages [65].

In this dissertation, we treated defect clusters by using defect pairs. Defect-pairs are special cases of clusters that consist only of two defects. We have assumed that the capture radii that we determined for defect-pairs are valid for clusters with more than two defects, as well. If the distance between two defects is less than the determined capture radius for those two defects, they are assumed to interact with each other. Following capture, we assume that the captured defects would trap and block each other from further migration. We used the methods described in Section 3.6.3 to determine the capture radii for defect-pairs in 4H-SiC.

2.4.3 Defect Recombination

Based on defect formation energies, if two defects become close to each other (closer than the capture radius), they may recombine to decrease the total energy of the system. A recombination may result in either defect annihilation (e.g. \( \text{I}_C + \text{V}_C \rightarrow \text{C} \) in its lattice site), or creating a new defect (e.g. \( \text{I}_C + \text{V}_{\text{Si}} \rightarrow \text{C}_{\text{Si}} \)).
We used the method described in Section 3.6.3 to determine the capture radii for defect recombination.

2.5 Influence of Temperature

Temperature has a dual impact on SiC detectors with opposite effects. On one hand, a high temperature may destroy the contact structure and produce defects inside the SiC detectors. On the other hand, the ambient temperature during reactor operation should be high enough that damage anneals and the SiC recovers. In fact, it seems that the SiC detector can tolerate a high fast neutron radiation environment only for a very short period of time at room temperature [81].

As it was stated by Kirschman [82], the electrical resistance of conductors and contacts, and chemical and metallurgical interactions between materials in the detector package are increased by increasing the temperature. Since SiC is a high band-gap semiconductor, it may tolerate at least up to 600-700 °C [83]. However, its contacts may not tolerate temperatures above 600 °C for long times. The SiC Schottky and ohmic contacts for high temperature environment are still in the development stage by several research groups [84-87].

On the other hand, at room temperature, 4H-SiC detectors rapidly degrade [81,146], depending on neutron flux, due to amorphization [145]. For fluxes that are typical of commercial nuclear reactors, this amorphization could happen at room temperature in a few hours. At high temperatures, SiC detectors have more chance to survive at least one reactor refueling cycle. Mclean et al. showed that at 300 °C, SiC
JFETs irradiated by neutrons are more stable than at lower temperature, but they found no evidence of annealing of damage [88].

On the contrary, Ruddy et al. [151] cited that at 230 °C irradiation temperature, the effect of neutron irradiation is reduced by a factor of at least 100, compared to room temperature. Though these results are arguable, defects move faster in the crystal at a high temperature and have more chance to capture each other. As a consequence, two defects may completely eliminate each other at high temperatures.

As a conclusion regarding the influence of temperature, there may be an optimum temperature for which the residual damage is minimized. This optimum temperature is not very well known, since it depends on several variables, such as, the Schottky and ohmic contacts, the irradiation time, and the neutron flux and its energy spectrum. Based on the literature review, the author thinks the total damage to the SiC detector and the contact is minimized at temperatures between 400-600 °C.

2.6 Displacement Damage Terms

There are some terms that are used to describe the sensitivity of the target material (i.e. SiC in our case) to the irradiation environment. Among those are: 1 MeV Equivalent Neutron Fluence (\( \Phi_{\text{Total}}^{\text{eq,1MeV}} \)), radiation hardness and the number of point defects per atom (\( PDPA \)). Each of these terms has some advantages and some limitations. In this section, these terms are briefly reviewed.
2.6.1 1 MeV Equivalent Neutron Fluence

A common term to characterize the damage dose received by a material, because of neutron interactions, is the 1 MeV Equivalent Neutron Fluence ($\Phi_{\text{Total_{eq,1MeV,mat}}}$) where $\text{mat}$ denotes the material of interest. $\Phi_{\text{Total_{eq,1MeV,mat}}}$ is defined as:

$$\Phi_{\text{Total_{eq,1MeV,mat}}} = \int_{0}^{\infty} \frac{F_{D,\text{mat}}(E)}{F_{D,1\text{MeV,mat}}} \Phi(E)dE$$

where $F_{D,\text{mat}}(E)$ is the damage function (the displacement damage kerma factor), which is given below in Figure 2.14 for Si and SiC. In this figure, $F_{D,\text{Si}}(E)$ is from ASTM 722-94 [87]. The values for $F_{D,\text{SiC}}(E)$ are not directly available in the literature. Instead, in Ref. [89] the values for the displacement cross section, $\sigma_d(E)$ (with the unit of barns), are given.
Figure 2.14: The damage functions (the displacement damage kerma factors) for Si and SiC logarithmic scales are used for the ordinate and for the abscissa.

Eq. 2.16 was used to calculate $F_{D, SiC}(E)$ [90-92], assuming the average $E_d$ for SiC is 22 eV [97,98]:

$$F_{D, SiC}(E) = \frac{2\sigma_d(E)E_d}{\beta} \times 10^{-3}$$

where $\beta$ is the atomic scattering correction factor and which is equal to 0.8. $\beta$ is used in Eq. 2.16 to take into account realistic atomic scattering (instead of the hard core
approximation) and recombination of defects in a cascade [93]. The $10^{-3}$ in the equation arises from matching the units of the different parameters.

2.6.2 $D\dot{P}A$

$\sigma_d(E)$ can be used to estimate the number of displacements per atom rate ($D\dot{P}A$) created by neutrons in a SiC crystalline structure [144] at a low temperature:

$$D\dot{P}A = \int_0^\infty \sigma_d(E) \times 10^{-24} \times \phi(E) dE$$  \hspace{1cm} 2.17

The $D\dot{P}A$ concept does not distinguish between stable defects and defects that may recover at a high temperature because of annealing.

2.6.3 Hardness

Another displacement damage parameter is the neutron energy spectrum hardness ($H_{\text{mat}}$). As stated in ASTM E722 [87], $H_{\text{mat}}$ is defined, as:

$$H_{\text{mat}} = \frac{\Phi_{\text{Total}}}{\Phi_{\text{Total}_{\text{eq.1MeV}}}}$$  \hspace{1cm} 2.18

$H_{\text{mat}}$ is a useful parameter for comparing two or more neutron energy spectra, on the basis of their propensity for creating displacement damage defects in a specific material (i.e. SiC in our case), assuming their total flux is equal [94]. In addition, if $H_{\text{mat}}$ is a small number, one can predict that the neutron count rate would be small, compared to the triton count rate for a SiC detector of the type shown in Figure 2.4.
It should be noted that since $H_{n_{\text{at}}}$ is not a function of the neutron fluence, it cannot be used alone to evaluate displacement damage.

2.6.4 PDPA

The number of point defects per atom (PDPA) is a useful term for comparing the number of displacements created by various fluences of various projectiles irradiating various target materials. In addition, it can be used to study the evolution of displacement damage defects over time at a higher temperature.

Another advantage of PDPA over $\Phi_{\text{eq,1MeV}_{n_{\text{at}}}}^{\text{Total}}$ is that the damage caused by all projectiles (e.g. neutrons and tritons) can be added up in PDPA [95]. This is particularly useful when the target is subjected to damage by more than one projectile. For instance, in our case, the SiC detector is subjected to damage from neutrons, tritons, and $^{29}\text{Si}$ and $^{13}\text{C}$ recoils.

A limitation of the PDPA as a damage assessment parameter, is that with the PDPA we treat defects in the target material as point defects. In other words, PDPA does not reflect the influence of clustering.

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$^6$ Previously, we used $N_{VP4}$ (number of vacancies per atom) in our papers [95-97]. Since $N_{VP4}$ does not cover the number of antisites; we have used PDPA in this dissertation. PDPA does not include the importance of different defects, since we are not aware of that yet.
2.7 Computer Codes

In this dissertation, six computer codes have extensively been used. Four of these codes are commercially available, including MCNP5 \[38\], TRIM \[99\], MARLOWE \[100,101\] and VASP \[102-105\]. The author of this dissertation wrote two other codes: MCASIC and DCRSIC, since there were no available codes for their purposes.

In addition to those six codes, two more molecular dynamic simulations (MD) codes, MOLDY and MDCASK, are introduced. Although, MD codes have not been run directly in this project, the MD data obtained by other researchers have been used in a part of the dissertation.

In this section, these computer codes are briefly reviewed. A description about how these codes were used is given in Chapter 3.

2.7.1 MCNP5, A MC Code

MCNP was developed by LANL. MCNP is a general purpose Monte Carlo N-Particle code that can be used for continuous-energy, generalized-geometry, time-dependent, neutron, photon, and electron or coupled neutron/photon/electron transport. When one uses MCNP to estimate desired quantities, one does not solve an explicit equation, such as the neutron transport equation, but rather one simulates the life histories of individual particles as they travel through the problem geometry. Large numbers of particles are followed and quantities of interest, such as particle fluxes or particle interaction rates, are inferred from the average behavior of the particles. A difficulty with
the Monte Carlo methods is that to achieve adequate accuracy for calculated averages, a large number of histories must be performed. For faster convergence of the averages, variance reduction techniques can be applied to get results that are more accurate in reasonable times.

MCNP5 covers neutron energies from $10^{-11}$ MeV to 20 MeV for all isotopes. In order to run MCNP5, the user needs to specify the geometry, materials, location and characteristics of the source, type of answer that is desired (tallies), and techniques to improve efficiency [106].

In this dissertation, we used MCNP5 to predict neutron flux and neutron energy spectra for various locations in the IRIS and GT-MHR, and to determine the number of created triton, $^{29}$Si and $^{13}$C recoils for detectors placed at various locations in the OSURR, IRIS and GT-MHR. In addition, we used this code to characterize collisions between neutrons and SiC primary knock-on atoms (PKAs) as inputs for TRIM.

2.7.2 TRIM, A BCA-MC Code

Transport of Ions in Matter (TRIM) is part of the Stopping and Range of Ions in Matter (SRIM) package [107-108]. TRIM is a binary collision approximation (BCA) code that, like MCNP5, is based on Monte Carlo methods. TRIM determines the collision characteristics between projectiles (ions or atoms) and the target atoms [109]. The inputs for TRIM are types, energies, positions and directions of incident projectiles, and densities, thicknesses, displacement energies and binding energies of target atoms.
TRIM only assumes an amorphous target at 0 K. Another TRIM deficiency for our purpose is that it gives the spatial distribution of vacancies, not interstitials. Therefore, the TRIM output cannot be directly used to determine the number of defects in the target (i.e. SiC in our case) after some period of time (e.g. a reactor refueling cycle) at reactor temperatures.

In this dissertation, we used TRIM to gain information about collisions between PKAs, tritons, $^{29}$Si and $^{13}$C projectiles and SiC atoms, including the numbers of different C- and Si-defects (vacancies, interstitials and antisites (TRIM assumes that an antisite is a kind of interstitial. However, approximately the number of replacements is equal to the number of antisites)). It should be noted that TRIM gives the number of interstitials, but not their positions.

2.7.3 MARLOWE, A BCA Code

MARLOWE is a program for simulating atomic collision processes in crystalline solids based on the binary collision approximation. MARLOWE has some advantages over TRIM. The most important one, regarding this dissertation, is that MARLOWE gives the positions of vacancies and interstitials\(^7\), within some uncertainties [143]. Another advantage of MARLOWE is that the target can be modeled as a crystal.

\[^7\] MARLOWE tracks the defects created before any possible recombination. Therefore, MARLOWE does not give the number or positions of antisites.
In spite of these benefits, MARLOWE is difficult to use; since in MARLOWE a user cannot directly define $E_d$ values for Si and C in SiC, as one can in TRIM. Therefore, we used TRIM to adjust two of MARLOWE’s input parameters (EBND\textsuperscript{8} and EQUIT\textsuperscript{9}) for each projectile energy that was analyzed, until the MARLOWE output for the number of C and Si-vacancies matched the TRIM output for these quantities.

2.7.4 VASP, An Ab Initio Code

The Vienna Ab-initio Simulation Package (VASP) is a software package for performing ab-initio quantum-mechanical atomistic calculations and molecular dynamics (MD) simulations using pseudopotentials and a plane wave basis set \cite{110}. VASP solves the quantum mechanical Kohn-Sham equations within density functional theory \cite{111} to determine the electronic structure and the interactions between target atoms.

VASP and other ab initio codes, such as SIESTA, have been extensively used by researchers like Rurali et al. \cite{112}, Mattausch et al. \cite{113}, Windl et al. \cite{114,115}, Torpo et al. \cite{70}, and Posselt et al. \cite{71} to calculate information about the SiC crystalline structure and defects. Since ab initio codes are slow, we used VASP to estimate the static energy of SiC lattices with and without defects, but did not use it to study dynamical processes with MD simulations.

\textsuperscript{8} EBND is the energy parameters of the binding model.

\textsuperscript{9} EQUIT is the minimum kinetic energy for an atom to continue in motion.
2.7.5 **MCASIC, A KMC Code**

The TRIM and MARLOWE codes assume that the target is at zero temperature, and that there is no annealing effect. In order to predict the impact of temperature and model annealing, we developed a Kinetic Monte Carlo (KMC) code for 4H-SiC which we currently call Monte Carlo Analysis of SiC (MCASIC). Some of the KMC input data, such as the point defect diffusion parameters, are available in the literature [75,80]. Where such information is missing, we used VASP and DCRSIC to estimate those parameters; for instance, the capture radii for defect-pairs.

2.7.6 **DCRSIC, A KMC Code**

If the distance between two defects becomes less than the capture radius for this defect pair, several different processes may occur. They may recombine and eliminate each other (such as $\text{V}_C^+ \text{I}_c \rightarrow \text{C}$ in its original site), or they may recombine and create one defect instead of two (such as $\text{V}_C^+ \text{I}_\text{Si} \rightarrow \text{SiC}$). Sometimes if two defects (such as I$_C^-$-I$_c$) become close enough, they may significantly influence their diffusion properties. In this case, a defect cluster is created. Usually, defect clusters have less mobility than point defects. We wrote Defect Capture Radius calculations for SiC (DCRSIC), which is a KMC code, to determine the capture radii for defect pairs in 4H-SiC. Assuming that defects will form pairs (recombine) once they are closer than their capture radii, the capture radii can be used as input parameters to speed up the KMC simulations in MCASIC.
2.7.7 *MOLDY* and *MDCASK, Classic MD Codes*

Classical MD codes use empirical or semi-empirical potentials to determine the interaction energies among atoms, but otherwise they perform the same types of atomistic simulations as VASP. MDCASK and MOLDY are two MD codes that have implemented Tersoff potentials for Si, C, and Si-C interactions [116-118] and can thus be used to perform MD simulations for SiC.

William Weber’s group at PNNL have used these codes to study defect properties in SiC, such as $E_d$ values for Si and C [53], the efficiency of damage production [119], amorphization [120-122], picosecond damage evolution [123-125], and defect migration [61]. Since the time step in MD simulation cannot exceed the order of femtoseconds (thermal vibrations with periods in the ps range need to be truthfully modeled), neither of these MD codes was used to study damage for longer annealing times.
CHAPTER 3

CALCULATIONAL METHODS

3.1 Nuclear Reactor Flux

3.1.1 OSURR

The values of $\phi(E)$ that are used in this dissertation for OSURR-AIF (Figure 2.6) and -BP1 (Figure 2.7) were measured using foil activation data and the SAND-II neutron energy spectrum deconvolution code, when the reactor power was 50 kW. Then assuming linearity between power and neutron flux, $\phi(E)$ values were determined at 500 kW.

$\phi^{\text{Total}}_{\text{eq},3\text{MeV},\text{SiC}}$ and $H_{\text{SiC}}$ were calculated using the method that is described in Section 0.

The Neutron flux spectrum measurements were taken at 11.65 cm (Position 1), 35.56 cm (Position 2) and 52.07 cm (Position 3) from the bottom of the core in the AIF.

In the BP1, the measurements were done at two positions in the Characterization Vessel (Figure 3.1), i.e. 7.6 cm (Position 3) and 17.6 cm (Position 1) from the edge of the reactor pool.
Figure 3.1: Characterization vessel that was used to measure neutron flux spectrum in the BP1. Ion-chamber pair was used for neutron and gamma dosimetry. The ion-chambers are in the balloons. The characterization vessel is shielded by a Cd layer.

We used MCNP5 to calculate the neutron flux in the TC as $1.4 \times 10^9$ cm$^{-2}$s$^{-1}$.$^{10}$

$^{10}$ One of my colleagues, Jeremy Chenkovich, did the MCNP modeling to calculate the neutron flux in TC.
3.1.2 IRIS

3.1.2.1 In-Vessel Placement of Detectors in the IRIS

The wide annular region surrounding the IRIS core (as a result of the in-vessel placement of the steam generators) leads to large neutron attenuation in the downcomer region that precludes the use of conventional ex-core detector technology for monitoring ex-vessel neutron fluxes. However, the wide downcomer region offers an opportunity to use novel detector technology for in-vessel monitoring. SiC detectors offer high temperature capability and radiation hardness along with small size and may be applied to IRIS in-vessel neutron monitoring. Conventional electronics (preamplifier and cabling) can be used with SiC detectors, which may be effectively routed within instrumentation tubes through the downcomer region to the core (Figure 3.2). The penetrations required for the instrumentation tubes can be made such that they comply with the safety goals of IRIS [37].
Figure 3.2: Routing vessel sidewall penetration [37]. The penetration is not in the main IRIS design.
3.1.2.2 *MCNP5-Model of IRIS*

The goal of the IRIS neutronics analysis was to calculate the neutron radial flux distribution resulting from fission events within the IRIS core, as input to predictions of SiC detector response. The contribution to the gamma-ray flux resulting from activation of materials within the RPV was not included in the calculations. A knowledge of the neutron and gamma-ray radial flux distributions is necessary in order to determine where to place the SiC detectors for a particular power range, since their placement must balance their sensitivity with their resistance to radiation resistance damage.

The IRIS reactor was modeled in 3-dimensions in MCNP5, accounting for radial and axial variations of the core power distribution. Figure 3.3 shows transverse and lateral views of the MCNP5 model of IRIS.

Some comments follow regarding the composition and density of materials used in the calculations:

1) The core is represented as a homogeneous mixture of UO$_2$, Zr, and H$_2$O, and the fraction of each element was calculated according to the core structure given by WEC. This is an acceptable approximation, since the primary interest is the fast neutron flux outside the core.

2) The reflector is made up of 90% stainless steel and 10% light water.

3) The density of H$_2$O is 0.702 g/cm$^3$. 
4) SS304 is used for stainless steel, with a density of 7.92 g/cm³.

5) AISI 100 is used for low carbon steel, with a density of 7.82 g/cm³.

6) The concrete density is 2.35 g/cm³.

Figure 3.3: The side and upper views of the MCNP5-model of IRIS.
The neutron flux distribution was calculated as functions of axial location for four radii in the downcomer region (155 cm, 170 cm, 185 cm, and 200 cm) in the instrumentation tube. We used these data to predict the detector count rate and the 1 MeV neutron equivalent flux in SiC.

Two instrumentation tube designs were considered. In all cases, the instrumentation tube was modeled as a 14-cm outer diameter stainless steel tube with a 4-cm thick wall. For one design (called simply the stainless-steel instrumentation tube), the instrumentation tube is empty except for the detector. For a second design (called the three-layer instrumentation tube), the instrumentation tube is lined with a 0.5-cm thick layer of Cd, which encircles a 2-cm thick polyethylene layer (Figure 3.4). The purpose of the Cd layer is to absorb thermal neutrons that are incident on the instrumentation tube from the outside. The purpose of the polyethylene layer is to thermalize energetic neutrons coming from outside the instrumentation tube which pass through the Cd, so that the neutrons more readily induce $n,\alpha$ reactions in the LiF radiator that is a part of the SiC diode neutron detector package. Together the Cd and polyethylene layers serve to: 1) make the detector more responsive to neutrons that reach the detector with fewer scattering events (higher energies), and 2) decrease the damage to the detector that results from Si and C neutron recoil events. By making the detector more responsive to energetic neutrons, we are effectively allowing the detector to peer more deeply into the core.
3.1.3  GT-MHR

The SiC neutron power monitors may be placed within the central reflector (in-core positions) or external to the core (ex-core positions). However, for the ex-core positions SiC detectors do not exhibit any particular advantage over traditional detectors. In fact, for ex-core positions, the neutron flux is so low that the count rate of SiC diode detectors may be too small to initiate protective actions in acceptably short times with good confidence.
This dissertation is directed toward the evaluation of semiconductor detectors for use as in-core neutron power monitors for the GT-MHR. For this purpose, a SiC diode detector has advantages, because of its wide band gap energy compared with conventional semiconductors, which make it resistant to the effects of temperature and radiation damage. Furthermore, its relatively small size permits measurement at discrete physical locations.

Although operation in the GT-MHR at temperatures as high as 850 °C (1123 K) might have some advantages for SiC detectors, by more completely annealing radiation damage, operation at such high temperatures would destroy the ohmic and Schottky contacts, for ohmic and Schottky contacts that are presently available for SiC devices. For this reason, we designed a cylindrical tube, which we shall hereafter call a “capsule”, in which to place SiC detectors within the GT-MHR central reflector. The purpose of the capsule is to maintain the temperature of the SiC detectors at values that are below the limits for degradation of the ohmic and Schottky contacts, but as high as possible within these limits, so as to maximize the annealing of the detector. It should be noted that these capsules are not a part of the GT-MHR original design.

We chose four radial locations, and given the hexagonal shape of the GT-MHR reactor, six azimuthally symmetrical azimuthal locations in the central reflector of the GT-MHR in which to place the capsules. Figure 3.5 [126] presents a cross section of the reactor vessel in which the locations of the capsules are identified. The capsules are
located at radii of 153 cm (R153\textsuperscript{11}) and 117 cm (R117), 81 cm (R81) and at the core center (R0). There would, of course, be only one capsule located at the center of the central reflector, since azimuthal angle cannot be defined for that position.

![Figure 3.5: GT-MHR core arrangement. R153, R117, R81 and R0 are shown in the schematic. The capsules are not in the original design and have been added by us.](image)

\textsuperscript{11} For the sake of simplicity, the notations R153, R117, R81 and R0 are used in the rest of this dissertation to refer to detector locations in the GT-MHR. The number after the R refers to the radial location of the capsule. For example, R153 refers to a capsule located at R=153 cm from the center of the GT-MHR.
3.1.3.1 Capsule Design

The capsule design is only conceptual at this point. In order to keep the SiC within a temperature range of 500-600 °C, it consists of two nested cooling systems (one that is passive and another that is active) circulating He coolant around and through, respectively, two nested steel cylinders that are insulated over their length by a third cylinder with larger radii (labeled in Figure 3.6 as insulator). The capsules enter the central reflector through the top of the core. The outer cooling system is a parasitic flow path (a diverted stream of reactor coolant) for the main coolant flow through the core. In the drawing below, this flow path is through the tube with tube walls that are labeled as insulator and the inwardly adjacent tube. This parasitic flow path cools the detectors, whenever coolant flows through the core. Although the term is not perfectly accurate, we will hereafter refer to it as a passive system. This system protects the detectors in the case of an accident event, for which the helium flow-rate for the active cooling system is interrupted. By the active cooling system we mean a forced-convection (pumped) loop moving heat energy from the capsule’s interior to the outside of the pressure vessel. Figure 3.6 shows the geometric arrangement of the two cooling systems.
3.1.3.2 *GT-MHR MCNP5 Model*

The GT-MHR reactor geometry was defined using MCNP5 input cards. Figure 3.7 presents axial and vertical cross sections for the MCNP5 GT-MHR model. The 3-D geometry was made up of a series of vertical surfaces and horizontal planes. Thus, all the regions of the reactor had finite lengths. Our model of the GT-MHR reactor geometry is described below in the following two paragraphs. In the first paragraph, we describe those parts of the MCNP5 model that are consistent with the General Atomics (GA)
The design of the GT-MHR, as that was the design provided to us by GA. The second paragraph describes those parts of the MCNP5 model that are particular to our envisioned modification of the GT-MHR reactor design to include capsules in the central reflector in which to place SiC neutron monitors.

The parts of the MCNP5 model that are consistent with the General Atomics design of the GT-MHR are described below, from smaller radii to larger radii. The central reflector consists of graphite hexagonal elements. These hexagonal elements are assembled in a manner so as to create a larger hexagon with a distance between flats (the distance between two opposite sides of the hexagon) of 280.592 cm. This larger hexagon defines the outer boundary of the central reflector and the inner boundary of the active (fueled region) of the GT-MHR core. The active core consists of an assembly of hexagonal graphite fuel elements (blocks) containing blind holes for fuel compacts and full-length channels for helium coolant flow. The fueled region of the GT-MHR core (1) was defined as existing between the hexagon that defines the outer boundary of the central reflector and a larger hexagon, with a distance between flats of 467.724 cm, which define the outer boundary of the active core. Neither the individual fuel compacts, nor the coolant channels, were modeled in detail. Also, six prismatic elements of the outer replaceable reflector were inserted into the hexagon defining the active core (compare the outside corners of the active core hexagon in Figure 3.5 and Figure 3.7), in order to model the real geometry, as closely as possible. The volume of the active core was divided into ten axial layers according to height of the hexagonal graphite fuel elements of which the core is composed. The height of the active core is 800 cm and the
height of one fuel element block is 80 cm. As can be seen in Figure 3.7, above and below the core, there are upper and lower replaceable reflector cells. The height of the upper reflector is one and one-half blocks (120 cm), and the height of the lower reflector is two blocks (160 cm). Although they are formed as blocks, three regions of the core that are outside of the active core region were, for simplicity, modeled as annuli with increasingly larger radii. The three regions are, in order of increasing radii, the outer replaceable reflector, the permanent side reflector, and the portion of the permanent side reflector that contains boron carbide pins. An annular core barrel, with a thickness of 5.5 cm, was defined as surrounding the portion of the permanent side reflector that contains boron carbide pins. The outer surface of the core barrel is modeled as being surrounded by two annular regions, which contain helium, that are divided by a gas duct shell. The helium is the working fluid in the power conversion system and the coolant for the core. The helium flows through the two annuli, before finally flowing down through the core. An annular region, which is at larger radius than the larger of the two helium-filled annuli, forms the reactor vessel. Two annular rings that are located at an elevation equal to that of the top of the active core, define the reactor flange. They are 68 cm thick, with a height of 100 cm. The reactor vessel is modeled as being surrounded by air, which fills the region between the outer surface of the reactor vessel and the Reactor Cavity Cooling System (RCCS). The RCCS removes heat from the reactor vessel. It surrounds the reactor vessel over its full circumference and height. In the model, an annular region with an inner diameter of 590 cm and an outer diameter of 606 cm defines the RCCS wall. We modeled an annular region of air with a thickness of 34 cm, behind the RCCS wall. Two cylinders, one with radius of 640 cm and the other with a radius of 640.6 cm define the
inner and outer walls of the RCCS cavity liner. The cavity liner is surrounded by the outermost component of the GT-MHR model, which is an annular region that represents the concrete wall of the silo. Finally, the model is surrounded by a sphere with a radius of 900 cm that forms the boundaries of the MCNP5 model. Particles are not transported outside beyond the boundaries of this sphere.

The parts of the MCNP5 model, which are particular to our envisioned modification of the GT-MHR reactor design to include capsules in the central reflector in which to place SiC neutron monitors, are described below. The capsules with the detectors and cables are envisioned to be placed at 0-, 60-, 120-, 180-, 240-, 300- degree locations, within the central reflector, as shown in Figure 3.7. Two annuli, with walls of steel, define each capsule. Each capsule is surrounded by a porous carbon annulus (which is identified as insulator in Figure 3.6) that provides thermal insulation for the capsule. The volumes within the inner steel annulus, and between the steel annuli, and between the outer steel annuli and the surrounding porous carbon insulator, are filled with helium. Four models were created with capsules at R153, R117, R81 and R0.
The fueled region of the core was represented in the MCNP5 model as a homogenous mixture of uranium, oxygen, silicon, boron and carbon. The same modeling simplification of homogenization was used for the permanent side reflector that contains boron carbide pins. The modeling is more detailed than is necessary beyond the reactor vessel. This detail was a remnant of a previous modeling effort where the intent was to
predict the response of detectors that were placed external to the reactor vessel. A more detailed description regarding our MCNP5 modeling of the GT-MHR can be found in [127,128].

3.2 Count Rate Calculations

Three general categories of events can contribute to the SiC detector count rate \((CR)_{all}^{12}\) in SiC detectors. The three categories of events are: 1) events that are initiated by the interaction of gamma rays; 2) events that are initiated by the interaction of thermal neutrons and epithermal neutrons with the radiator; and 3) events that are initiated by epithermal and fast neutron interactions with the SiC. Events that are initiated by gamma-rays produce counts in the detector in an indirect fashion, as the gamma-rays generate secondary electrons. The thickness of the depleted volume of the detector, that is shown in Figure 2.4, is so small (10 μm) that secondary electrons, that are created by gamma-ray interactions, pass through the diode depleted volume without creating many electron-hole pairs. Although gamma-ray events appear in recorded pulse height spectra, the gamma-ray events can be eliminated from the pulse height spectra by pulse height discrimination, by setting a sufficiently large lower level of discrimination (LLD). The events that are initiated by thermal and epithermal neutrons are, in the great majority of cases, due to the interaction of the thermal neutron with \(^6\text{Li}\) in the LiF radiator. The

\[\text{Ref}^{12}\] The subscript “all” stands for all projectiles related to the main variable. For instance, the count rate for the SiC diode detectors is due to either tritons or fast-neutron-induced PKAs. Therefore, “all” in \((CR)_{all}\) refers to the tritons and fast-neutron-induced PKAs.
resulting tritons have a range that is large enough that, for a 1 \( \mu \text{m} \) thick LiF radiator, most of the tritons, which are emitted in the direction of the diode, enter the diode active volume and create a pulse which is above the LLD setting for gamma-ray discrimination. In contrast with the events that are due to tritons, events that are initiated by epithermal and fast neutron interactions with SiC, create a pulse height distribution that has components that are both above and below the LLD, if the LLD is set to barely eliminate gamma-ray events from the pulse height spectra.

We have used MCNP to predict the count rates resulting from neutrons interacting with the LiF radiator and with the SiC. We have not concerned ourselves with modeling gamma-ray interactions, since events that are due to gamma-ray interactions can be eliminated from the detector count by pulse height discrimination.

The detector count rate was calculated in a two step process. As the first step of the process, we calculated the neutron flux within the desired SiC locations. As the next step in the process, a model of the detector was created in MCNP, and the MCNP-SiC detector model was run to estimate \((CR)_{\text{all}}\). In the MCNP-SiC detector model, the SiC detector was modeled as being at the center of a sphere. A source of neutrons was defined at the surface of the sphere, with neutron energy spectrum corresponding to the neutron flux that was calculated in step one. The neutron source was emitted from the spherical surface with a directional bias, which created a higher track density toward the center of the sphere, where our detector was placed. The radius of the sphere was 0.1 cm.
In order to calculate the fast neutron count rate \((CR)_{\text{neutron}}\), MCNP F4:N tally and PTRAC cards were used to determine the energy spectra for SiC-Primary Knock-on Atoms (PKA). Based upon experimental observations, we concluded that PKAs, that deposit more than 200 keV \((N_{e_{\text{PKA}>200\text{keV}}})\) within the detector active volume, create pulses which exceed the LLD and cause a count. Therefore, in our analysis, we counted the number of PKAs per sp in the MCNP-SiC detector model that have energies more than 200 keV \((N_{e_{\text{PKA}>200\text{keV}}})\). Because the active volume of the SiC detectors is very thin, the probability, of a single neutron creating more than one PKA, is exceedingly small. Therefore, the pulse height tally option in MCNP was not used.

Because a source particle, for the calculation of the neutron flux using the MCNP-Reactor model, is different from a source particle, for the calculation of the detector count rate using the MCNP-SiC detector model, Eq. 3.1 was used to determine \((CR)_{\text{neutron}}\):

\[
(CR)_{\text{neutron}} = \phi_{\text{reactor}} \cdot N_{e_{\text{PKA}>200\text{keV}}} / \Phi_{\text{MCNP}}
\]

where \(\phi_{\text{reactor}}\) is the neutron flux at the desired location calculated using the MCNP-Reactor model, and \(\Phi_{\text{MCNP}}\) is the neutron fluence per sp in the MCNP-SiC neutron detector model.

---

\(^{13}\) The methodology used to determine PKA specifications will be discussed in Section 3.6.1.
In addition, the MCNP FM card was used to determine the number of $^6$Li(n,α)$^3$He reactions in the LiF layer of a SiC diode detector. Then the triton count rate ((CR)$_{triton}$) was calculated using Eq. 3.2.

$$(CR)_{triton} = \phi_{reactor} \cdot N_{triton} \cdot 0.39 / \Phi_{MCNP}$$

where $N_{triton}$ is the number of (n,triton) reactions per sp in the MCNP-SiC detector model. The coefficient 0.39 accounts for 39% of the tritons that are born in the LiF reaching the SiC depleted layer (the geometric efficiency), for the SiC detector geometry shown in Figure 2.4.

$$(CR)_{all}$$ is the sum of (CR)$_{neutron}$ and (CR)$_{triton}$. It should be noted that our calculation of (CR)$_{all}$ assumes that the SiC detector records perfectly all of the calculated interactions.

### 3.3 Triton Reaction Rate

As it was stated in Section 2.1.3, our SiC diode monitoring system is based on interaction between SiC atoms with fast neutrons and/or tritons. The origin of tritons is from 1 μm $^6$Li 90%-enriched LiF layer. Figure 3.8 shows the macroscopic cross section for $^6$Li(n,triton)α reaction in the enriched LiF. This cross section is high for thermal neutrons where the damage, and counts due to the scattering interactions between neutrons and SiC atoms, are negligible. However, since the energy of emitted tritons is 2.73 MeV, tritons that reach the SiC can create displacement damage defects in SiC.
Figure 3.8: $^6\text{Li}(n,\text{triton})\alpha$ macroscopic cross section as a function of neutron energy.

Eq. 3.3 was used to estimate the rate at which tritons reach the SiC ($\dot{S}_{\text{triton}}$):

$$\dot{S}_{\text{triton}} = \phi_{\text{reactor}} \ast N_{\text{triton}} \ast 0.39 / \Phi_{\text{MCNP}} \ .$$

3.4 $^{29}\text{Si}$ and $^{13}\text{C}$ Production Rates

When a neutron hits a Si or C atom, either neutron scattering or absorption may occur. As shown in Figure 3.9 [52], the neutron absorption cross sections are important for some neutron energies for these atoms, particularly for Si.
If a thermal neutron is absorbed by a $^{28}\text{Si}$ atom, the kinetic energy of the $^{29}\text{Si}$ recoil ($E_{29\text{Si}}$) in the (n,$\gamma$) reaction can be calculated, using the following formula:

$$Q = [M_{^{28}\text{Si}} + m_n - M_{^{29}\text{Si}}]c^2 = [27.9769271 + 1.00866 - 28.9764949](931.5) = 8.469\text{MeV}$$

where $Q$ is the kinetic energy released in the absorption reaction. The rest mass energy of the recoil atom, $E_{\text{atom}}$, is:

$$E_{\text{Si atom}} = M_{^{29}\text{Si}}c^2 = (28.9764949\text{amu})(931.5\text{MeV/amu}) = 2.70 \times 10^4\text{MeV}.$$
Because $E_{\text{Si,atom}}$ is very big compared to $E_\gamma$, we can assume that $Q \approx E_\gamma$. Then based on conservation of momentum, we can calculate $E_{29\text{Si}}$ as follows:

$$2(M_{29\text{Si}} E_{29\text{Si}})^{1/2} = \frac{E_\gamma}{c} \implies E_{29\text{Si}} = \frac{E_\gamma^2}{2c^2 M_{29\text{Si}}} = \frac{(8.469\text{MeV})^2}{2(2.70 \times 10^4 \text{MeV})} \frac{1 \times 10^6 \text{eV}}{1 \text{MeV}} = 1.33 \text{keV}$$

As it can be seen, $E_{29\text{Si}}$ is bigger than the $E_d$ value for C (20 eV), and hence a $^{29}\text{Si}$ recoil is capable of creating displacement damage in SiC.

Using the same method, the energy of the $^{13}\text{C}$ recoil ($E_{13\text{C}}$) created by (n,$\gamma$) reactions for thermal neutrons is calculated to be 1.01 keV.

There are some other absorption reactions that might be important at high neutron energies. Since those reactions are very rare in the studied reactors, they are not cited in this dissertation. Similar procedure can be used to calculate those recoil energies.

### 3.5 Damage Terms Calculations

#### 3.5.1 1MeV Neutron Equivalent Flux and Hardness

To calculate $\phi_{\text{eq,1MeV,SiC}}^{\text{Total}}$, we first calculated the neutron flux, as stated in Section 3.1. Next we entered $\phi(E)$ and $F_{D,\text{SiC}}(E)$ from Figure 2.14 into an Excel spreadsheet. Then, using Eqs. 2.15 and 2.18, $\phi_{\text{eq,1MeV,SiC}}^{\text{Total}}$ (by substituting $\Phi(E)$ with $\phi(E)$) and $H_{\text{SiC}}$ were calculated.
3.5.2 PDPA/$\Phi$

We calculated $(PDPA/\Phi_{MCNP})_{\text{neutron}}$, the number of point defects created per atom (total number of atoms) in SiC per unit fluence by summing $(PDPA/\Phi_{MCNP})_{\text{neutron}}^i$ over species $i$ ($i=$Si or $i=$C). The quantity $(PDPA/\Phi_{MCNP})_{\text{neutron}}^i$ was calculated for each species by dividing the number of defects that were created in the SiC diode by the total number of atoms (that is the product of atom density and SiC volume) in the diode and then dividing the resulting quotient by the MCNP-fluence ($\Phi_{MCNP}$) that created the defects; i.e.

$$
(PDPA/\Phi_{MCNP})_{\text{neutron}} = \sum_i (PDPA/\Phi_{MCNP})_{\text{neutron}}^i
$$

where

$$
(PDPA)_{\text{neutron}}^i = \frac{\nu_{\text{neutron}}^i (N_{PKA})_{\text{neutron}}^i}{V n}
$$

where $\nu_{\text{neutron}}^i$ is the average number of defects that are created in the SiC layers per PKA for a neutron scattering event with atoms of species $i$, $(N_{PKA})_{\text{neutron}}^i$ is the total number of PKAs that are created by neutron scattering with atoms of species $i$, $V$ is the

\[\text{At a low temperature, where recombination of defects cannot happen, } \nu \simeq 2 \ast n(T), \text{ as } n(T) \text{ was described in Section 2.3.2.2.}\]
volume of the detector (the irradiated volume), and $n$ is the SiC atom density (the sum of
the number density for Si or C).

A similar methodology, with three differences, was used to calculate the number
of defects created per atom of species $i$, in the SiC layers per unit fluence for the three
other projectiles that initiate displacement damage ($^{29}\text{Si}$ particles, $^{13}\text{C}$ particles and
tritons). The similarity in the methodologies is in the mathematical approach that was
used, which is expressed in Eqs. 3.4 and 3.5; and that TRIM was used to determine the
number of defects that were created per projectile particle. A difference was that in the
implementation of the method, the 1.33-keV Si-recoils and the 1.01-keV C-recoils were
explicitly assumed to be uniformly distributed in the SiC layers. Also, the 2.73-MeV
tritons were explicitly assumed to be uniformly distributed in the LiF layer. A second
difference was that instead of extracting neutron pre and post collision properties from
the PTRAC cards and using these properties to deduce the properties of the PKAs, F4:N
tally and FM cards in MCNP5 were used to determine the number of $^{28}\text{Si}(n,\gamma)^{29}\text{Si},$
$^{12}\text{C}(n,\gamma)^{13}\text{C}$ and $^{6}\text{Li}(n,\alpha)^{3}\text{He}$ reactions occurring per cm$^3$ per sp in the MCNP-SiC
detector model. The third difference was that instead of calculating $N^{i}_{\text{PKA}}$ (i.e. the number of $^{29}\text{Si}$ recoils that are produced by neutron absorption), $N^{13}_{\text{C}}$ (i.e. the
number of $^{13}\text{C}$ recoils that are produced by neutron absorption) and $N_{\text{triton}}$ (i.e. the
number of tritons that are produced by neutron absorption) were used in Eq. 3.5
Therefore, $\nu^{i}$ for these three recoil projectiles is defined as the average number of defects
of species $i$ that are created per projectile $j$ (not PKA) in the SiC layers in the
simulation, where \( j \) refers to a \(^{29}\text{Si} \) recoil nucleus, a \(^{13}\text{C} \) recoil nucleus or a triton. Finally, \( (PDPA/\Phi_{MCNP})_{all} \) was calculated using Eq. 3.6

\[
(PDPA/\Phi_{MCNP})_{all} = (PDPA/\Phi_{MCNP})_{neutron} + \sum_{j} (PDPA/\Phi_{MCNP})_{j}
\]

thus combining, in one term, the effects of epithermal and fast neutron induced damage with the effects of damage that is initiated through the absorption of thermal and epithermal neutrons to produce \(^{29}\text{Si} \) recoil nuclei, \(^{13}\text{C} \) recoil nuclei and tritons \([94]\).

### 3.6 Displacement Damage Modeling

#### 3.6.1 Methods

In order to use TRIM or MARLOWE to determine the number of defects in SiC detectors resulting from neutron scattering interactions with SiC atoms, these two codes require as input the types, energies, initial positions and direction cosines of the PKAs. We determined these input parameters by modeling the transport of neutrons through SiC with MCNP5.

In this dissertation, we were concerned with displacement damage in Schottky SiC semiconductor diode detectors. As shown in Figure 2.4, these diodes are very thin (310 \( \mu \text{m} \)). Consequently, the majority of neutrons, which are incident upon the surface of the SiC diode, pass through the SiC without interacting. The PTRAC card in MCNP5 was used to determine the probability that a neutron, which enters the SiC volume, will interact with a Si or C atom therein. Furthermore, a C-program was written to extract
neutron characteristics (energy, position and direction cosines), before and after each collision, as well as the type of PKA that is created in a collision, from the PTRAC files that are created by MCNP5. Based on conservation of momentum, the PKA characteristics (atomic species, energy, position and direction cosines) were determined.

The output of the C-program is used as an input for TRIM and MARLOWE, which are used to estimate the number of displacements that are created, including the number of C- and Si-vacancies, interstitial or antisites.

We determined the stated PKA characteristics, using the equations described below:

Suppose $E_n$ and $E'_n$ are the energies of a neutron before and after collision with a PKA (either Si or C), respectively. Then the PKA kinetic energy, $E_{PKA}$, is calculated using Eq. 3.7. This equation is valid for both elastic and inelastic scattering.

$$E_{PKA} = \frac{m_n}{M} \left\{ E_n + E'_n - 2(E_n)^{\frac{1}{2}}(E'_n)^{\frac{1}{2}} \hat{\Omega}_n \cdot \hat{\Omega}'_n \right\}$$

where $m_n$ and $M$ are the masses of a neutron and the PKA nucleus, respectively; and

$$\hat{\Omega}_n \cdot \hat{\Omega}'_n$$ is:

$$\hat{\Omega}_n \cdot \hat{\Omega}'_n = \alpha_n \alpha'_n + \beta_n \beta'_n + \gamma_n \gamma'_n$$
where $\alpha_n$ and $\alpha'_n$ are the direction cosines of the neutron before and after collision with the x-axis, $\beta_n$ and $\beta'_n$ are the direction cosines of the neutron before and after collision with the y-axis and $\gamma_n$ and $\gamma'_n$ are the direction cosines of the neutron before and after collision with the z-axis.

The direction cosine of the PKA with the x-axis, $\alpha_{PKA}$, is calculated using Eq. 3.9:

$$
\alpha_{PKA} = \frac{(E_n)^{1/2} \alpha_n - (E_n')^{1/2} \alpha'_n}{\{E_n + E_n' - 2(E_n)^{1/2}(E_n')^{1/2} \hat{\Omega}_n \cdot \hat{\Omega}'_n\}^{1/2}}
$$

Similar equations are used to calculate the direction cosines of the PKA with the y-axis and z-axis, $\beta_{PKA}$ and $\gamma_{PKA}$.

3.6.2 Defect Specifications

As it is discussed in Chapter 4, the most appropriate locations, regarding the detector lifetime, for SiC detectors are where the neutrons are thermal. In those locations, tritons are the dominant projectiles, which create displacement damage defects in the SiC active volume layer and part of the substrate. 1.33-keV $^{29}$Si and 1.01-keV $^{13}$C recoils are projectiles that create damage in the SiC active volume and throughout the entire volume of the substrate. In order to evaluate how displacement damage defects, which are generated within the detector volume, evolve over time, because of their operation at high temperature; a histogram of the energy spectrum of tritons, which enter the SiC active
volume, was determined using TRIM. Then, we ran MARLOWE to obtain the initial types and positions of defects for tritons of various energies, and 1.33-keV $^{29}$Si and 1.01-keV $^{13}$C recoils. Finally, we used these initial types and positions of defects as inputs for MCASIC.

It should be noted that, as it was stated in Section 0.5.2.7.3, we used TRIM to adjust MARLOWE’s input parameters.

3.6.3 Capture Radius Calculations

The capture radii for all possible defect-pairs in 4H-SiC, except when both defects were antisites, were determined. We used a similar method to the method described by Beardmore et al. [128]. The method we used consists of three steps: 1) Total-energy calculations, 2) Distance-energy calculations, and 3) KMC calculations, as follows:

1) Total energy calculations: Using the Accelrys Material Studio modeling software [150], a tetragonal 192-atom supercell of 4H-SiC was created. The dimensions of this supercell were $12.31 \times 15.99 \times 10.05$ Å$^3$. Then, two defects were placed in specified positions in the supercell. The supercell containing the defect-pairs was relaxed using the ab-initio code VASP. We used the generalized gradient approximation (GGA) for the exchange-correlation energy in all calculations and a $2^3$ Monkhorst-Pack $k$-point
sampling for the Brillouin-zone integration. The total energy and the distance between
two defects after relaxation\textsuperscript{15} were determined.

2) Distance-energy potential calculations: For each set of defect pairs, the above
calculations were done for at least four defect pairs (hereafter, in this section, we call it
set of defect pairs), where the distance between defects in each defect pair was different
from other defect pairs in the set. In order to find a function for the distances between
defects and energies of the supercells, we assumed:

\[
E_j = E_0 + a_0 \left( \sum_i \frac{1}{d_{j,i}} + \sum_k \frac{1}{\lambda_{j,k}} \right)
\]

where the subscript \( j \) corresponds to a defect pair from the set of the defect pairs, \( E_j \) is
the energy of a supercell with the defect pair in the specific position, \( d_{j,s} \) are the
distances between a defect and the other defect or its periodic images (which stem from
the use of Periodic Boundary Conditions (PBC)) in the supercells, and \( \lambda_{j,s} \) are the
distances between a defect in the main supercell and its periodic images. The subscript \( i \)
is the cut-off distance for the interactions between a defect with the other defect and its
periodic images. The subscript \( k \) is the cut-off distance for the interactions between a
defect and its periodic images. \( E_0 \) and \( a_0 \) are constants. Then, the chi-square technique

\textsuperscript{15} The relaxation process lets atoms to find their positions such that the total energy of the system is
minimal.
was used to minimize the differences between $E_j$s and the total energies of the supercells, by changing $E_0$, $a_0$, $i$ and $k$.

We found that $E$ is a function of $\frac{1}{\min(d_i)}$ for each set of the defect pairs, which could indicate that the interaction is dominated by electrostatic interaction (Coulomb’s Law scales with $1/r$). We used the function to describe the interaction energy between two defects $x$ and $y$ as a function of distance.

The hopping rate can be written as Eq. 3.11:

$$R = R_0 \exp\left\{\left(\frac{-E_m}{k_B T}\right)\left(\frac{-E_f - E_i}{2k_B T}\right)\right\}$$

where $R$ is the hopping rate, $R_0$ is the hopping rate prefactor, $E_m$ is the defect migration energy, and $E_f$ and $E_i$ are the energies after and before hopping, respectively. $E_f$ and $E_i$ were determined using the fitted function that was stated in the above paragraph.

3) KMC calculations: We wrote a KMC code (DCRSIC) to determine the capture radius of defect-pairs in 4H-SiC. In DCRSIC, two specified defects were randomly placed in a $100 \times 100 \times 100$ Å$^3$ cell where the PBC for the system was active. These two defects randomly hopped$^{16}$ in the cell based on their hopping rate until the

$^{16}$ For the sake of simplicity, it was assumed that if two defects were different kinds, only the one that had a higher hopping rate would hop.
distance between those defects became less than the range of ab initio calculations (approximately 9.23 Å). At this point, the potential, stated in the above paragraph, became active accelerating the capture. When the distance between two defects became less than a hopping distance (the second nearest neighbor), we assumed that a capture happened. This process was repeated at least 14,000 times to have good statistics.

The rate coefficient, $k_{x,y}$, for defect $x$ and $y$ was calculated using Eq. 3.12:

$$k_{x,y} = \frac{\Omega}{<\tau>}$$ \hspace{1cm} 3.11

where $\Omega$ is the volume of the simulation box and $<\tau>$ is the average capture time. Finally, the capture radius, $a_{x,y}$, was calculated using Eq. 3.13:

$$a_{x,y} = \frac{k_{x,y}}{4\pi(D_x + D_y)}$$ \hspace{1cm} 3.12

where $D_x$ and $D_y$ are the diffusion coefficient of defects $x$ and $y$, respectively.

We did this calculation at different temperatures to determine the temperature dependence of the capture radii for defect pairs. For more information about the capture radius calculation methods, we refer the reader to Ref. [128].

3.6.4 Modeling of the Annealing Process

Most created defects will anneal out in a high-temperature environment, increasing the chance of SiC detectors being operational after at least one reactor
refueling cycle. We wrote a kinetic Monte Code (MCASIC) to model the annealing process in 4H-SiC crystals. In MCASIC, only defects (not atoms which are in their original sites) and their evolution are modeled. In addition, in the current version of MCASIC, only the interactions between defects are modeled and we have neglected the diffusion of defects to the boundaries and other drains.

Usually, KMC real time simulations for defect annealing are limited to the order of seconds [130-132,151]. Since we intended to estimate the number of defects after a nuclear reactor refueling cycle, we wrote MCASIC such that it anneals defects in four steps. In the last two steps, we made some assumptions to speed up the modeling process. The four steps in the MCASIC modeling process are described in below:

1) When an energetic projectile enters the target, it collides with target atoms. Those struck atoms may hit other atoms in the target, and so on. Sometimes, the distance between the interstitials that are initially created and the vacancies that are initially created is less than the defect hopping distance. In this case, the interstitials will recombine with the vacancies, creating normal atom sites, or antisites. In this step (hereafter, we call it preliminary recombination), since interstitials and vacancies are very close, defects do not need to pass through the energy barriers stated in Section 2.4.

Using MARLOWE’s output data as the input, MCASIC finds those interstitial-vacancy pairs whose distance is below the second-neighbor distance (3.078 Å). Then, the code recombines those defects and creates perfect lattice sites or antisites. This step of modeling is not based on the kinetic Monte Carlo method, and happens very fast, with a
timescale that is on the order of ps. The author used the preliminary recombination time cited in Ref. [125], i.e. 1 ps.

2) The second step in the MCASIC modeling process is performed as in traditional KMC codes. In this step, each defect may jump to an available site. MCASIC finds the closest defect to the migrant defect. If the distance between these two defects is less than their capture radius, the code decides if the defects should recombine, create defect clusters, or stay as they were. Figure 3.10 shows a brief schematic diagram of the second step in the MCASIC annealing method.

![Figure 3.10: Schematic of second annealing step of MCASIC.](image)

Figure 3.10: Schematic of second annealing step of MCASIC.
For each hop, MCASIC estimates the real time ($\tau$) and advances the clock. A common equation to model the real time in KMC is [133,134]:

$$\tau = \frac{\chi}{\sum_i N_i R_i}$$  \hspace{1cm} (3.13)

where $\chi$ is a Poisson distributed random number (natural logarithm of a uniform random number between 0 and 1), $N_i$ is number of defects than can hop of defect type $i$, and $R_i$ is the hopping rate (or jump rate) of defect type $i$. MCASIC stochastically, based on the various values of $R$ and $N$, chooses the hopping defect.

Knowing the diffusion pre-exponential factor ($D_0$) from Section 2.4.1, the rate of event prefactors ($R_0$ s) are calculated [135] for each defect species:

$$R_0 = \frac{6}{\delta^2} D_0$$  \hspace{1cm} (3.14)

where $\delta$ is the defect jump distance. $R$ for each defect is:

$$R = R_0 \exp\left(-\frac{E_m}{k_B T}\right)$$  \hspace{1cm} (3.15)

where $T$ is the ambient temperature, and $E_m$ is:

$$E_m = Q - E_f$$  \hspace{1cm} (3.16)
where $Q$ values are cited in Section 2.4.1, and $E^f$ is defect formation energy and can be found in Ref [75].

MCASIC assumes that defect clusters are immobile, until a mobile defect finds and recombines with one of the defects in the cluster. In this case, MCASIC decides, based on their distances of separation and capture radii, whether the other defects in the cluster are still immobile or whether they are free to hop.

Usually, traditional KMC codes simulate the damage annealing from $1 \times 10^{-3}$ s up to 100 s. In this dissertation, step 2 covers 10 s of the annealing process at 500 K.

3) To speed up the modeling process, we forced the fastest defects, which are mobile ICS, to interact with their closest defects, and then advanced the real time based on the average real capture time. This third step is based on the first-passage probability [136]; that is, the probability that a diffusing particle first reaches a specified site in a specified time. The algorithm for this step is:

1. MCASIC chooses a mobile I$_C$. A mobile I$_C$ is an I$_C$ that is not trapped in a defect cluster.

17 A cluster may have more than 2 defects, in the case that a mobile defect is trapped by a cluster. This process makes the cluster bigger.
2. MCASIC finds the closest defect (with the exception of $C_{SiS}$ which do not interact with $I_{Cs}$) and it assumes that the $I_C$ is captured by the closest defect. The distance ($\lambda$) between the main $I_C$ and its closest defect is calculated.

3. Based on Eq. 3.17, $\tau$ is calculated.

$$\tau = \frac{\lambda^2}{6D}$$  \hspace{2cm} 3.17

If both defects are $I_{Cs}$, the right side of Eq. 3.17 is divided by 2.

4. The real time clock is advanced by $\tau$.

5. Calculations are repeated for other mobile $I_{Cs}$, until there is no mobile $I_C$.

4) In this step of modeling, we let all remaining mobile defects (that are mobile $I_{SiS}$, $V_{Cs}$ and $V_{SiS}$) hop around in random directions for a constant real time, $\tau$. However, the hopping is not performed by regular KMC, but is rather done in one step, advancing each defect in a random direction by an amount equal to its diffusion length ($\lambda$) which was calculated using Eq. 3.17. Then MCASIC finds the defect that is closest to each hopped defect. If the distance between a mobile defect and its closest defect is less than their capture radius, the code assumes that the defect pair interacts. If there were no defects within the capture radius for a mobile defect, then the code assumes that the mobile defect is still mobile. In order to have more accurate results, we chose $\tau$ such that $\lambda$ was a small distance for the fastest defect in this step, which are $I_{SiS}$. This allows defects to have more chance to interact with each other. This process was repeated for a period of
time equal to the reactor refueling cycle. We determined the number of defects in a cascade after each month.

In this dissertation, we have studied the evolution of defects for SiC detectors placed in a thermal neutron environment at 227 °C (500 K)\textsuperscript{18}, highlighting GT-MHR R0. The important projectiles, in this case, are tritons and 1.33-keV \textsuperscript{29}Si recoils.

Using TRIM, we made a histogram, with 100 keV increments, for the energy of tritons which would enter\textsuperscript{19} the SiC. One triton from the middle point of each energy interval was chosen; then, MARLOWE was used to have the spatial distribution of defects in defect cascade created by those tritons and an 1.33-keV \textsuperscript{29}Si recoil in SiC at 0 K. Then, MCASIC was used to study how the numbers of different defects in a defect cascade would be changed during 15.7-month operation at 500 K. The numbers of defects after 10 sec annealing time and then after each month were recorded.

A Monte Carlo program was written to create $1 \times 10^8$ defect cascades induced by tritons and 1.33-keV \textsuperscript{29}Si recoils. The numbers of tritons and \textsuperscript{29}Si recoils in the code corresponded to the number of tritons which enter the SiC and the number of \textsuperscript{28}Si (n,γ)\textsuperscript{29}Si reactions during a reactor refueling cycle. In order to model 15.7 months of damage creation and annealing, defect cascades were created at different reactor

\textsuperscript{18} 500 K was chosen to allow both I\textsubscript{C} and I\textsubscript{Si} to migrate, also while the computations could still finish in a reasonable processing time. In addition, this temperature is close to the LWR coolant temperature.

\textsuperscript{19} In MCASIC, the SiC active volume and substrate have not been separated.
operational times, with one-month increment time. For example, if a defect cascade was created at month 5, its annealing time was 10.7 (=15.7-5) months, and if a defect cascade was created at month 14, its annealing time was only 1.7 months. The number of defects remained in each defect cascade was added up to the remained defects in other defect cascades to determine how the number of defects in SiC changes during the 15.7-months operational time. Finally, knowing the number of tritons and $^{29}$Si projectiles born over a GT-MHR refueling cycle, the number of defects created by these projectiles in the SiC was calculated after 15.7-month months of reactor operation.
CHAPTER 4

RESULTS

4.1 Capture Radii of Defect-pairs

Table 4.1 in column 1 presents the number of trials taken to determine the $E_j$ values. Table 4.1 in column 2 presents $\chi^2$ that is a criterion for quality of fittings. Table 4.1 in columns 3 and 4 presents $a_o$ and $E_o$ values as discussed in Section 3.6.3.
<table>
<thead>
<tr>
<th></th>
<th>Number of trials</th>
<th>$\chi^2$</th>
<th>$a_0$</th>
<th>$E_0$</th>
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<td>-1415.63</td>
</tr>
<tr>
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<td>2.72</td>
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<tr>
<td>ISi-VC</td>
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<td>-9.04</td>
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<tr>
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</tr>
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<td>4</td>
<td>0.01</td>
<td>-0.44</td>
<td>-1427.94</td>
</tr>
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</table>

Table 4.1: Number of trials, $\chi^2$, $a_0$ and $E_0$

$^{20} \chi^2 = \sum_j (\text{VASP\ Calculated\ Energy}_j - E_j)^2$
Figure 4.1 displays the fitted curves for \(1/\text{min}(d_i)\) (from \(d_i = 3.078\) Å to \(d_i = 9.23\) Å) vs. energy for defect pairs in SiC, as calculated by VASP. Defect pairs that have curves with higher slope have larger capture radii (for instance, \(\text{I}_\text{Si}-\text{V}_\text{Si}\) and \(\text{C}_\text{Si}-\text{I}_\text{Si}\)).

![Graph showing fitted curves for 1/min(d_i) vs. energy for defect pairs in SiC, determined by the ab initio code, VASP.](image)

Figure 4.1: The fitted curves for \(1/\text{min}(d_i)\) vs. energy for defect pairs in SiC, determined by the ab initio code, VASP.

Figure 4.2 shows the capture radii as functions of temperature, for temperatures from 200 K to 1000 K, for defect pairs in 4H-SiC. The capture radii for defect pairs decrease with increasing temperature. The temperature dependence of capture radii
changes with the type of defect pair. For instance, the absolute value of the slope of the capture radius curve for $A_{Si}-I_{Si}$ is larger than that for $I_{C}-I_{C}$. Considering some computational fluctuations, the largest capture radius in the studied temperature range belongs to $I_{Si}-V_{Si}$. These two defects can capture each other at a distance of 1.46 nm when the temperature is 500 K. The smallest capture radii belong to $A_{Si}-V_{Si}$ and $V_{Si}-V_{Si}$, respectively. At 500 K, those defect pairs may not interact with each other until their distances fall below 0.48 nm and 0.5 nm, respectively. We found that there is no appreciable interaction between $A_{C}$ and $I_{C}$ defects.

Figure 4.2: Capture radii for defect pairs in 4H-SiC at different temperatures.
4.2 Damage at 0 K

4.2.1 Monoenergetic Neutrons

The scattering cross sections for Si and C are presented in Figure 4.3 [52]. For values of $E_n$ less than approximately 50 keV, the scattering cross section for C is about 2 times greater than the scattering cross section for Si. When $E_n$ is greater than 50 keV, the scattering cross section for Si atoms is comparable to, or slightly larger than, that for C atoms. Figure 4.3 is important because it helps to explain some of results, plotted in the next figures in this section.

![Figure 4.3: Scattering cross sections for Si and C atoms.](image-url)
We used MCNP5 to determine the fraction of neutrons that collide while passing through the SiC detector. Figure 4.4 shows the fraction of neutrons that collide while passing through a 310-μm thick SiC detector versus $E_n$, assuming the neutrons are isotropically directed.

Figure 4.4: Fraction of neutrons that collide, while passing through a 310 μm thick SiC detector.
Except at resonance energies, only a small fraction (about 0.6%) of the neutrons that are incident upon the detector interact with Si or C atoms within the detector. Consequently, the probability that a particular neutron interacts two times within the SiC detector, before leaving the detector, is approximately 0.004%. This probability (i.e. the probability that a particular neutron interacts twice within the SiC detector) is an important parameter in distinguishing between thin and thick SiC layers, since the thickness of the layer affects the dependence of the volume averaged displacement damage on $E_n$. As an illustration of the effect, assume a neutron with energy $E_n$ interacts within a SiC target that is thick enough that a neutron is likely to interact twice within the target. In this case, if a neutron scatters on a C atom, after the scattering event, the energy of the neutron decreases to $E_{n,C}^\prime$; if a different neutron with the same energy, $E_n$, interacts with a Si atom, the energy of the neutron decreases to $E_{n,\text{Si}}^\prime$. Since on average, $E_{n,C}^\prime < E_{n,\text{Si}}^\prime$, the dependence of the volume averaged displacement damage on $E_n$ would be less dramatic for a thick SiC target than for a thin SiC target; because, for the thick SiC target, the neutron that interacts first with a C atom, and in so doing deposits more energy in the SiC on average than a neutron which interacts first with a Si atom, would have less energy available on average to create additional displacements, if it were to interact a second time within the detector. Conversely, a neutron that interacts first with a Si atom, and in so doing deposits less energy in the SiC on average than a neutron which interacts first with a C atom, would have more energy available on average to create
additional displacements, if it were to interact a second time within the detector. Therefore, as stated above, the dependence of the volume averaged displacement damage on $E_n$ would be less dramatic for a thick SiC target than for a thin SiC target, because of the balancing of greater and lesser energy losses that occurs between the first and second collisions in a thick target. For our case, where the SiC target is very thin, the probability of interaction between neutrons and SiC atoms is very small, on a per neutron basis, and the dependence of the displacement damage on $E_n$ is most pronounced. Figure 4.5 presents the ratio of C-PKAs to the total number of PKAs (the ratio of the C scattering cross section to the SiC scattering cross section) as a function of neutron energy. For low neutron energies, this fraction is 0.70. For larger neutron energies, this fraction varies due to variations in the scattering cross sections of C and Si.

![Figure 4.5: Fraction of C-PKAs as a function of neutron energy.](image)

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Figure 4.6 shows the maximum and average C- and Si-PKA energies as a function of $E_n$. Theoretically, the ratio of the average PKA energy to the maximum PKA energy should be 0.5 for elastic and isotropic scattering. Our calculations show that this ratio is 0.50, for $E_n$ less than 50 keV for C and for $E_n$ less than 20 keV for Si. For $E_n$ greater than 50 keV to 7 MeV for C, our calculations show that this ratio is slightly less than 0.5, because the scattering is not purely isotropic. For $E_n$ ranging from 20 keV to 1 MeV for Si, our calculations show that this ratio varies between 0.29 and 0.58. For $E_n$ values greater than 1 MeV the ratio changes more significantly for both C and Si atoms.

Since the atomic mass of C is less than the atomic mass of Si, for equal $E_n$, the average C-PKA energy is greater than the average Si-PKA energy. Theoretically, the ratio of the average-C-PKA energy to the average-Si-PKA energy should be 2.13 for elastic and isotropic scattering. Our calculations reveal that the ratio of these two average energies is 2.14 for low $E_n$ (where collisions are elastic and isotropic), but that due to anisotropic scattering, this ratio changes dramatically as $E_n$ increases.
Figure 4.6: Maximum and average PKA energies versus neutron energy for: (a) C-PKAs and (b) Si-PKAs.

Figure 4.7 shows the number of displacements per PKA, determined by our method, as a function of $E_n$. For comparison, the number of displacements per PKA calculated by the simple NRT model is plotted as well. As it can be seen in the figure, these two results are in good agreement, particularly for small $E_n$. For larger $E_n$, the difference between the two methods is a little greater, since in the NRT model it is assumed that the neutron scattering angle is isotropic and that it is not a function of $E_n$. This assumption is not very accurate for large $E_n$, depending on the type of PKA. In addition, the NRT model was originally developed to estimate the number of displacements for elements, not compounds.
Figure 4.7: Number of displacements per PKA, determined by two methods: our method (MCNP+TRIM) and the NRT model.

The results of our calculations of $PDPA/\Phi$ from the previous results are presented as a function of $E_n$ in Figure 4.8, along with calculations of $2*DPA/\Phi$,\textsuperscript{21} that we determined using SPECTER. One interesting point is that, according to both methods, the MCNP+TRIM calculations and the SPECTER calculations, $PDPA/\Phi$ and $DPA/\Phi$ are almost constants, for $E_n$ greater than 200 keV but less than 1 MeV.

As can be seen in Figure 4.8, the results of the MCNP+TRIM and SPECTER calculations are comparable, except for low $E_n$. We believe that the main reason for the

\textsuperscript{21} The factor of two is because each displacement includes two defects, i.e. one vacancy and one interstitial.
differences between the code calculations for low $E_n$ is that the codes SPECTER and TRIM use different formalisms to predict the number of displaced atoms per PKA as a function of the kinetic energy of the PKA. The authors refer interested readers to the SPECTER and TRIM manuals [11,12] for details regarding the differences in the formalisms.\(^{22}\)

One advantage of using MCNP+TRIM is that MCNP+TRIM uses cross sections which are continuous functions of energy. Another advantage of using MCNP+TRIM, compared to SPECTER, is that MCNP+TRIM yields additional information; including, for example, the number of Si- and C-vacancies and replacements, the fraction of collided neutrons and the fraction of C-PKAs. Furthermore, when necessary, the spatial distribution of displacements can be studied. Finally, since TRIM is a code that was developed principally to study displacement damage resulting from ions, the MCNP+TRIM approach allows one to compare, in a consistent manner, the displacement damage caused by neutrons with the displacement damage caused by ions (for example protons to determine the effect of adding Coulomb interaction into the picture) [58].

\(^{22}\) The main reason for the difference might be that the modified Kinchin-Pease model is not built into TRIM, but is built into SPECTER.
Figure 4.8: $PDPA/\Phi$ determined by SPECTER and $2\,*DPA/\Phi$ and determined by our method (MCNP+TRIM) as functions of neutron energy.

4.2.2 Tritons, and $^{29}$Si and $^{13}$C Recoils

Figure 4.9 presents $\nu$, as it was explained in Section 3.5.2, for tritons, and $^{13}$C and $^{29}$Si recoils in SiC. Figure 4.9 shows that, on average, $^{29}$Si recoil atoms are more destructive than the other two projectiles, because, among these particles, $^{29}$Si has the biggest $\nu$. On the contrary, among these particles, the damage caused by $^{13}$C recoils is expected to be smallest, since their $\nu$ is smallest. Also, as it was shown in Figure 3.9, the absorption cross section for $^{12}$C is small compared to that for $^{28}$Si and $^6$Li. Because of these two facts for C (small $\nu$ and small absorption cross section), the displacement
damage caused by $^{13}\text{C}$ recoils is of negligible importance.\textsuperscript{23} In the next, related sections, we will again show $\nu$ values for tritons, and $^{13}\text{C}$ and $^{29}\text{Si}$ recoils, in order to compare those with $\nu$ values for neutron scattering of $^{12}\text{C}$ and $^{28}\text{Si}$. We will show that even damage caused by $^{29}\text{Si}$ recoils is negligible compared to the damage caused by fast neutron scattering. However, damage caused by $^{29}\text{Si}$ recoils is important when the SiC detector is placed in the thermal region of a nuclear reactor. In such a region, damage caused by $^{29}\text{Si}$ recoils is the dominant form of damage in that part of the SiC substrate, which tritons cannot reach and the only important projectile is $^{29}\text{Si}$.\textsuperscript{24}

\textsuperscript{23} Since the damage caused by $^{13}\text{C}$ recoils is very small, we have neglected them in MCASIC.

\textsuperscript{24} It is assumed that the SiC detector does not have any pre-irradiation defects.
Figure 4.9: $\nu$ for 2.73-MeV triton, 1.01-keV $^{13}\text{C}$ and 1.33-keV $^{29}\text{Si}$, as calculated by TRIM.

Contrarily to $^{29}\text{Si}$ and $^{13}\text{C}$, the damage induced by tritons is significant in the SiC active volume and part of the SiC substrate to the point that all tritons will stop (the range of tritons in the series of Al, Au and SiC layers for the SiC detector shown in Figure 2.4). The energy of the tritons, when born in $^6\text{Li}(n,\alpha)$ reactions, is 2.73 MeV. However, the tritons lose energy while passing through the LiF, Al and Au layers. Figure 4.10 shows, as a histogram, the results of a TRIM calculation for the distribution of the triton energies as the tritons enter the SiC. The height of the elements in the histogram in Figure 4.10 represents the conditional probability that a triton, which enters the SiC, does so with an
energy within the indicated energy bin. The maximum energy with which a triton enters the SiC is approximately 2200 keV. The mode and the average energy of tritons as they enter the SiC are 1750 keV and 1300 keV, respectively.

Figure 4.10: A histogram representing the energy of tritons as they enter the SiC, for the SiC detector shown in Figure 2.4.

Figure 4.11 is the histogram of the estimated numbers of C- and Si-defects in the SiC for tritons \( \nu_{C,\text{triton}} \) and \( \nu_{Si,\text{triton}} \), respectively) that enter the SiC with energies within the specified energy bin. Figure 4.12 shows \( \nu_{C,\text{triton}} \) and \( \nu_{Si,\text{triton}} \) is not a strong function of triton energy, since by increasing the triton energy from 50 keV to 2050 keV (41 times...
increase in triton energy), the sum of the numbers of C- and Si-defects is increased by less than two fold. This occurs for two reasons: 1) because the dominant stopping power for tritons in the SiC is electronic, not nuclear, and 2) because the thickness of the SiC active volume is limited, so that although increases in triton energy correspond to additional defects being created, those defects are not created within the SiC active volume and are therefore not included in the calculation of $\nu_{\text{triton}}^C$ and $\nu_{\text{triton}}^\text{Si}$.

Figure 4.11 shows that $\nu_{\text{triton}}^C$ is larger than $\nu_{\text{triton}}^\text{Si}$, by a factor of 1.4-1.5. The main reasons are: 1) In SiC, $E_d$ for C is bigger than $E_d$ for Si; and 2) the triton atomic mass is closer to the C atomic mass than the Si atomic mass; therefore based on Eqs. 2.6 and 2.7 on average, the energy transferred from tritons to C-PKAs is more than the energy transferred from tritons to Si-PKAs. Those C-PKAs, also transfer more energy to the secondary C-knock-on atoms rather than the secondary Si-knock-on atoms, and so on. Therefore, C-struck atoms would move out from their original sites more than Si-struck atoms.
Figure 4.11: $v_{\text{triton}}^C$ and $v_{\text{triton}}^\text{Si}$ as a function of the triton energy, as determined by TRIM.

The TRIM calculations show that the range of 1750 keV tritons in the SiC is approximately 15 μm; and according to Figure 4.11, $v_{\text{triton}}$ for 1750 keV tritons is 144. Therefore, if we assume that all defects are created on a line corresponding to the triton track, the average distance between two consecutive defects in a defect cascade ($\bar{d}$) created by a 1750 keV triton is 1042 Å (15 μm/144). By increasing the triton energy, $\bar{d}$ significantly increases. For example, $\bar{d}$ for a 2150 keV triton is 1400 Å. These high $\bar{d}$s reduce the chance of defect recombination for SiC detectors irradiated by tritons. MARLOER+MCASIC results prove this conclusion, as discussed in Section 4.3.4.
Based on the TRIM calculations, one $^{29}$Si and one $^{13}$C recoil, on average, create 133 and 29 defects, respectively. The $d$ values for two consecutive defects in a defect cascade resulting from these two recoils are very small (less than 1 Å). These small $d$ values allow that defects rapidly recombine after creation.

4.3 Reactor Displacement Damage at 0 K and Count Rates

4.3.1 OSURR

Table 4.2 presents in column 2, $\phi^{Total}$ for some TC, BP1 and AIF positions, as described in Section 3.1.1. $\phi^{Total}$ for these positions varies between $1.4 \times 10^9$ cm$^{-2}$s$^{-1}$ (at TC) to $8.9 \times 10^{12}$ cm$^{-2}$s$^{-1}$ (at AIF Position 2).

Table 4.2 presents $\phi^{Total}_{eq,3MeV,SC}$ in column 3. $\phi^{Total}_{eq,3MeV,SC}$ for TC is 2-3 orders of magnitude less than $\phi^{Total}_{eq,3MeV,SC}$ for BP1 and AIF, since in the TC most neutrons are thermal and thermal neutrons cannot create damage through scattering.

Table 4.2 presents $H_{SiC}$ in column 4. The average $H_{SiC}$ values for BP1 and AIF positions are 0.66 and 0.40, respectively. Hence, the neutron energy spectrum is harder in BP1 than in AIF. Therefore, at the same neutron flux, we anticipate that a bare (without LiF layer) SiC detector degrades faster in BP1 than in the AIF.

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As it mentioned previously, the Characterization Vessel in the BP1 that was used for modeling is shielded by a Cd layer.
Table 4.2 presents in column 5, $\dot{S}_{\text{trion}}$ for the SiC detector shown in Figure 2.4 for the stated positions in the OSURR. As can be seen, $\dot{S}_{\text{trion}}$ per neutron flux is maximal in the TC where most neutrons are thermalized.

<table>
<thead>
<tr>
<th></th>
<th>$\phi^{\text{Total}}$ (cm$^{-2}$s$^{-1}$)</th>
<th>$\phi^{\text{Total}}_{\text{eq.1MeV,SiC}}$ (cm$^{-2}$s$^{-1}$)</th>
<th>$H_{\text{SiC}}$</th>
<th>$\dot{S}_{\text{trion}}$ (cm$^{-2}$s$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>TC</td>
<td>1.4x10$^9$</td>
<td>3.1x10$^5$</td>
<td>&lt;0.005</td>
<td>4.7x10$^3$</td>
</tr>
<tr>
<td>BP1, Position 1</td>
<td>6.1x10$^{11}$</td>
<td>4.0x10$^{11}$</td>
<td>0.66</td>
<td>4.1x10$^4$</td>
</tr>
<tr>
<td>BP1, Position 3</td>
<td>1.1x10$^{12}$</td>
<td>7.2x10$^{11}$</td>
<td>0.66</td>
<td>7.3x10$^4$</td>
</tr>
<tr>
<td>AIF, Position 1</td>
<td>7.4x10$^{12}$</td>
<td>2.8x10$^{12}$</td>
<td>0.38</td>
<td>1.3x10$^7$</td>
</tr>
<tr>
<td>AIF, Position 2</td>
<td>8.9x10$^{12}$</td>
<td>3.5x10$^{12}$</td>
<td>0.39</td>
<td>1.5x10$^7$</td>
</tr>
<tr>
<td>AIF, Position 3</td>
<td>6.4x10$^{12}$</td>
<td>2.7x10$^{12}$</td>
<td>0.42</td>
<td>1.1x10$^7$</td>
</tr>
</tbody>
</table>

**Table 4.2:** Total flux, 1MeV equivalent neutron flux, hardness and triton production rate, for the stated positions in the TC, BP1, and AIF.

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Figure 4.12 shows \( \nu \) for 2.73-MeV tritons, 1.01-keV \(^{13}\text{C}\), 1.33-keV \(^{29}\text{Si}\) and neutron scattering in TC, BP1 and AIF. As can be seen, neutrons cannot create damage in the SiC detector placed in TC through scattering. On the contrary, neutron scattering at BP1 and AIF is very destructive.

![Graph showing neutron scattering](image)

Figure 4.12: \( \nu \) for 2.73-MeV triton, 1.01-keV 13C, 1.33-keV 29Si and neutrons scatterings in various locations at OSU RR, as calculated by MCNP and TRIM.
Figure 4.13 shows the estimated $PDPA$ of the SiC depleted region and substrate for SiC detectors placed in TC, BP1 and AIF, after one-month radiation by neutron fluxes cited in Table 4.2. These $PDPA$ values show that if SiC detectors would be placed at the stated positions for a month and the reactor would work at the full power, what fraction of atoms would be displaced from their origin sites\(^{26}\). For instance, in the AIF Position 2, $1.7\%\(^{27}\)$ of the atoms in the SiC depleted region have been displaced after one month irradiation at the full power. Still, we do not know at what $PDPA$ value, SiC detectors fail; but our experimental results [81] show that detectors placed in AIF fail rapidly. One interesting result is that the $PDPA$ in the active and substrate regions of SiC detectors placed in the BP1 are almost similar. This happens since the damage resulting from neutron scattering is very dominant for SiC detectors in the BP1, and damage in both SiC regions (depleted region and substrate) is controlled by neutron scattering.

\[^{26}\] Recall that for detectors at high temperatures, a majority of defects may be eliminated because of the annealing.

\[^{27}\] Recall that each displacement creates two defects, approximately.
Figure 4.13: *PDPA* of the SiC depleted region and substrate placed in various OSURR positions, after one month radiation.

Table 4.3 presents the modeling estimation of total count rates (*CR*\(_{all}\)) for SiC detectors placed in TC, BP1 and AIF, when the reactor operates at full power. As it can be seen, *CR*\(_{all}\) is largest for detectors placed in the AIF, because *ϕ*\(_{Total}\) is maximal at the AIF.
Figure 4.13 shows that after one-month radiation, the depleted region of SiC detectors placed in the TC has 5300 times less defects than that in the AIF Position 1. However, as it is shown in Table 4.3, \((CR)_{all}\) for detectors placed in the AIF Position 1 is only 2900 times more than \((CR)_{all}\) for detectors placed in the TC. Hence, on a per count basis, the number of defects in detectors placed in the AIF is more than the number of defects for detectors placed in the TC. Therefore, we expect that for the same \((CR)_{all}\), the lifetime of detectors in the TC is longer than the lifetime of detectors in the AIF.

<table>
<thead>
<tr>
<th></th>
<th>TC</th>
<th>BP1, Position 1</th>
<th>BP1, Position 3</th>
<th>AIF, Position 1</th>
<th>AIF, Position 2</th>
<th>AIF, Position 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total Count Rate (cps)</td>
<td>4.7x10³</td>
<td>7.5x10⁴</td>
<td>1.4x10⁵</td>
<td>1.3x10⁷</td>
<td>1.5x10⁷</td>
<td>1.1x10⁷</td>
</tr>
</tbody>
</table>

Table 4.3: Modeling estimation of \((CR)_{all}\) for the detectors placed in various positions of OSURR
Figure 4.14 illustrates the C- and Si-PKA spectra for a SiC detector at AIF Position 1. Considering that SiC detectors can count only PKAs that have energy more than 200 keV, if it is functioning perfectly, given the stated LLD for pulse counting, the detector may count 6.4% of C-PKAs and 3.6% of Si-PKAs. PKAs with energies less than 200 keV can create significant damage, but the detector is unable to count them.

Figure 4.14: The C- and Si-PKA energy spectra as a result of neutron scattering for a SiC detector at AIF Position 1. The detector can only count the PKAs that have energy more than 200 keV. The last value for the C-PKA (at 1x10^6 eV) corresponds to the number of C-PKAs that have energy more than 1x10^6 eV.
Figure 4.15 displays the percent of the triton count rate \((CR)_{trion}\) to \((CR)_{all}\). For detectors placed in the TC and AIF, almost all the count rates are due to tritons. Even for the detectors placed in the BP1, that has a harder neutron spectrum, \((CR)_{trion}\) is more than 50% of \((CR)_{all}\).

Figure 4.15: Percent of \((CR)_{trion}\) to the total count rate for SiC detectors placed in various positions at OSURR.
4.3.2 IRIS

4.3.2.1 Stainless-Steel Instrumentation Tube

Figure 4.16 shows $\phi_{\text{Total}}$ and $\phi_{\text{Total,1MeV,SC}}$ as the detector radial location is varied from 155 cm to 200 cm in the IRIS downcomer, for the case of the empty instrumentation tube. As it can be seen, and is expected, the neutron flux decreases as the radius of the location of the instrumentation tube in the IRIS downcomer is increased.

Figure 4.16: Total flux and 1MeV neutron equivalent flux for four radii in the IRIS downcomer, inside of the stainless steel instrumentation tube.
One interesting result is that, although $\phi^{Total}_{eq,1\text{MeV},SiC}$ decreases as the radius of the location of the instrumentation tube in the IRIS downcomer is increased, $H_{SiC}$ increases, as it is shown in Figure 4.17. This is a consequence of a relative diminution of the epithermal portion of the neutron flux energy spectrum in comparison to the thermal and fast portions of the spectrum, and the dependence of $F_{D,1\text{MeV},SiC}$ on neutron energy. As it is shown in Figure 2.14, $F_{D,\text{SiC}(\text{epithermal})}$ is less than $F_{D,\text{SiC}(\text{thermal})}$ and $F_{D,\text{SiC}(\text{fast})}$. Therefore, an epithermal neutron flux has a smaller $H_{SiC}$ than a thermal- or fast-neutron flux. In Figure 4.18 and Figure 4.19, the contributions of thermal ($1 \times 10^{-4} \text{ eV} - 1\text{eV}$), epithermal and fast neutrons ($500 \text{ keV} - 18 \text{MeV}$), are shown when the radial location of the instrumentation tube is 155 cm and 170 cm, respectively.

Figure 4.17: $H_{SiC}$ for four radii in the IRIS downcomer, inside of the stainless steel instrumentation tube.
Figure 4.18: Neutron flux vs. the axial position in the stainless steel instrumentation tube when R = 155 cm.
Figure 4.19: Neutron flux vs. the axial position in the stainless steel instrumentation tube when \( R = 170 \text{ cm} \).

Hardness is a linear function of the radial location of the instrumentation tube from \( R =155 \) cm to \( R = 200 \) cm. In this range, \( \phi^{Total}_{eq,13MeV,SC} \) decrease exponentially (Figure 4.20).
Figure 4.20: 1MeV equivalent neutron flux for four radii in the IRIS downcomer, inside of the stainless steel instrumentation tube.

Figure 4.21 shows the triton count rate as a function of the radial distance of the instrumentation tube from the center of the core, assuming that tritons, that are born in $(n,\alpha)$ reactions in the $^6\text{LiF}$ radiator, are recorded with a detection efficiency of 39%. As it is seen, all triton count rates are between $5.0 \times 10^2$ and $1.8 \times 10^5$ cps. These count rates, particularly at locations from $R = 170$ cm to $R = 200$ cm, are too low for a neutron monitoring system to respond with sufficient quickness in the event of a transient. The total count rate\footnote{There are two sources for count rate: 1) tritons, 2) fast neutrons.} might be high enough to yield an adequate neutron monitoring system response time for some of these positions. As a remedy, the LiF thickness can be
increased to enhance the count rate. The count rate can also be enhanced by increasing the area of the diodes or the number of diodes (or both).

![Figure 4.21: Triton count rate for four radii in the IRIS downcomer, inside of the stainless steel instrumentation tube.](image)

4.3.2.2 Three-Layer Instrumentation Tube

The calculations that are discussed in Section 4.3.2.1 were repeated for the case of an instrumentation tube that is lined with a 0.5-cm thick layer of Cd, which encircles a 2-cm thick polyethylene layer (the three–layer instrumentation tube). Except for R=155cm, adding Cd and polyethylene layers to the inside of the empty instrumentation tube increases $H_{sc}$ (Figure 4.22) by about 8%. For example, $H_{sc}$ for the three-layer
instrumentation tube is around 7.5% more than $H_{SiC}$ for the stainless-steel instrumentation tube for R=170 cm. At R=155 cm, the contribution of thermal neutrons, compared to the fraction of epithermal neutrons, is very small. Therefore, adding Cd and polyethylene layers does not increase $H_{SiC}$.

\[ \phi_{ep,1MeV, SiC}^{Total} \] and \[ \phi_{ep,1MeV, SiC}^{Total} \] are not significantly influenced by adding Cd and polyethylene layers, and their orders remain the same as for the stainless steel instrumentation tube (Figure 4.23).

![Graph showing hardness and linear hardness against radial location of the instrumentation tube](image)

Figure 4.22: $H_{SiC}$ for four radii in the IRIS downcomer, inside of three-layer instrumentation tube.
Figure 4.23: Total flux and 1MeV equivalent neutron flux for four radii in the IRIS downcomer, inside of the three-layer instrumentation tube.

Figure 4.24 shows the values of the triton count rate in a SiC diode for various radii of the location of the three-layer instrumentation tube. Considering statistical errors, these triton count rates are almost the same as triton count rates determined for the stainless instrumentation tube.
4.3.2.3 Section Conclusion

Using MCNP5, $\phi^{\text{Total}}$, $\phi^{\text{Total}}_{\text{eq.,1MeV,\text{SiC}}}$, $H_{\text{SiC}}$ and triton count rates were determined at four radii in the downcomer region of IRIS, inside of two different designs of instrumentation tube. In the three-layer instrumentation tube, at R = 155 cm, where the triton count rate is more appropriate than for other locations, $\phi^{\text{Total}}_{\text{eq.,1MeV,\text{SiC}}}$ and $\phi^{\text{Total}}$ are $8.67 \times 10^{10}$ cm$^{-2}$s$^{-1}$ and $2.26 \times 10^{11}$ cm$^{-2}$s$^{-1}$, respectively. At this location $H_{\text{SiC}}$ is 0.38 and the triton count rate is $1.40 \times 10^5$ cps. In this calculation, we assumed that the detector
(\(^6\)LiF radiator and SiC diode) radius is 250 μm and that tritons that are born in \((n,\alpha)\)
reactions in the \(^6\)LiF radiator are recorded with a detection efficiency of 39%.

4.3.3 GT-MHR

4.3.3.1 Displacement Damage and Count Rates

Figure 4.25 shows the differential neutron flux vs. energy for locations R153L5\(^{29}\),
R117L5, R81L5 and R0L5 in the capsule. Although, there is some lack of good statistics,
particularly at R81L5, it is seen that the fast neutron flux declines dramatically by
decreasing the radial location of the capsule in the GT-MHR central reflector. The
thermal neutron flux at R117L5, R81L5 and R0L5 are comparable.

\(^{29}\) This notation refers to the position in the GT-MHR, where the calculation was made. As it was stated
previously, R\(#\) is the radial location of the capsule in the GT-MHR. L\(#\) is the axial position. For instance,
R153L5 refers to a capsule located at R=153cm and into layer 5 (for 10-fuel layers where layer 1 is the top
layer).
However, within the capsules, above about 10 eV, the neutron flux at R153L5 is greater than the neutron flux at other specified positions. On this basis, one can conclude that at R153L5, fast neutrons contribute more to the count rate, and to the displacement damage rate, than at R117L5, R81L5 and R0L5. However, the flux spectrum exhibits a thermal peak at these three locations and consequently the triton count rate \((\text{(CR)}_{\text{triton}})\), at R117L5, R81L5 and R0L5, can be expected to be significant in comparison to the triton count rate at R153L5. Figure 4.25 presents the total (integrated over all energies) neutron flux versus position for the ten layers of the GT-MHR core for the active core and at the specified axial locations within the capsule for capsules at R153, R117, R81 and R0.
The total neutron flux within the active core is one and two orders of magnitude greater than the total neutron flux at R153 and R117, respectively. It can be seen from Figure 4.26, that for the Beginning of Life (BOL) Source Spectra that was used in the MCNP-GT-MHR model, the total neutron flux decreases nearly linearly with increasing layer number, for the active core and at locations R153, R117, R81 and R0. Therefore, for purposes of brevity, hereafter, results averaged over layers 3, 5 and 8 are presented as being representative of results for the GT-MHR as a whole.

Figure 4.26: Total neutron flux for various axial layers for the active core and for four radii: R153, R117, R81 and R0.
Table 4.4 presents results regarding neutron fluxes and count rates averaged over axial layers, 3, 5 and 8 with detector radial location as a parameter. Columns 2 and 3 present $\phi_{\text{Total}}^{\text{eq,1MeV,SiC}}$ and $H_{\text{SiC}}$; $\phi_{\text{Total}}^{\text{eq,1MeV,SiC}}$ for R153 is $2.0 \times 10^{13}$ cm$^{-2}$s$^{-1}$. The values of $\phi_{\text{Total}}^{\text{eq,1MeV,SiC}}$ for R117, R81 and R0 are, respectively, one, three and five orders of magnitude less than the value of $\phi_{\text{Total}}^{\text{eq,1MeV,SiC}}$ for R153. The decrease in $\phi_{\text{Total}}^{\text{eq,1MeV,SiC}}$ with decreasing detector radial location is due to the decrease of the total neutron flux with decreasing detector radial location that is shown in Figure 4.26, plus the softening of the neutron flux energy spectra with decreasing detector radial location that is shown in column 3 of Table 4.4. Columns 4, 5, 6 and 7 present $(CR)_{\text{neutron}}$, $(CR)_{\text{triton}}$, $(CR)_{\text{neutron}}/(CR)_{\text{all}}$, and $(CR)_{\text{triton}}/(CR)_{\text{all}}$. Regarding column 4, since thermal neutron absorption events in Si and C do not deposit, within the Si and C, enough energy for the energy deposition events to be recorded as counts, $(CR)_{\text{neutron}}$ decreases with decreasing detector radial location in approximately the same manner as $\phi_{\text{Total}}^{\text{eq,1MeV,SiC}}$. Regarding column 5, despite the decrease in the total neutron flux with decreasing detector radial location (as shown in Figure 4.26), $(CR)_{\text{triton}}$ increases with decreasing detector radial location, due to softening of the neutron flux. $(CR)_{\text{neutron}}/(CR)_{\text{all}}$, in column 6, like $H_{\text{SiC}}$, is a ratio. The variation of $(CR)_{\text{neutron}}/(CR)_{\text{all}}$ with detector radial location is similar, but not identical to that for $H_{\text{SiC}}$. $(CR)_{\text{triton}}/(CR)_{\text{all}}$, in column 7, on the other hand, increases with decreasing detector radial location, as a consequence of softening of the neutron flux energy spectra, since the sum of $(CR)_{\text{neutron}}/(CR)_{\text{all}}$ and $(CR)_{\text{triton}}/(CR)_{\text{all}}$ equals unity.
<table>
<thead>
<tr>
<th>Detector Radial Location (cm)</th>
<th>$\phi_{\text{Total}}^{\text{eq,1MeV,SiC}}$ (cm$^{-2}$s$^{-1}$)</th>
<th>$H_{\text{SiC}}$ (cps)</th>
<th>$(CR)_{\text{neutron}}$ (cps)</th>
<th>$(CR)_{\text{triton}}$</th>
<th>$(CR)<em>{\text{neutron}}/(CR)</em>{\text{all}}$</th>
<th>$(CR)<em>{\text{triton}}/(CR)</em>{\text{all}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1.9x10$^8$</td>
<td>8.9x10$^{-4}$</td>
<td>0.0</td>
<td>1.6x10$^5$</td>
<td>0.0</td>
<td>1.0</td>
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<td>81</td>
<td>4.3x10$^{10}$</td>
<td>1.0x10$^{-1}$</td>
<td>2.7x10$^3$</td>
<td>2.2x10$^5$</td>
<td>0.1x10$^{-1}$</td>
<td>9.9x10$^{-1}$</td>
</tr>
<tr>
<td>117</td>
<td>1.1x10$^{12}$</td>
<td>2.1x10$^{-1}$</td>
<td>1.3x10$^4$</td>
<td>5.8x10$^5$</td>
<td>0.2x10$^{-1}$</td>
<td>9.8x10$^{-1}$</td>
</tr>
<tr>
<td>153</td>
<td>2.0x10$^{13}$</td>
<td>4.5x10$^{-1}$</td>
<td>5.7x10$^5$</td>
<td>6.4x10$^5$</td>
<td>4.7x10$^{-1}$</td>
<td>5.3x10$^{-1}$</td>
</tr>
</tbody>
</table>

Table 4.4: Average 1MeV equivalent neutron flux, $H_{\text{SiC}}$, $(CR)_{\text{neutron}}$, $(CR)_{\text{triton}}$, $(CR)_{\text{neutron}}/(CR)_{\text{all}}$ and $(CR)_{\text{triton}}/(CR)_{\text{all}}$ for R153, R117, R81 and R0 within the GT-MHR.

At R153, $(CR)_{\text{neutron}}$ and $(CR)_{\text{triton}}$ contribute almost equally to $(CR)_{\text{all}}$. To the contrary, $(CR)_{\text{triton}}$ contributes 98% to $(CR)_{\text{all}}$ at R117, and 100% to $(CR)_{\text{all}}$ at R0.

Table 4.5 presents values of $\nu$ (the average number of defects that are created in the SiC layers per projectile particle for $^{29}\text{Si}$ and $^{13}\text{C}$ recoil particles and tritons; or per PKA for neutron scattering (neutron-PKA)). $\nu$ is presented for 1.33-keV $^{29}\text{Si}$ and 1.01-keV $^{13}\text{C}$ recoil particles and 2.73-MeV tritons, and for neutron induced PKAs (for neutrons with energy spectra that are consistent with the stated location of the...
detector in the core). As is the case for Table 4.4, Table 4.5 presents results averaged over axial layers, 3, 5 and 8 with detector radial location as a parameter, as indicated. Also, the value of $\nu$ is calculated irrespective of where in the SiC diode the defects are created (either in the diode’s active volume or in the substrate). For 1.33-keV $^{29}$Si and 1.01-keV $^{13}$C recoil particles and neutron PKAs the value of $\nu$ is independent of location in the diode, since the 1.33-keV $^{29}$Si and 1.01-keV $^{13}$C recoil particles and PKAs are born within the SiC. For the tritons, the number of defects that are created per triton is a function of location in the diode, since the tritons are born external to the diode. Regarding neutron induced PKAs, on average, each neutron induced PKA at R153 produces more damage in the SiC layers than the other projectiles, because of the neutrons’ high energies at this radial location. Regarding tritons, although the energy of tritons is 2.73 MeV at their birth in the LiF radiator, tritons create less damage than the other projectiles, except $^{13}$C; since in contrast to the other projectile particles, they are born external to the SiC, and therefore part of their energy is absorbed by the LiF, Al and Au layers. Also, a large fraction of the triton’s energy is spent in creating ionizations, not displacement damage.
<table>
<thead>
<tr>
<th>Projectile</th>
<th>1.33-keV $^{29}\text{Si}$</th>
<th>1.01-keV $^{13}\text{C}$</th>
<th>2.73-MeV triton</th>
<th>Neutron - PKA at R0</th>
<th>Neutron - PKA at R81</th>
<th>Neutron - PKA at R117</th>
<th>Neutron - PKA at R153</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\nu$</td>
<td>133</td>
<td>29</td>
<td>52</td>
<td>0</td>
<td>60</td>
<td>116</td>
<td>252</td>
</tr>
</tbody>
</table>

Table 4.5: $\nu$ for various projectile species.

Table 4.6 presents additional results that are averaged over axial layers, 3, 5 and 8 with detector radial location as a parameter. However, the location of the defects within the SiC diode is noted (either averaged over the diode’s active volume and substrate, or in the diode’s active volume only). This distinction is made, because the doping levels of the diode’s active volume and the substrate are different; and, therefore, the effect of a given concentration of defects on the performance of the diode may be different for these locations within the diode. Table 4.6 presents, respectively in columns 2 and 3, the values of $(PDPA/\Phi_{MCNP})_{all}$, averaged over the whole SiC volume ($<(PDPA/\Phi_{MCNP})_{all}\text{whole}>$) and averaged over the SiC depleted region (active volume) only ($<(PDPA/\Phi_{MCNP})_{all}\text{depleted}>$). From column 2 it can be seen that $<(PDPA/\Phi_{MCNP})_{all}\text{whole}>$ for R153 is twice as large as its corresponding value for R117 and is approximately 36 times larger than its corresponding value for R0. At R153, the capsule is very close to the fuel, and consequently, fast
neutron interactions with Si and C atoms contribute significantly to the concentration of displacement damage defects in the SiC. On the contrary, at R117, R81 and R0, the concentration of displacement damage defects due to fast neutrons decreases dramatically with decreasing radial location, and the effect of tritons increases.

<table>
<thead>
<tr>
<th>Detector Radial Location (cm)</th>
<th>〈(PDPA/Φ)<em>{all}^{whole}〉</em>{MCNP} (cm²)</th>
<th>〈(PDPA/Φ)<em>{all}^{depleted}〉</em>{MCNP} (cm²)</th>
<th>〈(PDPA)_{all}^{whole}〉</th>
<th>〈(CR)<em>{all}^{all}/(PDPA)</em>{all}^{whole}〉</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>2.4x10^{-23}</td>
<td>4.0x10^{-22}</td>
<td>1.7x10^{-4}</td>
<td>9.5x10^{8}</td>
</tr>
<tr>
<td>81</td>
<td>2.2x10^{-22}</td>
<td>4.4x10^{-22}</td>
<td>3.8x10^{-3}</td>
<td>0.6x10^{8}</td>
</tr>
<tr>
<td>117</td>
<td>2.0x10^{-22}</td>
<td>4.6x10^{-22}</td>
<td>8.0x10^{-2}</td>
<td>0.9x10^{7}</td>
</tr>
<tr>
<td>153</td>
<td>8.8x10^{-22}</td>
<td>8.8x10^{-22}</td>
<td>1.54</td>
<td>0.8x10^{6}</td>
</tr>
</tbody>
</table>

Table 4.6: The values of (PDPA/Φ)_{all}^{MCNP}, averaged over the whole SiC volume and averaged over the SiC depleted region, 〈(PDPA)_{all}^{whole}〉 and 〈(CR)_{all}/(PDPA)_{all}^{whole}〉 in different detector radial locations.
Because at R0 the thermal flux is large in comparison to the fast neutron flux, 
\[
<\left(\frac{PDPA}{\Phi_{MCNP}}\right)_{\text{depleted}}^{\text{whole}} >
\]
is significantly more than 
\[
<\left(\frac{PDPA}{\Phi_{MCNP}}\right)_{\text{whole}}^{\text{whole}} >
\]. This is because the damage caused by tritons is greater in the depleted region than in the substrate due to the limited range of the tritons in the SiC.

Table 4.6 presents in column 4, the axially averaged value of \((PDPA)_{\text{all}}\) averaged over the whole SiC volume for the detector radial location as a parameter, for the neutron fluence that would be experienced by the SiC detectors for the GT-MHR refueling cycle, i.e. 15.7 months \((<PDPA>_{\text{whole}}^{\text{whole}}>)\). \((PDPA)_{\text{all}}\) for detectors located at R153 is 1.54. This means that \(77\%^{30}\) of SiC atoms would be displaced from their original sites in one refueling cycle, if the reactor works at full power and the temperature in the capsule is low. The corresponding percentages for detectors located at R117, R81 and R0 are 4.0%, 0.19% and \(8.5\times10^{-3}\%\), respectively.

Table 4.6 presents in column 5, the axially averaged \((CR)_{\text{all}}\) averaged over the whole SiC volume for SiC detectors at R153, R117, R81 and R0, for the GT-MHR refueling cycle \((<CR>_{\text{whole}}^{\text{whole}}>)\). As can be seen, by moving the SiC detectors further from the fuel elements (from R153 to R0) in the Central Reflector of the GT-MHR, the number of counts per \((PDPA)_{\text{whole}}\) decreases, by approximately three orders of

\[\]

\[^{30}\text{Recall that approximately each displacement consists of two defects.}\]
magnitude. Hence, a specified count rate, would result in many fewer defects for detectors located at R0, compared to detectors located at R153.

The cited results show that SiC detectors placed at R0 and R81 have more chance to survive, at least one GT-MHR refueling cycle, than SiC detectors at R153.

4.3.3.2 Selection of the Optimum Detector Location

Appropriate locations for the SiC detectors are locations where: 1) the detector sensitivity is adequately large to monitor the reactor power with acceptable accuracy in acceptable times, and 2) the detector survives for at least a refueling cycle period. The power monitoring system sensitivity is an essentially important parameter in the design of the nuclear power plant power monitoring instrumentation. For a system that operates in pulse mode, such as the SiC detector system that is the subject of this discussion, the channel sensitivity is limited by the maximum allowable count rate of the channel. The detector count rate should not exceed the level at which corrections for the electronic channel dead time become unacceptably large. Our calculations show that a power monitoring system electronic channel that we have designed and tested for SiC detectors is able to process count rates as high as $5 \times 10^7$ cps with less than 10% dead time [96]. We somewhat arbitrarily assume here that the count rate upper limit is $5 \times 10^7$ cps. As presented in Table 4.7, the detector count rates for R0, R81, R117 and R153 are far less than this upper limit.
Table 4.7: The SiC detector sensitivity and \( (CR)_{\text{all}} \) (averaged over axial layers 3, 5 and 8) at four GT-MHR in-core locations.

<table>
<thead>
<tr>
<th></th>
<th>R0</th>
<th>R81</th>
<th>R117</th>
<th>R153</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sensitivity ( (\text{cps/ cm}^2 \text{s}^{-1}) )</td>
<td>( 9.2 \times 10^{-7} )</td>
<td>( 5.3 \times 10^{-7} )</td>
<td>( 1.3 \times 10^{-7} )</td>
<td>( 2.8 \times 10^{-8} )</td>
</tr>
<tr>
<td>( (CR)_{\text{all}} ) ( (\text{cps}) )</td>
<td>( 1.6 \times 10^5 )</td>
<td>( 2.3 \times 10^5 )</td>
<td>( 6.2 \times 10^5 )</td>
<td>( 1.2 \times 10^6 )</td>
</tr>
</tbody>
</table>

As shown, four radial locations were identified in which to place the detectors. Firstly, assuming arbitrarily a 1 second counting time, these detectors are only able to monitor reactor power for reactor powers in the power range, at most, due to their limited sensitivity. Although modifications to the detector configuration can be made that will increase the channel sensitivity (the details of those modifications will not be discussed here), the sensitivity is nevertheless bounded on its high side. Consequently, depending on the detector counting time and count rate, there is a power level, for each potential detector location, for which the count rate is too low to obtain good statistics for the counting period. Even for their use in the power range, we cannot calculate with good confidence the acceptable operation of the power monitoring system, since the system’s required dynamic range at full power, response time, and accuracy are not known to us. These system specifications are interrelated in a way such that improving one
specification may adversely affect another specification. As an example, if the power range is expanded to more than three orders of magnitude, the uncertainty of the channel count rate, at the lower limit of the range, can become unacceptably large, assuming a 1 second counting time and that the detector dead-time does not exceed 10% at full power.

4.3.3.3 Section Conclusion

Our final goal is to be able to predict the operational lifetime of SiC detectors, in different nuclear reactors, as neutron monitors, as a function of their flux and temperature histories. Towards this goal, highlighting the GT-MHR, we have developed a method to estimate the count rate and number of defects at 0 K created per atom using two well-known codes: MCNP and TRIM. It was shown that, for the stated SiC detector geometry, in comparison with detectors placed at R153, for detectors place at R117, the count rate for the detectors is one-half, but the average \((PDPA)_{all}\) over a GT-MHR refueling cycle is twenty times smaller. For SiC detectors placed at R81 and R0, the reduction in the average \((PDPA)_{all}\) over a GT-MHR refueling cycle is much more significant. Based on available data in literature [153], SiC detectors placed in a capsule that is located at R0 may tolerate at least one GT-MHR refueling cycle. However, more study is needed to define the detector failure, and then find the \(PDPA\) for the corresponding neutron fluence and energy spectrum that caused the SiC detector to fail.
4.3.4  Evolution of Defects in SiC at GT-MHR R0

MCNP5 modeling shows that $1.7 \times 10^{13}$ tritons are born in the LiF$^{31}$ for a SiC detector at GT-MHR R0 during one GT-MHR refueling. Figure 4.27 displays the ratio of the number of defects before and after annealing at 500 K for two annealing time periods, 10 sec and 1 month to the number of defects before annealing, calculated by MARLOWE+MCASIC. As can be seen in Figure 4.27, by increasing the triton energy the effectiveness of the annealing process decreases. For example, if a 50-keV triton hits the SiC target, after 10 sec annealing time, approximately 70% of defects created by the triton will have vanished. However, if a 2050-keV triton hits the target, only approximately 28% of defects would vanish after 10-sec annealing time. Another important result from Figure 4.27 is that at 500 K the majority of recombinations happen during the first 10 sec of annealing, when some defects in a cascade are close enough for recombination. After this time period, the average distance between two consecutive defects in a defect cascade $\bar{d}$ (this term has been defined in Section 4.2.2) increases dramatically such that annealing via defect recombination almost does not impact the number of defects anymore. It is possible that this conclusion might be true even for higher temperature annealing (i.e. 800 °C); except at those temperatures, the migration of defects to the SiC boundaries (that act as drains) becomes important. This happens since, at high temperatures, defects diffuse faster in the material and have more chance to reach the boundaries in 15.7 months. In addition, at high temperatures, defects from different

\[31\text{The } ^6\text{Li burnup has been neglected.}\]
cascades have a higher chance to interact with each other. It should be noted that migration of defects to the boundaries and interaction between cascades are not modeled in MCASIC yet. Damage created by tritons is important for the first 21 μm thickness of SiC close to the Au layer. Beyond this thickness, damage in SiC is limited to damage resulting from $^{29}$Si recoils$^{32}$

Figure 4.27: The fraction of defects remained after 10 sec annealing and 1 month annealing to the number of defects before annealing, calculated by MARLOWE+MCASIC.

$^{32}$ The damage caused by $^{13}$C and some other rare recoils (such as $^{30}$Si that is born from the $^{29}$Si(n,γ)$^{30}$Si reaction) is neglected.
MCNP5 modeling shows that $8.9 \times 10^{11}$ $^{29}$Si recoils are born in the SiC, during one GT-MHR refueling cycle. Initially, the average number of defects created is 86 per each $^{29}$Si recoil. The MARLOWE+MCASIC results show that the number of defects created by a $^{29}$Si recoil reduces to 9 and 7 after 10 sec and one month annealing at 500 K, respectively. In other words, 90% of defects created by $^{29}$Si recoils are diminished in the first 10 sec of annealing. This shows that damage induced by $^{29}$Si recoils is negligible.

Our modeling shows that $PDPA$ for the depleted region of a SiC detector placed at GT-MHR R0 is $1.5 \times 10^{-3}$ after 15.7 months of operation at 500 K. Without the annealing effect, $PDPA$ would have been $2.9 \times 10^{-3}$. Therefore, the annealing (via defects recombination) process decreases the amount of defects by a factor of two. Assuming that the importance of defects is the same, the decrease in the number of defects by a factor of two means that the detector can tolerate the environment for a longer time, compared to the case where annealing may not happen.

As it was stated previously, most of the defects anneal out very quickly after damage creation. For instance, if no recombination happens after 10 sec of damage creation, $PDPA$ would have been $1.7 \times 10^{-3}$.

$PDPA$ for the SiC substrate where the triton particles cannot reach is $2.1 \times 10^{-7}$, i.e. four orders of magnitude less than $PDPA$ in the depleted region. The defect density in the stated region in the SiC substrate is so low that we think the detector performance cannot be controlled by defects created in the part of the substrate out of the triton range. Therefore, the SiC substrate may act as a drain for defects created by tritons.
CHAPTER 5

DISCUSSION

5.1 In-Core Neutron Monitoring

SiC diode detectors are usually considered as ex-core neutron monitors for nuclear reactors [139,140], or where the neutron flux is low (such as nuclear waste [141]), or where they can be quickly exchanged with new detectors without significant additional cost (such as in boron neutron capture therapy [142]). On the other hand, if possible, the use of SiC detectors as in-core neutron monitors provides some advantages over traditional in-core detectors. SiC detectors have a very small volume and may be operated in the pulse mode. In addition, the SiC detectors ability for high counting rates makes it sensitive to small changes in the neutron flux, allowing reactors to be operated closer to the safety limit. The problem of using SiC as in-core neutron monitors is that SiC detectors may not tolerate an environment with a high fast neutron flux for a long irradiation time [81].

Fast neutrons are very destructive for SiC and other semiconductors. Since neutrons have no charge, they lose their energy by collision to the target atoms. The transferred energy from fast neutrons to the primary knock-on atoms (PKAs) may be
more than the minimum energy ($E_d$) that is needed to move away the PKAs from their original lattice sites [40]. As a consequence, displacement damage defects, such as vacancies and interstitials, will be created. Those defects degrade the electrical properties of detectors. The accumulation of defects eventually amorphizes the semiconductor; and in the end, the damaged semiconductor fails to detect the collided neutrons.

In contrast to fast neutrons, thermal neutrons do not have enough energy to create damage in SiC through neutron scattering. The contribution of thermal neutrons in creating damage in SiC via neutron absorption is also not significant, since the neutron absorption cross sections for both C and Si atoms are small. Furthermore, $^{29}$Si and $^{13}$C recoils created by (n,$\gamma$) reactions would lose a big part of their energies due to electronic stopping. For these reasons, SiC detectors with a LiF triton convertor layer might be operable in a thermal neutron environment for an acceptable time period in nuclear reactors.

Our study on the IRIS showed that it is very difficult, if it is not impossible, to find a location in a light water reactor (LWR) for SiC detectors where: 1) the detector count rate is acceptably high (approximately $1 \times 10^6$ cps); and 2) the fast-neutron contribution to the neutron flux energy spectrum is a sufficiently small fraction of the total neutron flux. Mainly, this is because: 1) the fractional (with respect to the mean) standard deviation of the logarithmic energy loss for neutrons scattering on H is large; and 2) the neutron absorption cross section for H is high. Therefore, where the neutron flux energy spectrum is sufficiently thermalized, the count rate is too low.
The conditions in the graphite moderated reactors are very different. Graphite is a superior moderator. The average change in lethargy in an elastic collision, $\xi$, for graphite is 0.158, whereas $\xi$ for light water is 0.920. Because the mean logarithmic energy decrement is smaller for graphite than for light water the energy loss of neutrons is more continuous, and the neutron flux energy distribution in a graphite moderated reactor may be very thermal, with a very small fast neutron component, in graphite regions that are located far from fission sources in the fuel. C atoms moderate neutrons without too much absorption. The moderating ratio of graphite is 192 (the second best after D$_2$O), compared to the moderating ratio of H$_2$O that is only 71. Therefore, it might be possible to find locations in graphite moderated reactors where the neutron flux is very thermal, with little fast neutron contamination, and where the thermal neutron flux is large. Our study has shown that indeed these conditions are available in some radial locations, such as the core center, in the central reflector of the Gas Turbine-Modular Helium Reactor (GT-MHR). The central reflector is a large volume of graphite in the center of the GT-MHR, and its center is far from fission sources.

5.2 Damage and Annealing Modeling

The simulation methods that we used have some advantages over other methods, such as using the simple NRT model or SPECTER. Those methods were originally developed to estimate the damage dose, not the annealing effect. The advantages of our methods are:
a) The PKA spectrum determined by MCNP5 is continuous in energy.

b) The PKA-neutron collision characteristics, like the fraction of collided neutrons and the fraction of C-PKAs, can be determined.

c) The PKA characteristics, like the average and maximum energy transferred to the C- and Si-PKAs and positions of PKAs, can be studied.

d) The number of various kinds of defects can be estimated.

e) The distribution of defects can be approximated.

f) Damage created by different kinds of projectiles (for instance neutrons and protons) can be compared.

g) For the case that there are two or more projectile species, the number of defects created due to each projectile species and their can be estimated. For instance, the number of defects created by neutron scattering events and tritons can be summed.

h) By knowing the distribution and types of defects, the time-temperature evolution of defects can be studied.

In spite of the stated advantages, there are several sources of uncertainties (both epistemic and aleatory), as follows:

a) Some Monte Carlo codes were used. Since Monte Carlo codes are based on random numbers, they have some aleatory uncertainties.
b) Several sets of data were used that were not perfectly suited to the calculations and in using these data sets epistemic uncertainties were incorporated into the calculations. For instance it was assumed that data for 3C-SiC is valid for 4H-SiC.

c) Another instance in which epistemic uncertainties were included in the calculation is in using MARLOWE. Although one can define crystalline matter in MARLOWE, with different properties in different directions, there was not enough data available for 4H-SiC (for example the direction dependence of $E_d$ values), for us to do so. Consequently, we have incorporated epistemic uncertainties in our calculations, when we treated an anisotropioic crystalline material as though it possessed isotropic properties.

d) As a consequence of the assumptions that were made regarding the isotropy of SiC, as discussed in the comment above, some important phenomena that affect the spatial distributions of defects are not included in MARLOWE, such as channeling.

e) The defect capture radii for defect pairs increases by increasing the supercell size, and it seems that it does not converge with increasing cell size. Therefore, the cited defect capture radii are relative values.

f) It was assumed that the defect capture radii that were calculated for defect pairs are valid for defect cascades with more than two defects, as well.

g) Steps 3 and 4 of MCASIC are not among standardly used KMC methods. We developed them since, based on our best knowledge, there is no KMC method that is able to model defect annealing that can happen over a time-span of several months.

h) In MCASIC, it was assumed that the SiC is infinite. Therefore, it was assumed that defects anneal out only by interactions among themselves. In reality, for long annealing times at a high temperature, the trapping of defects in drains is important.
i) In calculating $PDPA$, we assumed that each defect type has the same impact on the SiC electrical properties. For example, we assumed that there is no difference between a $V_C$ and an $I_C$, with respect to its impact on electron or ion mobilities or charge trapping.

The results for the damage at low temperature are valid and consistent with results obtained by other methods. However, based on the above comments here and discussions in the text, the MCASIC results are uncertain, especially since properties of 4H-SiC, such as defect diffusion properties, are not well-enough validated yet. Also, more advanced methods are needed to model the annealing of defects for long annealing times, for instance several months.
CONCLUSION AND FUTURE WORK

Our final goal is to be able to predict the operational lifetime of SiC detectors, in different nuclear reactor types, as neutron monitors, as a function of their flux and temperature histories. Towards this goal, using several computer codes, we have developed computer simulation methods to estimate PDPA and count rates for SiC power monitors placed in nuclear reactors. MCNP5 was used to determine the neutron spectrum, and triton and $^{29}$Si production rates. TRIM was used to estimate the number of defects created by each projectile and the range of projectiles in SiC. MARLOWE was used to determine the spatial distribution of defects of various types for each defect cascade. VASP and DCRSIC were used to calculate the capture radii for defect pairs at different temperatures. Finally, MCASIC was used to estimate PDPA, after a specified period of time.

We found that at 500 K, $PDPA$ is $1.5 \times 10^{-3}$ in the depleted region for SiC detectors placed at GT-MHR R0 for a refueling cycle. At this location, $(CR)_{all}$ is $1.6 \times 10^5$ that is one order of magnitude less than the stated preferable count rate. Therefore, some
changes in the SiC design might be needed, such as using SiC diode detectors with larger
diameter and/or thicker LiF layer.

We still do not know at what PDPA we could say that a detector has failed. Using simulation codes and experimental data, my colleagues in the Nuclear Engineering Program and Department of Materials Science and Engineering are working to find that out.

MCASIC needs some modifications to be able to model the damage recovery at higher temperatures. These modifications include the migration of defects to the drains and the interaction of defects created in more than one defect cascade. We also intend to study how the ambient temperature affects PDPA. It will help us to find the most appropriate temperatures for SiC neutron monitors placed in a thermal neutron environment. The final step in our modeling process will be to evaluate how each defect influences the carrier mobility and other electrical properties of SiC, and to predict how these changes in the electrical properties of SiC affect the count rate of the power monitor.
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APPENDIX A

SYMBOLS AND ABBREVIATIONS
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
<th>Symbol</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Reactors:</strong></td>
<td></td>
<td><strong>Reactors:</strong></td>
<td></td>
</tr>
<tr>
<td>IRIS</td>
<td>International Reactor Innovative &amp; Secure</td>
<td>GT-MHR</td>
<td>Gas Turbine-Modular Helium Reactor</td>
</tr>
<tr>
<td>OSURR</td>
<td>Ohio State University Research Reactor</td>
<td>LWR</td>
<td>Light Water Reactor</td>
</tr>
<tr>
<td>AIF</td>
<td>Auxiliary Irradiation Facility</td>
<td>BP1</td>
<td>Beam Port One</td>
</tr>
<tr>
<td>TC</td>
<td>Thermal Column</td>
<td>RPV</td>
<td>Reactor Pressure Vessel</td>
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<td>Containment Vessel</td>
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<td><strong>Codes:</strong></td>
<td></td>
<td><strong>Codes:</strong></td>
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</tr>
<tr>
<td>MCNP</td>
<td>Monte Carlo N-Particle</td>
<td>MCASIC</td>
<td>Monte Carlo Analysis for SiC</td>
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<tr>
<td>DCRSIC</td>
<td>Defect Capture Radius calculations for SiC</td>
<td>VASP</td>
<td>Vienna Ab-initio Simulation Package</td>
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<tr>
<td>TRIM</td>
<td>Transport of Ions in Matter</td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Count Rate</strong></td>
<td></td>
<td><strong>Count Rate</strong></td>
<td></td>
</tr>
<tr>
<td>cps</td>
<td>Counts per second</td>
<td>CR</td>
<td>Count Rate</td>
</tr>
<tr>
<td>LLD</td>
<td>Lower level of discrimination</td>
<td>$N_{E_{PKA}&gt;200keV}$</td>
<td>Number of PKAs which have energy more than 200 keV</td>
</tr>
<tr>
<td>Symbol</td>
<td>Definition</td>
<td>Symbol</td>
<td>Definition</td>
</tr>
<tr>
<td>-----------------</td>
<td>-------------------------------------</td>
<td>-----------------</td>
<td>-------------------------------------</td>
</tr>
<tr>
<td><strong>Displacement Damage:</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$PDPA$</td>
<td>Point Defects Per Atom</td>
<td>$PKA$</td>
<td>Primary Knock-on Atom</td>
</tr>
<tr>
<td>$\Phi_{\text{Total}}^{\text{eq},1\text{MeV},\text{mat}}$</td>
<td>1 MeV equivalent neutron fluence</td>
<td>$F_{D,\text{mat}}(E)$</td>
<td>Damage function</td>
</tr>
<tr>
<td>$\sigma_{d}(E)$</td>
<td>Displacement cross section</td>
<td>$DPA$</td>
<td>Displacement Per Atom</td>
</tr>
<tr>
<td>$H_{\text{mat}}$</td>
<td>Neutron spectrum hardness</td>
<td>$mat$</td>
<td>Material of interest</td>
</tr>
<tr>
<td>$E_{n}$</td>
<td>Neutron energy after collision</td>
<td>$\bar{d}$</td>
<td>Average distance between two defects in a defect cascade, if all defects placed in a line</td>
</tr>
<tr>
<td>$T$</td>
<td>Temperature, PKA energy</td>
<td>$E$</td>
<td>Projectile energy</td>
</tr>
<tr>
<td>$E_{n}$</td>
<td>Neutron Energy</td>
<td>$E_{d}$</td>
<td>The minimum kinetic energy that a struck atom should gain to move away from its original site</td>
</tr>
<tr>
<td>$E_{n}^{th}$</td>
<td>Threshold neutron energy</td>
<td>$M, m$</td>
<td>Mass</td>
</tr>
<tr>
<td>$\Lambda$</td>
<td>Defined in Eq. 7</td>
<td>$E^*$</td>
<td>Excitation energy</td>
</tr>
<tr>
<td>Symbol</td>
<td>Definition</td>
<td>Symbol</td>
<td>Definition</td>
</tr>
<tr>
<td>--------</td>
<td>------------</td>
<td>--------</td>
<td>------------</td>
</tr>
<tr>
<td>Φ</td>
<td>Fluence</td>
<td>φ</td>
<td>Flux</td>
</tr>
<tr>
<td>$\dot{S}_{\text{triton}}$</td>
<td>Rate of tritons which reach to the SiC</td>
<td>$N$</td>
<td>Number of projectiles</td>
</tr>
<tr>
<td>$E_{\text{atom}}$</td>
<td>Rest mass energy of the recoil</td>
<td>$\nu$</td>
<td>Number of defects per PKA (in the case of neutron scattering), or projectile</td>
</tr>
<tr>
<td>$V_C$</td>
<td>C vacancy</td>
<td>$V_Si$</td>
<td>Si vacancy</td>
</tr>
<tr>
<td>$SiC$</td>
<td>Si antisite</td>
<td>$C_{Si}$</td>
<td>C antisite</td>
</tr>
</tbody>
</table>

**Material Properties:**

<table>
<thead>
<tr>
<th>H (in 2H-, 4H-, or 6H-SiC)</th>
<th>Hexagonal</th>
<th>C (in 3C-SiC)</th>
<th>Cubic</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_F$</td>
<td>Fermi energy</td>
<td>$E_{Fi}$</td>
<td>Fermi energy for intrinsic semiconductors</td>
</tr>
<tr>
<td>$E_{Fn}$</td>
<td>Fermi energy for $n$-type semiconductors</td>
<td>$E_v$</td>
<td>Valence band edge</td>
</tr>
<tr>
<td>$E_g$</td>
<td>Bandgap energy</td>
<td>$m_e^*$</td>
<td>Effective electron mass</td>
</tr>
<tr>
<td>$m_h^*$</td>
<td>Effective hole mass</td>
<td>$m_0$</td>
<td>Electron mass</td>
</tr>
<tr>
<td>$k_B$</td>
<td>Boltzmann constant</td>
<td>$\hbar$</td>
<td>Plank constant</td>
</tr>
<tr>
<td>$N_d$</td>
<td>Donor concentration</td>
<td>$n_i$</td>
<td>intrinsic carrier concentration</td>
</tr>
<tr>
<td>$D$</td>
<td>Diffusion coefficient</td>
<td>$D_0$</td>
<td>Diffusion prefactor</td>
</tr>
<tr>
<td>Symbol</td>
<td>Definition</td>
<td>Symbol</td>
<td>Definition</td>
</tr>
<tr>
<td>--------</td>
<td>------------</td>
<td>--------</td>
<td>------------</td>
</tr>
<tr>
<td>$\mu_F$</td>
<td>Fermi level</td>
<td>$\Delta \mu$</td>
<td>Chemical potential difference</td>
</tr>
<tr>
<td>$T$</td>
<td>Temperature, PKA energy</td>
<td>$Q$</td>
<td>Activation energy, Energy given off in a nuclear reaction</td>
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</tbody>
</table>

**Kinetic Monte Carlo**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
<th>Symbol</th>
<th>Definition</th>
</tr>
</thead>
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<tr>
<td>$R$</td>
<td>Hopping rate</td>
<td>$k_{x,y}$</td>
<td>Rate coefficient</td>
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<tr>
<td>$E_m$</td>
<td>Defect migration energy</td>
<td>$a_{x,y}$</td>
<td>Capture radius</td>
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<tr>
<td>$KMC$</td>
<td>Kinetic Monte Carlo</td>
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**Capture Radius Calculations**

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<tbody>
<tr>
<td>$d_{j,s}$</td>
<td>Distances between a defect and the other defect or its periodic images (which stem from the use of PBC) in the supercells.</td>
</tr>
<tr>
<td>$\lambda_{j,s}$</td>
<td>Distances between a defect in the main supercell and its periodic images.</td>
</tr>
<tr>
<td>$i$</td>
<td>Cut-off distance for the interactions between a defect with the other defect and its periodic images</td>
</tr>
<tr>
<td>$k$</td>
<td>Cut-off distance for the interactions between a defect and its periodic images</td>
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APPENDIX B

CALCULATED AND FITTED ENERGIES OF DEFECT PAIRS
I_{Si-V_{Si}}:

<table>
<thead>
<tr>
<th>Min($d_i$) (Å)</th>
<th>0.00</th>
<th>3.93</th>
<th>6.73</th>
<th>7.24</th>
<th>6.58</th>
</tr>
</thead>
<tbody>
<tr>
<td>Energy calculated (eV)</td>
<td>-1449.45</td>
<td>-1436.96</td>
<td>-1434.21</td>
<td>-1434.55</td>
<td>-1434.79</td>
</tr>
<tr>
<td>Energy fitted (eV)</td>
<td>-1449.45</td>
<td>-1436.9</td>
<td>-1434.63</td>
<td>-1434.34</td>
<td>-1434.70</td>
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C_{Si-I_{Si}}:

<table>
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<tr>
<th>Min($d_i$) (Å)</th>
<th>2.15</th>
<th>3.27</th>
<th>5.16</th>
<th>8.60</th>
<th>2.15</th>
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</thead>
<tbody>
<tr>
<td>Energy calculated (eV)</td>
<td>-1452.10</td>
<td>-1446.03</td>
<td>-1446.09</td>
<td>-1445.91</td>
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<tr>
<td>Energy fitted (eV)</td>
<td>-1451.08</td>
<td>-1448.04</td>
<td>-1446.06</td>
<td>-1444.94</td>
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I_{C-V_{Si}}:

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<tr>
<th>Min($d_i$) (Å)</th>
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<th>3.39</th>
<th>8.91</th>
<th>8.97</th>
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<tr>
<td>Energy calculated (eV)</td>
<td>-1449.68</td>
<td>-1440.26</td>
<td>-1438.65</td>
<td>-1441.34</td>
<td>-1438.13</td>
<td>-1437.50</td>
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<tr>
<td>Energy fitted (eV)</td>
<td>-1449.68</td>
<td>-1440.55</td>
<td>-1438.18</td>
<td>-1441.14</td>
<td>-1438.09</td>
<td>-1437.96</td>
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**I_{Sr}-I_{Si}:**

<table>
<thead>
<tr>
<th>Min($d_i$) (Å)</th>
<th>3.10</th>
<th>2.64</th>
<th>5.10</th>
<th>8.80</th>
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</thead>
<tbody>
<tr>
<td>Energy calculated (eV)</td>
<td>-1443.50</td>
<td>-1443.83</td>
<td>-1440.98</td>
<td>-1440.89</td>
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<tr>
<td>Energy fitted (eV)</td>
<td>-1443.15</td>
<td>-1443.97</td>
<td>-1441.49</td>
<td>-1440.62</td>
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**I_{C}-I_{C}:**

<table>
<thead>
<tr>
<th>Min($d_i$) (Å)</th>
<th>2.43</th>
<th>2.23</th>
<th>4.85</th>
<th>6.24</th>
<th>8.17</th>
<th>9.42</th>
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<tbody>
<tr>
<td>Energy calculated (eV)</td>
<td>-1459.63</td>
<td>-1458.01</td>
<td>-1455.44</td>
<td>-1455.31</td>
<td>-1455.24</td>
<td>-1455.37</td>
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<tr>
<td>Energy fitted (eV)</td>
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**I_{Sr}-V_{C}:**

<table>
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<th>Min($d_i$) (Å)</th>
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<td>Energy calculated (eV)</td>
<td>-1441.84</td>
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<td>Energy fitted (eV)</td>
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<td>-1432.72</td>
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**Ic-Vc:**

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<tr>
<th>Min($d_i$) (Å)</th>
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<th>1.18</th>
<th>4.08</th>
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<tr>
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<td>-1449.59</td>
<td>-1443.79</td>
<td>-1443.49</td>
<td>-1438.51</td>
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<tr>
<td>Energy fitted (eV)</td>
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<td>-1440.03</td>
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<table>
<thead>
<tr>
<th>Min($d_i$) (Å)</th>
<th>5.59</th>
<th>7.92</th>
<th>8.76</th>
<th>9.80</th>
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<tbody>
<tr>
<td>Energy calculated (eV)</td>
<td>-1438.65</td>
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<td>-1438.56</td>
<td>-1438.56</td>
</tr>
<tr>
<td>Energy fitted (eV)</td>
<td>-1439.75</td>
<td>-1440.27</td>
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</table>

**Vc-Vc:**

<table>
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<tr>
<th>Min($d_i$) (Å)</th>
<th>3.11</th>
<th>3.08</th>
<th>4.45</th>
<th>5.38</th>
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</thead>
<tbody>
<tr>
<td>Energy calculated (eV)</td>
<td>-1423.50</td>
<td>-1423.30</td>
<td>-1422.09</td>
<td>-1422.12</td>
</tr>
<tr>
<td>Energy fitted (eV)</td>
<td>-1423.31</td>
<td>-1423.30</td>
<td>-1422.54</td>
<td>-1422.24</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>Min($d_i$) (Å)</th>
<th>6.03</th>
<th>6.91</th>
<th>7.41</th>
</tr>
</thead>
<tbody>
<tr>
<td>Energy calculated (eV)</td>
<td>-1422.23</td>
<td>-1422.24</td>
<td>-1422.38</td>
</tr>
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<td>Energy fitted (eV)</td>
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Ic-Isi:

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<th>Min($d_i$) (Å)</th>
<th>1.03</th>
<th>1.71</th>
<th>7.85</th>
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<td>-1452.55</td>
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<td>-1448.71</td>
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<td>Energy fitted (eV)</td>
<td>-1452.56</td>
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<td>-1448.91</td>
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Csii-Vsi:

<table>
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<th>Min($d_i$) (Å)</th>
<th>2.31</th>
<th>5.62</th>
<th>7.16</th>
<th>8.41</th>
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<tr>
<td>Energy calculated (eV)</td>
<td>-1437.01</td>
<td>-1436.02</td>
<td>-1436.06</td>
<td>-1436.01</td>
</tr>
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<td>Energy fitted (eV)</td>
<td>-1436.97</td>
<td>-1436.17</td>
<td>-1436.00</td>
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SiC-Ic:

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<tr>
<th>Min($d_i$) (Å)</th>
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<td>-1445.83</td>
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<td>Energy fitted (eV)</td>
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VC-V_{Si}:

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<th>Min(d_i) (Å)</th>
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<td>Energy calculated (eV)</td>
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<td>-1423.48</td>
</tr>
<tr>
<td>Energy fitted (eV)</td>
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<td>-1425.21</td>
<td>-1423.93</td>
<td>-1423.96</td>
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Si_{C}-I_{Si}:

<table>
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<tr>
<th>Min(d_i) (Å)</th>
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<th>4.08</th>
<th>7.17</th>
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</thead>
<tbody>
<tr>
<td>Energy calculated (eV)</td>
<td>-1438.74</td>
<td>-1437.73</td>
<td>-1438.19</td>
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<tr>
<td>Energy fitted (eV)</td>
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<td>-1438.11</td>
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V_{Si}-V_{Si}:

<table>
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<th>Min(d_i) (Å)</th>
<th>3.10</th>
<th>3.16</th>
<th>4.38</th>
<th>4.66</th>
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<tbody>
<tr>
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<td>-1422.71</td>
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<td>-1422.67</td>
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Min\(d_i\) (Å) | 7.59  | 8.20  | 8.93  |
<table>
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<td>-1422.63</td>
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<td>Energy fitted (eV)</td>
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SiC-V_{Si}:

<table>
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<td>Energy fitted (eV)</td>
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<td>-1428.45</td>
<td>-1428.44</td>
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</tr>
</tbody>
</table>
APPENDIX C

EXAMPLE OF MCNP-SIC DETECTOR MODEL
SiC Detector Model

c Mode N

c Inside the Inner Reflector

c

c ==============================================================

c                         Cell Cards

c ==============================================================

10 1 -2.640  -10  1  -2   imp:n=1 imp:p=1               $ LiF   1 um
20 2 -2.702  -10  2  -3   imp:n=1 imp:p=1               $ Al    8 um
25 5 -19.311 -10  3  -4   imp:n=1 imp:p=1               $ Au    1 um
30 3 -3.21   -10  4  -6   imp:n=1 imp:p=1               $ SiC   310um
50 4 3.437E-5  (-1:10:6) -999      imp:n=1 imp:p=1
52 0 999                  imp:n=0 imp:p=0                    $ External World

c ==============================================================

c                     Surface Cards

c ==============================================================

1   px  0.00000             $ Start LiF
2   px  0.00010             $ Start Al
3   px  0.00090             $ Start Au
4   px  0.00100             $ Start SiC
6   px  0.0320              $ Stop SiC
10  cx  0.0250              $ Detector radius = 250 um
888 so  0.1                   $ Source
999 so  0.5                   $ Sphere around assembly

c ==============================================================

c                               Problem Type

c ==============================================================

c


c ==============================================================

c                                    Energy Cards

c ==============================================================

phys:n    20.0 0.0                 $ >20 MeV neutron XSNs expunged
tmp1 3.645E-8 4r 0.0          $ Take care of temperature!!!

c ==============================================================

c                                    Source

c ==============================================================

sdef sur=888 nrm=-1 dir=d1 wgt=1 erg=d701
sb1 -21 2
si701 h   1.00E-10
<table>
<thead>
<tr>
<th>Value</th>
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<tbody>
<tr>
<td>1.00E-09</td>
</tr>
<tr>
<td>1.00E-08</td>
</tr>
<tr>
<td>2.30E-08</td>
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<td>5.00E-08</td>
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<td>7.60E-08</td>
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Tally

fc4
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fm14 (0.122581 21 105) (0.122581 21 107)
   (0.122581 21 205) (0.122581 21 33)

f34:n 30

fm44 0.0964211 3 102

f54:n 30

fm54 0.04821055 6 102

f64:n 30

fm64 0.04821055 7 102

f74:n 30

fm74 (0.0964211 3 1) (0.0964211 3 2) (0.0964211 3 51:52:53:54:55:91)

Material

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**Cutoff Cards**

ctme 40
nps 99999999

**Peripherals**

print -85
prdmp 2j 1 4
APPENDIX D

EXAMPLE OF THE MARLOWE’S INPUT
100 keV C ==> 4H-SiC
Displacement Cascade in SiC

&XTAL
UNIT=-1,
BASE=1.0,ALAT=3.078003,5.33128,10.0460,90.0,90.0,90.0,DMAX=7.5,
RZ=0.0,0,0,1.88865,0,0,0,6.91165,1.5390015,0.8885644,4.410194,1.5390015,-
0.8885644,9.433194,0,0,0,0,0,0,0,0,0,5.023,1.5390015,0.8885644,2.5195368,1.5390015,-
0.8885644,7.5425368,&END
&ATOM NTYPE=2,TYPE='C','Si',Z=6.0,14.0,W=12.0107,28.0855,EBND=12*3,12*7,
EQUIT=15,15,LOCK=1,1,1,1,2,2,2,&END
&OUTP LOOK=4,INFORM=4*.TRUE,&END
&PROJ
MAXRUN=1,RANX=5,THA=55 PHI=35,RAIP=0,0,0,0,0,0,LEAP=6,EKIP=100000,&END
&END
APPENDIX E

EXAMPLE OF DCRSIC
CHARACTER line*80

* Maximum # of Hops = Hopmax
  parameter(Hopmax = 2)

* Position of atoms = r (x,y,z)
  dimension xC(3,8),xSi(3,8),a(3,3)

* Data needs to begin AND CLOSE with / values need to be separated by,
  data a / 3.078003, 0.0000, 0.0000,
  &  0.0000, 5.331258, 0.0000,
  &  0.0000, 0.0000, 10.046 /

* Position of the 8 C atoms in 4H-SiC cell
  data xC / 0.00000, 0.00000, 0.18800,
  &  0.50000, 0.50000, 0.18800,
  &  0.00000, 0.33333, 0.43900,
  &  0.50000, 0.83333, 0.43900,
  &  0.00000, 0.00000, 0.68800,
  &  0.50000, 0.50000, 0.68800,
  &  0.00000, 0.66667, 0.93900,
  &  0.50000, 0.16667, 0.93900 /

* Position of the 8 Si atoms in 4H-SiC cell
  data xSi / 0.00000, 0.00000, 0.00000,
  &  0.50000, 0.50000, 0.00000,
  &  0.00000, 0.33333, 0.25080,
  &  0.50000, 0.83333, 0.25080,
  &  0.00000, 0.00000, 0.50000,
  &  0.50000, 0.50000, 0.50000,
  &  0.00000, 0.66667, 0.75080,
  &  0.50000, 0.16667, 0.75080 /

INTEGER*4 seed

* IC and Hop are counters
  INTEGER nHop,counter,DefSel,NonSel,Hop,iPBC,IC,
  &  Digit(7),Migr(7),C

DOUBLE PRECISION dcomp,Temp,TVC,dist,ReaRad,
&  XNew1,YNew1,ZNew1,XOld1,YOld1,ZOld1,
&  Xpos1(Hopmax),Ypos1(Hopmax),Zpos1(Hopmax),
&  EmVC0,EmVC2P,EmVSi2N,EmVSi1N,EmVSi0,mu3,mu4,mu5,mu6,mu7,mu8,
&  EmIC1N,EmIC1P,EmIC2P,EmISi0,EmISi4P,kBeV,
&  xCarbon,yCarbon,zCarbon,Def2Dist,Coef(14),aX,bY,cZ,Rate,Diffu,
&  Xoption(12),Yoption(12),Zoption(12),OptDis(12),MinDist,RangeP
DOUBLE PRECISION DVC,DVSi,DIC,DISi,D3,D4,D5,D6,
& R3,R4,R5,R6,TotRate,RealTime,
& mSe,mSh,kBJ,Ph,Eg,n,i,n,p,Nd,nni,pni,MioF,Ev,axy,Diffu5,EChange,
& ni1,ni2,ni3,ni4,ni5,nni,PeakTime,MDTime,kxy,omega,Diff,
& TotHop,Hopping,HopRate(12),AngSel,xt(13),HopR,
& OptEner(12),Energy,EqValid,EqVal(4),
& Xpos27(27),Ypos27(27),Zpos27(27),PBCDis(27),
& xPBC(27),yPBC(27),zPBC(27),PBC,B(14)

OPEN(UNIT=10,FILE='inputpdbDiDef.dat',STATUS='old')
* dcomp = atoms bond length
READ(10,*)dcomp
* nDef = number of defects
READ(10,*)nDef
* Seed = random generator seed
READ(10,*)Seed
* nHop = number of hops, mHop = number of hops for each movie frame
READ(10,*)nHop
* Nd is the density of dopant
READ(10,*)Nd
* aX, bY & cZ are box dimensions
READ(10,*)aX, bY, cZ
* ArbCR is an arbitrary capture radius to find the real capture radius.
READ(10,*)ArbCR
* EqValid are the max distances where the potential is valid.
READ(10,*)EqValid
* MinDist is the minimum distance between two defects that the potential is valid.
READ(10,*)MinDist
* RangeP is the range of the potential
Read(10,*)RangeP
* E = -Coef/dist - B, The following are Coef# and B# for capture Radii.
* Order: ASi-VC, AC-VSi
READ(10,*)Coef(1),Coef(2)
READ(10,*)B(1),B(2)
* Digit is the number of active migrants (if the defect are the same, then Digit=2,
otherwise Digit=1), Migr is the immigrant defect
READ(10,*)Digit(1),Digit(2)
READ(10,*)Migr(1),Migr(2)

CLOSE(UNIT=10)

OPEN(UNIT=60,FILE='Temp.o',STATUS='Unknown')
WRITE(60,*)' Temp(K), Capture_Radius(nm), Captures, IC,
& EqValid'

DO 58 i10 = 1,2
Temp = 200

DO 56 iTemp = 1,17

*---------------------------------------------------------
* S.1. Set Diffusion Parameters
*---------------------------------------------------------

* kBeV is the Boltzmann Constant in eV/k, kBJ is the Boltzmann Constant in J/k
* mSe = Effective mass of an electron, hP = Planks Constant,
* mSh = Effective mass of a hole, Eg = band gap in eV
kBeV = 8.617343E-5
kBJ = 1.38E-23
hP = 6.62E-34
mSe = 3.2305E-31
mSh = 9.1E-31
Eg = 3.2
Ev = 8

ni1 = 2*(2*3.14159265*kBJ*Temp) ** (1.5)
ni2 = (mSe*mSh)**(0.75)
ni3 = hP**3
ni4 = EXP(-Eg/(2*kBeV*Temp))
ni = ni1*ni2*ni4/ni3 * 1E-6

n = Nd
p = ni**2 / Nd

nni = n/ni
pni = p/ni

* MioF is the Fermi level - Valence band, EFi is the intrinsic Fermi level,EFn is the Fermi level,

* 3=C-Vac, 4=Si-Vac, 5=C-Int, 6=Si-Int, 7=C-Ant, 8=Si-Ant

EFi = Ev + Eg/2 - 0.75*kBeV*Temp*LOG(mSe/mSh)
EFn = EFi + kBeV*Temp*LOG(Nd/ni)
MioF = EFn - Ev

c write(*,*)'MioF =', MioF

* Most of the following mu (defect formation energy) and Em (defect migration energy)
* are from "ab initio study of the migration of intrinsic defects in 3C-SiC,

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* Assuming an stoichiometric SiC ($\Delta \text{Mio} = 0$)

* $\mu_3$ is the defect formation energy of C-Vac of n-type SiC where 0 charged C-Vac is dominant.
  \[ \mu_3 = 3.1 + 2 \times \text{MioF} \]
  \[ \text{EmVC}^0 = 3.5 \]
  \[ \text{EmVC}^2P = 5.2 \]

* $\mu_4$ is the defect formation energy of Si-Vac of n-type SiC where 2- charged Si-Vac is dominant.
  \[ \mu_4 = 10.7 - 2 \times \text{MioF} \]
  \[ \text{EmVS}^2N = 2.4 \]
  \[ \text{EmVS}^1N = 3.2 \]
  \[ \text{EmVS}^0 = 3.4 \]

* $\mu_5$ is the defect formation energy of C-Int of n-type SiC where 1- charged C-Int is dominant.
  \[ \mu_5 = 8.5 - \text{MioF} \]
  \[ \text{EmIC}^1N = 0.6 \]
  \[ \text{EmIC}^0 = 0.5 \]
  \[ \text{EmIC}^1P = 0.9 \]
  \[ \text{EmIC}^2P = 1.4 \]

* $\mu_6$ is the defect formation energy of Si-Int of n-type SiC where 0 charged Si-Int is dominant.
  \[ \mu_6 = 8.5 \]
  \[ \text{EmIS}^0 = 1.4 \]
  \[ \text{EmIS}^4P = 3.45 \]
  \[ \mu_7 = 3.55 \]
  \[ \mu_8 = 4.27 \]

* $D_0$s are diffusion prefactors from F. Gao et al, Atomistic study of intrinsic defect migration in 3C-SiC,

  \[ D_0C = 1.23 \times 10^{-3} \]
  \[ D_0Si = 3.30 \times 10^{-3} \]

  \[ R_0C = D_0C \times \frac{6}{(a(1,1)^{**2} \times 10^{-16})} \]
  \[ R_0Si = D_0Si \times \frac{6}{(a(1,1)^{**2} \times 10^{-16})} \]

  \[ D_3 = R_0C \times (\exp(-\text{EmVC}^0/\text{kBeV} \times \text{Temp})) \]
  \[ D_4 = R_0Si \times (\exp(-\text{EmVS}^2N/\text{kBeV} \times \text{Temp})) \]
  \[ D_5 = R_0C \times (\exp(-\text{EmIC}^1N/\text{kBeV} \times \text{Temp})) \]
  \[ D_6 = R_0Si \times (\exp(-\text{EmIS}^0/\text{kBeV} \times \text{Temp})) \]
D7 = 0.
D8 = 0.

IF(Migr(i10).EQ.3)THEN
  Diff = D3
ELSEIF(Migr(i10).EQ.4)THEN
  Diff = D4
ELSEIF(Migr(i10).EQ.5)THEN
  Diff = D5
ELSEIF(Migr(i10).EQ.6)THEN
  Diff = D6
ELSE
ENDIF

RealTime = 0.

write(*,*)'D3,               D4,            D5,           D6,'
&             Temp, RealTime'
write(*,*) D3, D4, D5, D6, Temp, RealTime

counter is to count the number of times that two defects has less distance than ArbCr.
  counter = 0
  Hop = 0

*---------------------------------------------------------
*              S.4. Choosing the diffusitive and migration
*---------------------------------------------------------

ICs are to be sure the the random generator works
  IC1 = 0
  IC2 = 0
  IC3 = 0
  IC4 = 0
  IC5 = 0
  IC6 = 0
  IC7 = 0
  IC8 = 0
  IC9 = 0
  IC10 = 0
  IC11 = 0
  IC12 = 0

nHop is the number of Hops
  Xpos1(1) = aX * ran0(seed)
  Ypos1(1) = bY * ran0(seed)
  Zpos1(1) = cZ * ran0(seed)
  Xpos1(2) = aX * ran0(seed)
  Ypos1(2) = bY * ran0(seed)
  Zpos1(2) = cZ * ran0(seed)
Zpos1(2) = cZ * ran0(seed)

write(*,*)'Xpos1(1), Xpos1(2)'  
write(*,*) Xpos1(1), Xpos1(2) 
DO 59 j = 1,nHop  
   IC=counter+IC1+IC2+IC3+IC4+IC5+IC6+IC7+IC8+IC9+IC10+IC11+IC12 
   * DefecSel is to choose the migrant defect  
   IF(Digit(i10).EQ.2)THEN  
      DefecSel = ran0(seed) * 2  
      IF(DefecSel.LE.1)THEN  
         DefSel = 1  
         NonSel = 2  
      ELSE  
         DefSel = 2  
         NonSel = 1  
      ENDIF  
   ELSE  
      DefSel = 2  
      NonSel = 1  
   ENDIF  
   CALL PBCImp(Xpos1,YPos1,ZPos1,j,aX,bY,cZ,NonSel,DefSel,iPBC)  
   Def2Dist = sqrt((Xpos1(DefSel)-Xpos1(NonSel))**2 + 
                   (Ypos1(DefSel)-Ypos1(NonSel))**2 + 
                   (Zpos1(DefSel)-Zpos1(NonSel))**2)  
   IF(Def2Dist.LE.ArbCR)THEN  
      counter = counter + 1  
      IC=counter+IC1+IC2+IC3+IC4+IC5+IC6+IC7+IC8+IC9+IC10+IC11+IC12  
      c  
      Type1(1) = 4  
      Xpos1(1) = aX * ran0(seed)  
      Ypos1(1) = bY * ran0(seed)  
      Zpos1(1) = cZ * ran0(seed)  
      c  
      Type1(2) = 5  
      Xpos1(2) = aX * ran0(seed)  
      Ypos1(2) = bY * ran0(seed)  
      Zpos1(2) = cZ * ran0(seed)  
      C = 1  
      GOTO 59  
   ELSE  
      C = 0  
   ENDIF  
   ZDefect = Zpos1(DefSel)  
   IF(Migr(i10).EQ.5.OR.Migr(i10).EQ.6)THEN  
      CALL Interstitial(a,xC,xSi,ZDefect,x1,y1,z1,z2,Znear)  
   ENDIF  
END
ELSEIF(Migr(i10).EQ.3)THEN
CALL Cvacancy(a,xC,ZDefect,x1,y1,z1,z2,Znear)
ELSEIF(Migr(i10).EQ.4)THEN
CALL Sivacancy(a,xSi,ZDefect,x1,y1,z1,z2,Znear)
ELSE
ENDIF

IF(Def2Dist.LE.MinDist)THEN
Energy = (-Coef(i10) / MinDist - B(i10)) +
& (-Coef(i10) / RangeP - B(i10)) -
& (-Coef(i10) / EqValid - B(i10))
ELSEIF(Def2Dist.GT.MinDist.AND.Def2Dist.LE.EqValid)THEN
Energy = (-Coef(i10) / Def2Dist - B(i10)) +
& (-Coef(i10) / RangeP - B(i10)) -
& (-Coef(i10) / EqValid - B(i10))
ELSEIF(Def2Dist.GT.EqValid)THEN
Energy = -Coef(i10) / RangeP - B(i10)
ENDIF

******* 1st migration option:
Xoption(1) = Xpos1(DefSel)+a(1,1)
Yoption(1) = Ypos1(DefSel)
Zoption(1) = Zpos1(DefSel)
OptDis(1) = SQRT((Xoption(1) - Xpos1(NonSel))**2 +
& (Yoption(1) - Ypos1(NonSel))**2 +
& (Zoption(1) - Zpos1(NonSel))**2)
IF(OptDis(1).LE.MinDist)THEN
OptEner(1) = (-Coef(i10) / MinDist - B(i10)) +
& (-Coef(i10) / RangeP - B(i10)) -
& (-Coef(i10) / EqValid - B(i10))
ELSEIF(OptDis(1).GT.MinDist.AND.OptDis(1).LE.EqValid)THEN
OptEner(1) = (-Coef(i10) / OptDis(1) - B(i10)) +
& (-Coef(i10) / RangeP - B(i10)) -
& (-Coef(i10) / EqValid - B(i10))
ELSEIF(Def2Dist.GT.EqValid)THEN
OptEner(1) = -Coef(i10) / RangeP - B(i10)
ENDIF

HopRate(1) = Diff*EXP(-(OptEner(1)-Energy)/(2*kBeV*Temp))

******* 2nd migration option:
Xoption(2) = Xpos1(DefSel)-a(1,1)
Yoption(2) = Ypos1(DefSel)
Zoption(2) = Zpos1(DefSel)
OptDis(2) = SQRT((Xoption(2) - Xpos1(NonSel))**2 +
& (Yoption(2) - Ypos1(NonSel))**2 +
& (Zoption(2) - Zpos1(NonSel))**2)

IF(OptDis(2).LE.MinDist)THEN
OptEner(2) = (-Coef(i10) / MinDist - B(i10)) +
& (-Coef(i10) / RangeP - B(i10)) -
& (-Coef(i10) / EqValid - B(i10))
ELSEIF(OptDis(2).GT.MinDist.AND.OptDis(2).LE.EqValid)THEN
OptEner(2) = (-Coef(i10) / OptDis(2) - B(i10)) +
& (-Coef(i10) / RangeP - B(i10)) -
& (-Coef(i10) / EqValid - B(i10))
ELSEIF(Def2Dist.GT.EqValid)THEN
OptEner(2) = -Coef(i10) / RangeP - B(i10)
ENDIF

HopRate(2) = Diff*EXP(-(OptEner(2)-Energy)/(2*kBeV*Temp))

******* 3rd migration option:
Xoption(3) = Xpos1(DefSel)+a(1,1)/2
Yoption(3) = Ypos1(DefSel)+a(1,1)*sqrt(3.)/2
Zoption(3) = Zpos1(DefSel)
OptDis(3) = SQRT((Xoption(3) - Xpos1(NonSel))**2 +
& (Yoption(3) - Ypos1(NonSel))**2 +
& (Zoption(3) - Zpos1(NonSel))**2)

IF(OptDis(3).LE.MinDist)THEN
OptEner(3) = (-Coef(i10) / MinDist - B(i10)) +
& (-Coef(i10) / RangeP - B(i10)) -
& (-Coef(i10) / EqValid - B(i10))
ELSEIF(OptDis(3).GT.MinDist.AND.OptDis(3).LE.EqValid)THEN
OptEner(3) = (-Coef(i10) / OptDis(3) - B(i10)) +
& (-Coef(i10) / RangeP - B(i10)) -
& (-Coef(i10) / EqValid - B(i10))
ELSEIF(Def2Dist.GT.EqValid)THEN
OptEner(3) = -Coef(i10) / RangeP - B(i10)
ENDIF

HopRate(3) = Diff*EXP(-(OptEner(3)-Energy)/(2*kBeV*Temp))

******* 4rd migration option:
Xoption(4) = Xpos1(DefSel)+a(1,1)/2
Yoption(4) = Ypos1(DefSel)-a(1,1)*sqrt(3.)/2
Zoption(4) = Zpos1(DefSel)
OptDis(4) = SQRT((Xoption(4) - Xpos1(NonSel))**2 +...
(Yoption(4) - Ypos1(NonSel))**2 +
& (Zoption(4) - Zpos1(NonSel))**2)

IF(OptDis(4).LE.MinDist)THEN
OptEner(4) = (-Coef(i10) / MinDist - B(i10)) +
& (-Coef(i10) / RangeP - B(i10)) -
& (-Coef(i10) / EqValid - B(i10))
ELSEIF(OptDis(4).GT.MinDist.AND.OptDis(4).LE.EqValid)THEN
OptEner(4) = (-Coef(i10) / OptDis(4) - B(i10)) +
& (-Coef(i10) / RangeP - B(i10)) -
& (-Coef(i10) / EqValid - B(i10))
ELSEIF(Def2Dist.GT.EqValid)THEN
OptEner(4) = -Coef(i10) / RangeP - B(i10)
ENDIF

HopRate(4) = Diff*EXP(-(OptEner(4)-Energy)/(2*kBeV*Temp))

****** 5th migration option:
Xoption(5) = Xpos1(DefSel)-a(1,1)/2
Yoption(5) = Ypos1(DefSel)+a(1,1)*sqrt(3.)/2
Zoption(5) = Zpos1(DefSel)
OptDis(5) = SQRT((Xoption(5) - Xpos1(NonSel))**2 +
& (Yoption(5) - Ypos1(NonSel))**2 +
& (Zoption(5) - Zpos1(NonSel))**2)

IF(OptDis(5).LE.MinDist)THEN
OptEner(5) = (-Coef(i10) / MinDist - B(i10)) +
& (-Coef(i10) / RangeP - B(i10)) -
& (-Coef(i10) / EqValid - B(i10))
ELSEIF(OptDis(5).GT.MinDist.AND.OptDis(5).LE.EqValid)THEN
OptEner(5) = (-Coef(i10) / OptDis(5) - B(i10)) +
& (-Coef(i10) / RangeP - B(i10)) -
& (-Coef(i10) / EqValid - B(i10))
ELSEIF(Def2Dist.GT.EqValid)THEN
OptEner(5) = -Coef(i10) / RangeP - B(i10)
ENDIF

HopRate(5) = Diff*EXP(-(OptEner(5)-Energy)/(2*kBeV*Temp))

****** 6th migration option:
Xoption(6) = Xpos1(DefSel)-a(1,1)/2
Yoption(6) = Ypos1(DefSel)-a(1,1)*sqrt(3.)/2
Zoption(6) = Zpos1(DefSel)
OptDis(6) = SQRT((Xoption(6) - Xpos1(NonSel))**2 +
& (Yoption(6) - Ypos1(NonSel))**2 +
& (Zoption(6) - Zpos1(NonSel))**2)
IF(OptDis(6).LE.MinDist)THEN
OptEner(6) = (-Coef(i10) / MinDist - B(i10)) +
& (-Coef(i10)/RangeP - B(i10)) -
& (-Coef(i10)/EqValid - B(i10))
ELSEIF(OptDis(6).GT.MinDist.AND.OptDis(6).LE.EqValid)THEN
OptEner(6) = (-Coef(i10) / OptDis(6) - B(i10)) +
& (-Coef(i10)/RangeP - B(i10)) -
& (-Coef(i10)/EqValid - B(i10))
ELSEIF(Def2Dist.GT.EqValid)THEN
OptEner(6) = -Coef(i10)/RangeP - B(i10)
ENDIF

HopRate(6) = Diff*EXP(-(OptEner(6)-Energy)/(2*kBeV*Temp))

******* 7th migration option:
yproduct = 2
IF(Znear.EQ.xC(3,1).OR.Znear.EQ.xC(3,2).OR.
& Znear.EQ.xC(3,3).OR.Znear.EQ.xC(3,4).OR.
& Znear.EQ.xSi(3,1).OR.Znear.EQ.xSi(3,2).OR.
& Znear.EQ.xSi(3,3).OR.Znear.EQ.xSi(3,4))THEN
ysign = -1
ELSE
ysign = 1
END IF

Xoption(7) = Xpos1(DefSel)
Yoption(7) = Ypos1(DefSel) + ysign*y1*yproduct
Zoption(7) = Zpos1(DefSel) + z1
OptDis(7) = SQRT((Xoption(7) - Xpos1(NonSel))**2 +
& (Yoption(7) - Ypos1(NonSel))**2 +
& (Zoption(7) - Zpos1(NonSel))**2)

IF(OptDis(7).LE.MinDist)THEN
OptEner(7) = (-Coef(i10) / MinDist - B(i10)) +
& (-Coef(i10)/RangeP - B(i10)) -
& (-Coef(i10)/EqValid - B(i10))
ELSEIF(OptDis(7).GT.MinDist.AND.OptDis(7).LE.EqValid)THEN
OptEner(7) = (-Coef(i10) / OptDis(7) - B(i10)) +
& (-Coef(i10)/RangeP - B(i10)) -
& (-Coef(i10)/EqValid - B(i10))
ELSEIF(Def2Dist.GT.EqValid)THEN
OptEner(7) = -Coef(i10)/RangeP - B(i10)
ENDIF

HopRate(7) = Diff*EXP(-(OptEner(7)-Energy)/(2*kBeV*Temp))
8th migration option:

\[ y_{\text{product}} = 2 \]

\[
\text{IF}(Z_{\text{near}}.EQ.\, xc(3,1).\, OR.\, Z_{\text{near}}.EQ.\, xc(3,2).\, OR. \\
& \quad Z_{\text{near}}.EQ.\, xc(3,7).\, OR.\, Z_{\text{near}}.EQ.\, xc(3,8).\, OR. \\
& \quad Z_{\text{near}}.EQ.\, xSi(3,1).\, OR.\, Z_{\text{near}}.EQ.\, xSi(3,2).\, OR. \\
& \quad Z_{\text{near}}.EQ.\, xSi(3,7).\, OR.\, Z_{\text{near}}.EQ.\, xSi(3,8)) \text{THEN} \\
\]

\[ y_{\text{sign}} = 1 \]

ELSE

\[ y_{\text{sign}} = -1 \]

END IF

\[ X_{\text{option}}(8) = X_{\text{pos1}}(\text{DefSel}) \]

\[ Y_{\text{option}}(8) = Y_{\text{pos1}}(\text{DefSel}) + y_{\text{sign}} \cdot y_{\text{product}} \]

\[ Z_{\text{option}}(8) = Z_{\text{pos1}}(\text{DefSel}) + z_{2} \]

\[ \text{OptDis}(8) = \sqrt{X_{\text{option}}(8) - X_{\text{pos1}}(\text{NonSel})^2 + \\
& \quad Y_{\text{option}}(8) - Y_{\text{pos1}}(\text{NonSel})^2 + \\
& \quad Z_{\text{option}}(8) - Z_{\text{pos1}}(\text{NonSel})^2} \]

\[
\text{IF}(\text{OptDis}(8).LE.\, \text{MinDist}) \text{THEN} \\
\text{OptEner}(8) = (-\text{Coef}(i10) / \, \text{MinDist} - \, B(i10)) + \\
& \quad (-\text{Coef}(i10) / \, \text{RangeP} - \, B(i10)) - \\
& \quad (-\text{Coef}(i10) / \, \text{EqValid} - \, B(i10)) \]

ELSEIF(\text{OptDis}(8).GT.\, \text{MinDist. AND. OptDis}(8).LE.\, \text{EqValid}) \text{THEN} \\
\text{OptEner}(8) = (-\text{Coef}(i10) / \, \text{OptDis}(8) - \, B(i10)) + \\
& \quad (-\text{Coef}(i10) / \, \text{RangeP} - \, B(i10)) - \\
& \quad (-\text{Coef}(i10) / \, \text{EqValid} - \, B(i10)) \]

ELSEIF(\text{Def2Dist.GT. EqValid}) \text{THEN} \\
\text{OptEner}(8) = -\text{Coef}(i10) / \, \text{RangeP} - \, B(i10) \]

ENDIF

\[ \text{HopRate}(8) = \text{Diff} \cdot \exp\left(\frac{-\text{OptEner}(8) - \text{Energy}}{2 \cdot k_{\text{BeV}} \cdot \text{Temp}}\right) \]

9th migration option:

\[ y_{\text{product}} = 1 \]

\[
\text{IF}(Z_{\text{near}}.EQ.\, xc(3,1).\, OR.\, Z_{\text{near}}.EQ.\, xc(3,2).\, OR. \\
& \quad Z_{\text{near}}.EQ.\, xc(3,3).\, OR.\, Z_{\text{near}}.EQ.\, xc(3,4).\, OR. \\
& \quad Z_{\text{near}}.EQ.\, xSi(3,1).\, OR.\, Z_{\text{near}}.EQ.\, xSi(3,2).\, OR. \\
& \quad Z_{\text{near}}.EQ.\, xSi(3,3).\, OR.\, Z_{\text{near}}.EQ.\, xSi(3,4)) \text{THEN} \\
\]

\[ y_{\text{sign}} = 1 \]

ELSE

\[ y_{\text{sign}} = -1 \]

END IF

\[ X_{\text{option}}(9) = X_{\text{pos1}}(\text{DefSel}) - \, x_{1} \]

\[ Y_{\text{option}}(9) = Y_{\text{pos1}}(\text{DefSel}) + \, y_{1} \cdot y_{\text{product}} \cdot y_{\text{sign}} \]
Z\text{option}(9) = Z\text{pos}_1(\text{DefSel}) + z_1
Opt\text{Dis}(9) = \sqrt{\left( X\text{option}(9) - X\text{pos}_1(\text{NonSel}) \right)^2 +}
\left( Y\text{option}(9) - Y\text{pos}_1(\text{NonSel}) \right)^2 +
\left( Z\text{option}(9) - Z\text{pos}_1(\text{NonSel}) \right)^2
\]

IF(Opt\text{Dis}(9).LE.Min\text{Dist})THEN
Opt\text{Ener}(9) = (-\text{Coef}(i10) / \text{MinDist} - B(i10)) +
& (-\text{Coef}(i10) / \text{RangeP} - B(i10)) -
& (-\text{Coef}(i10) / \text{EqValid} - B(i10))
ELSEIF(Opt\text{Dis}(9).GT.Min\text{Dist}.AND.Opt\text{Dis}(9).LE.Eq\text{Valid})THEN
Opt\text{Ener}(9) = (-\text{Coef}(i10) / \text{Opt\text{Dis}(9)} - B(i10)) +
& (-\text{Coef}(i10) / \text{RangeP} - B(i10)) -
& (-\text{Coef}(i10) / \text{EqValid} - B(i10))
ELSEIF(Def2\text{Dist}.GT.Eq\text{Valid})THEN
Opt\text{Ener}(9) = -\text{Coef}(i10) / \text{RangeP} - B(i10)
ENDIF

Hop\text{Rate}(9) = \text{Diff} \times \text{EXP}\left(\frac{-(Opt\text{Ener}(9) - \text{Energy})}{2 \times k\text{BeV} \times \text{Temp}}\right)

******* 10th migration option:
y\text{product} = 1
\]
IF(Z\text{near}.EQ.x\text{C}(3,1).OR.Z\text{near}.EQ.x\text{C}(3,2).OR.
& Z\text{near}.EQ.x\text{C}(3,7).OR.Z\text{near}.EQ.x\text{C}(3,8).OR.
& Z\text{near}.EQ.x\text{Si}(3,1).OR.Z\text{near}.EQ.x\text{Si}(3,2).OR.
& Z\text{near}.EQ.x\text{Si}(3,7).OR.Z\text{near}.EQ.x\text{Si}(3,8))THEN
ysign = -1
ELSE
ysign = 1
END IF

X\text{option}(10) = X\text{pos}_1(\text{DefSel}) - x_1
Y\text{option}(10) = Y\text{pos}_1(\text{DefSel}) + y_1*\text{y\text{product}*ysign}
Z\text{option}(10) = Z\text{pos}_1(\text{DefSel}) + z_2
Opt\text{Dis}(10) = \sqrt{\left( X\text{option}(10) - X\text{pos}_1(\text{NonSel}) \right)^2 +}
\left( Y\text{option}(10) - Y\text{pos}_1(\text{NonSel}) \right)^2 +
\left( Z\text{option}(10) - Z\text{pos}_1(\text{NonSel}) \right)^2
\]

IF(Opt\text{Dis}(10).LE.Min\text{Dist})THEN
Opt\text{Ener}(10) = (-\text{Coef}(i10) / \text{MinDist} - B(i10)) +
& (-\text{Coef}(i10) / \text{RangeP} - B(i10)) -
& (-\text{Coef}(i10) / \text{EqValid} - B(i10))
ELSEIF(Opt\text{Dis}(10).GT.Min\text{Dist}.AND.Opt\text{Dis}(10).LE.Eq\text{Valid})THEN
Opt\text{Ener}(10) = (-\text{Coef}(i10) / \text{Opt\text{Dis}(10)} - B(i10)) +
& (-\text{Coef}(i10) / \text{RangeP} - B(i10)) -
& (-\text{Coef}(i10) / \text{EqValid} - B(i10))
ELSEIF(Def2\text{Dist}.GT.Eq\text{Valid})THEN
188
OptEner(10) = -Coef(i10) / RangeP - B(i10)
ENDIF

HopRate(10) = Diff*EXP(-(OptEner(10)-Energy)/(2*kBeV*Temp))

***** 11th migration option:
    yproduct = 1
    IF(Znear.EQ.xC(3,1).OR.Znear.EQ.xC(3,2).OR.
      & Znear.EQ.xC(3,3).OR.Znear.EQ.xC(3,4).OR.
      & Znear.EQ.xSi(3,1).OR.Znear.EQ.xSi(3,2).OR.
      & Znear.EQ.xSi(3,3).OR.Znear.EQ.xSi(3,4))THEN
      ysign = 1
    ELSE
      ysign = -1
    END IF

    Xoption(11) = Xpos1(DefSel) + x1
    Yoption(11) = Ypos1(DefSel) + y1*yproduct*ysign
    Zoption(11) = Zpos1(DefSel) + z1
    OptDis(11) = SQRT((Xoption(11) - Xpos1(NonSel))**2 +
                      (Yoption(11) - Ypos1(NonSel))**2 +
                      (Zoption(11) - Zpos1(NonSel))**2)
    IF(OptDis(11).LE.MinDist)THEN
      OptEner(11) = (-Coef(i10) / MinDist - B(i10)) +
      & (-Coef(i10) / RangeP - B(i10)) -
      & (-Coef(i10) / EqValid - B(i10))
    ELSEIF(OptDis(11).GT.MinDist.AND.OptDis(11).LE.EqValid)THEN
      OptEner(11) = (-Coef(i10) / OptDis(11) - B(i10)) +
      & (-Coef(i10) / RangeP - B(i10)) -
      & (-Coef(i10) / EqValid - B(i10))
    ELSEIF(Def2Dist.GT.EqValid)THEN
      OptEner(11) = -Coef(i10) / RangeP - B(i10)
    ENDIF

    HopRate(11) = Diff*EXP(-(OptEner(11)-Energy)/(2*kBeV*Temp))

***** 12th migration option:
    yproduct = 1
    IF(Znear.EQ.xC(3,1).OR.Znear.EQ.xC(3,2).OR.
      & Znear.EQ.xC(3,7).OR.Znear.EQ.xC(3,8).OR.
      & Znear.EQ.xSi(3,1).OR.Znear.EQ.xSi(3,2).OR.
      & Znear.EQ.xSi(3,7).OR.Znear.EQ.xSi(3,8))THEN
      ysign = -1
    ELSE
      ysign = 1

189
END IF

Xoption(12) = Xpos1(DefSel) + x1
Yoption(12) = Ypos1(DefSel) + y1*yproduct*ysign
Zoption(12) = Zpos1(DefSel) + z2
OptDis(12) = SQRT((Xoption(12) - Xpos1(NonSel))**2 +
& (Yoption(12) - Ypos1(NonSel))**2 +
& (Zoption(12) - Zpos1(NonSel))**2)

IF(OptDis(12).LE.MinDist)THEN
  OptEner(12) = (-Coef(i10) / MinDist - B(i10)) +
& (-Coef(i10) / RangeP - B(i10)) -
& (-Coef(i10) / EqValid - B(i10))
ELSEIF(OptDis(12).GT.MinDist.AND.OptDis(12).LE.EqValid)THEN
  OptEner(12) = (-Coef(i10) / OptDis(12) - B(i10)) +
& (-Coef(i10) / RangeP - B(i10)) -
& (-Coef(i10) / EqValid - B(i10))
ELSEIF(Def2Dist.GT.EqValid)THEN
  OptEner(12) = -Coef(i10) / RangeP - B(i10)
ENDIF

HopRate(12) = Diff*EXP(-(OptEner(12)-Energy)/(2*kBeV*Temp))

********************************************************************************

xt(1) = 0
xt(2) = HopRate(1)
do 51 i = 3,13
  xt(i) = xt(i-1) + HopRate(i-1)
51         Continue

AngSel = ran0(seed)
********************************************************************************

* Since second hop is dominant, only that is activated.
* However, the code can easily be modified for more complex situations.

IF(AngSel.GE.xt(1)/xt(13).AND.AngSel.LT.xt(2)/xt(13))THEN
  IC1 = IC1 + 1
  Hop = 1
  Xpos1(DefSel)=Xpos1(DefSel)+a(1,1)
  Ypos1(DefSel)=Ypos1(DefSel)
  Zpos1(DefSel)=Zpos1(DefSel)

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ELSEIF(AngSel.GE.xt(2)/xt(13).AND.AngSel.LT.xt(3)/xt(13))THEN

    IC2 = IC2 + 1
    Hop = 2

    Xpos1(DefSel)=Xpos1(DefSel)-a(1,1)
    Ypos1(DefSel)=Ypos1(DefSel)
    Zpos1(DefSel)=Zpos1(DefSel)

ELSEIF(AngSel.GE.xt(3)/xt(13).AND.AngSel.lt.xt(4)/xt(13))THEN

    IC3 = IC3 + 1
    Hop = 3

    Xpos1(DefSel)=Xpos1(DefSel)+a(1,1)/2
    Ypos1(DefSel)=Ypos1(DefSel)+a(1,1)*sqrt(3.)/2
    Zpos1(DefSel)=Zpos1(DefSel)

ELSEIF(AngSel.GE.xt(4)/xt(13).AND.AngSel.lt.xt(5)/xt(13))THEN

    IC4 = IC4 + 1
    Hop = 4

    Xpos1(DefSel)=Xpos1(DefSel)+a(1,1)/2
    Ypos1(DefSel)=Ypos1(DefSel)-a(1,1)*sqrt(3.)/2
    Zpos1(DefSel)=Zpos1(DefSel)

ELSEIF(AngSel.GE.xt(5)/xt(13).AND.AngSel.lt.xt(6)/xt(13))THEN

    IC5 = IC5 + 1
    Hop = 5

    Xpos1(DefSel)=Xpos1(DefSel)-a(1,1)/2
    Ypos1(DefSel)=Ypos1(DefSel)+a(1,1)*sqrt(3.)/2
    Zpos1(DefSel)=Zpos1(DefSel)

ELSEIF(AngSel.GE.xt(6)/xt(13).AND.AngSel.lt.xt(7)/xt(13))THEN

    IC6 = IC6 + 1
    Hop = 6

    Xpos1(DefSel)=Xpos1(DefSel)-a(1,1)/2
    Ypos1(DefSel)=Ypos1(DefSel)-a(1,1)*sqrt(3.)/2
    Zpos1(DefSel)=Zpos1(DefSel)

ELSEIF(AngSel.GE.xt(7)/xt(13).AND.AngSel.lt.xt(8)/xt(13))THEN

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IC7 = IC7 + 1
Hop = 7

yproduct = 2
IF(Znear.EQ.xC(3,1).OR.Znear.EQ.xC(3,2).OR.
& Znear.EQ.xC(3,3).OR.Znear.EQ.xC(3,4).OR.
& Znear.EQ.xSi(3,1).OR.Znear.EQ.xSi(3,2).OR.
& Znear.EQ.xSi(3,3).OR.Znear.EQ.xSi(3,4))THEN
ysign = -1
ELSE
ysign = 1
END IF

Xpos1(DefSel)=Xpos1(DefSel)
Ypos1(DefSel)=Ypos1(DefSel)+y1*ysign*yproduct
Zpos1(DefSel)=Zpos1(DefSel)+z1

ELSEIF(AngSel.GE.xt(8)/xt(13).AND.AngSel.lt.xt(9)/xt(13))THEN

IC8 = IC8 + 1
Hop = 8

yproduct = 2
IF(Znear.EQ.xC(3,1).OR.Znear.EQ.xC(3,2).OR.
& Znear.EQ.xC(3,7).OR.Znear.EQ.xC(3,8).OR.
& Znear.EQ.xSi(3,1).OR.Znear.EQ.xSi(3,2).OR.
& Znear.EQ.xSi(3,7).OR.Znear.EQ.xSi(3,8))THEN
ysign = 1
ELSE
ysign = -1
END IF

Xpos1(DefSel)=Xpos1(DefSel)
Ypos1(DefSel)=Ypos1(DefSel)+y1*ysign*yproduct
Zpos1(DefSel)=Zpos1(DefSel)+z1

ELSEIF(AngSel.GE.xt(9)/xt(13).AND.AngSel.LT.xt(10)/xt(13))THEN

IC9 = IC9 + 1
Hop = 9

yproduct = 1
IF(Znear.EQ.xC(3,1).OR.Znear.EQ.xC(3,2).OR.
& Znear.EQ.xC(3,3).OR.Znear.EQ.xC(3,4).OR.
& Znear.EQ.xSi(3,1).OR.Znear.EQ.xSi(3,2).OR.
& Znear.EQ.xSi(3,3).OR.Znear.EQ.xSi(3,4)) THEN
  ysign = 1
  ELSE
  ysign = -1
  END IF

  Xpos1(DefSel)=Xpos1(DefSel)-x1
  Ypos1(DefSel)=Ypos1(DefSel)+y1*ysign*yproduct
  Zpos1(DefSel)=Zpos1(DefSel)+z1

ELSEIF(AngSel.GE.xt(10)/xt(13).AND.AngSel.LT(xt(11)/xt(13))) THEN
  IC10 = IC10 + 1
  Hop = 10

  yproduct = 1
  IF(Znear.EQ.xC(3,1).OR.Znear.EQ.xC(3,2).OR.
    & Znear.EQ.xC(3,7).OR.Znear.EQ.xC(3,8).OR.
    & Znear.EQ.xSi(3,1).OR.Znear.EQ.xSi(3,2).OR.
    & Znear.EQ.xSi(3,7).OR.Znear.EQ.xSi(3,8)) THEN
    ysign = -1
    ELSE
    ysign = 1
    END IF

  Xpos1(DefSel)=Xpos1(DefSel)-x1
  Ypos1(DefSel)=Ypos1(DefSel)+y1*ysign*yproduct
  Zpos1(DefSel)=Zpos1(DefSel)+z2

ELSEIF(AngSel.GE.xt(11)/xt(13).AND.AngSel.LT(xt(12)/xt(13))) THEN
  IC11 = IC11 + 1
  Hop = 11

  yproduct = 1
  IF(Znear.EQ.xC(3,1).OR.Znear.EQ.xC(3,2).OR.
    & Znear.EQ.xC(3,3).OR.Znear.EQ.xC(3,4).OR.
    & Znear.EQ.xSi(3,1).OR.Znear.EQ.xSi(3,2).OR.
    & Znear.EQ.xSi(3,3).OR.Znear.EQ.xSi(3,4)) THEN
    ysign = 1
    ELSE
    ysign = -1
    END IF

  Xpos1(DefSel)=Xpos1(DefSel)+x1
  Ypos1(DefSel)=Ypos1(DefSel)+y1*ysign*yproduct

193
\[ Z_{pos1}(DefSel) = Z_{pos1}(DefSel) + z1 \]

ELSEIF (AngSel \( \geq \) xt(12)/xt(13) \( \text{AND} \) AngSel \( \leq \) xt(13)/xt(13)) THEN

\[ IC12 = IC12 + 1 \]
\[ \text{Hop} = 12 \]
\[ \text{yp} = 1 \]
\[ \text{IF} (Z_{near} \text{EQ} xC(3,1) \text{OR} Z_{near} \text{EQ} xC(3,2) \text{OR} \]
\[ \quad \text{AND} \]
\[ \quad Z_{near} \text{EQ} xC(3,7) \text{OR} Z_{near} \text{EQ} xC(3,8) \text{OR} \]
\[ \quad \text{AND} \]
\[ \quad Z_{near} \text{EQ} xSi(3,1) \text{OR} Z_{near} \text{EQ} xSi(3,2) \text{OR} \]
\[ \quad \text{AND} \]
\[ \quad Z_{near} \text{EQ} xSi(3,7) \text{OR} Z_{near} \text{EQ} xSi(3,8)) \text{THEN} \]
\[ \text{ys} = -1 \]
ELSE
\[ \text{ys} = 1 \]
ENDIF

\[ X_{pos1}(DefSel) = X_{pos1}(DefSel) + x1 \]
\[ Y_{pos1}(DefSel) = Y_{pos1}(DefSel) + y1 \times \text{ys} \times \text{yp} \]
\[ Z_{pos1}(DefSel) = Z_{pos1}(DefSel) + z2 \]

ENDIF

\[ X_{pos1}(NonSel) = X_{pos1}(NonSel) \]
\[ Y_{pos1}(NonSel) = Y_{pos1}(NonSel) \]
\[ Z_{pos1}(NonSel) = Z_{pos1}(NonSel) \]

WRITE (*,*) j, X_{pos1}(DefSel), Y_{pos1}(DefSel), Z_{pos1}(DefSel)

* To find the real time
* \( R# \) is dissociation and migration rate for each defect
*****

Do 53 i = 1, 12
\[ \text{IF} (i \text{EQ} \text{Hop}) \text{THEN} \]
\[ \text{Rate} = \text{HopRate}(i) \]
ELSE
ENDIF
53 CONTINUE

*****

\[ \text{TotRate} = \text{Digit}(i10) \times \text{Rate} \times 1E-12 \]

65 \[ \text{U} = \text{ran0(seed)} \]
If(U.EQ.0)THEN
  GOTO 65
ELSE
END IF

IF(C.EQ.0)THEN
  RealTime = RealTime - LOG(U)/TotRate
ELSE
  RealTime = RealTime
ENDIF

59 CONTINUE

***********************
c    omega is the vlume of the box in Ang^3
  omega=aX*bY*cZ
  kxy = omega * 1E-24 / ((RealTime/counter) * 1E-12)

write(*,*)'----------------------'
write(*,*)'kxy, RealTime, omega, counter, Digit(i10), Diff'
write(*,*)'----------------------'

IF(Migr(i10).EQ.3)THEN
  Diffu  = D0C*(EXP(-EmVC0/(kBeV*Temp)))
ELSEIF(Migr(i10).EQ.4)THEN
  Diffu  = D0Si*(EXP(-EmVSi2N/(kBeV*Temp)))
ELSEIF(Migr(i10).EQ.5)THEN
  Diffu  = D0C*(EXP(-EmIC1N/(kBeV*Temp)))
ELSEIF(Migr(i10).EQ.6)THEN
  Diffu  = D0Si*(EXP(-EmISi0/(kBeV*Temp)))
ELSE
ENDIF

c    axy is in nm
  axy = 1E7 * kxy / (4*3.14159265*Digit(i10)*Diffu)

write(*,*)'----------------------'
write(*,*)'Capture_Radius(nm), counter, Temp, diffu'
write(*,*) axy, counter, Temp, diffu

IC=counter+IC1+IC2+IC3+IC4+IC5+IC6+IC7+IC8+IC9+IC10+IC11+IC12

c    write(*,*)'----------------------'

c    write(*,*)'IC1, IC2, IC3, IC4, IC5, IC6'
c    write(*,*) IC1, IC2, IC3, IC4, IC5, IC6
WRITE(60,*) Temp, axy, counter, IC, EqValid

Temp = Temp + 50
RealTime = 0

56 CONTINUE
58 CONTINUE
c CLOSE(UNIT=30)
c CLOSE(UNIT=40)
c CLOSE(UNIT=50)
CLOSE(UNIT=60)
STOP
END

*-------------------------------------------------------------
Subroutine PBCImp(Xpos1,YPos1,ZPos1,j,aX,bY,cZ,NonSel,
& DefSel,iPBC)
*-------------------------------------------------------------
* Maximum # of Hops = Hopmax
parameter(Hopmax = 2)
INTEGER j,NonSel,DefSel,iPBC
DOUBLE PRECISION Xpos1(Hopmax),
& Ypos1(Hopmax),Zpos1(Hopmax),
& aX,bY,cZ,Xpos27(27),Ypos27(27),Zpos27(27),PBC,PBCDis(27),
& xPBC(27),yPBC(27),zPBC(27)
Xpos27(1) = Xpos1(NonSel)
Ypos27(1) = Ypos1(NonSel)
Zpos27(1) = Zpos1(NonSel)
Xpos27(2) = Xpos1(NonSel)+aX
Ypos27(2) = Ypos1(NonSel)
Zpos27(2) = Zpos1(NonSel)
Xpos27(3) = Xpos1(NonSel)
Ypos27(3) = Ypos1(NonSel)+bY
Zpos27(3) = Zpos1(NonSel)
Xpos27(4) = Xpos1(NonSel)
Ypos27(4) = Ypos1(NonSel)
Zpos27(4) = Zpos1(NonSel)+cZ
Xpos27(5) = Xpos1(NonSel)-aX
Ypos27(5) = Ypos1(NonSel)
Zpos27(5) = Zpos1(NonSel)
Xpos27(6) = Xpos1(NonSel)
Ypos27(6) = Ypos1(NonSel)-bY
Zpos27(6) = Zpos1(NonSel)
Xpos27(7) = Xpos1(NonSel)
Ypos27(7) = Ypos1(NonSel)
Zpos27(7) = Zpos1(NonSel)-cZ
Xpos27(8) = Xpos1(NonSel)+aX
Ypos27(8) = Ypos1(NonSel)+by
Zpos27(8) = Zpos1(NonSel)
Xpos27(9) = Xpos1(NonSel)+aX
Ypos27(9) = Ypos1(NonSel)
Zpos27(9) = Zpos1(NonSel)+cZ
Xpos27(10) = Xpos1(NonSel)
Ypos27(10) = Ypos1(NonSel)+bY
Zpos27(10) = Zpos1(NonSel)+cZ
Xpos27(11) = Xpos1(NonSel)-aX
Ypos27(11) = Ypos1(NonSel)-by
Zpos27(11) = Zpos1(NonSel)
Xpos27(12) = Xpos1(NonSel)-aX
Ypos27(12) = Ypos1(NonSel)
Zpos27(12) = Zpos1(NonSel)-cZ
Xpos27(13) = Xpos1(NonSel)
Ypos27(13) = Ypos1(NonSel)-bY
Zpos27(13) = Zpos1(NonSel)-cZ
Xpos27(14) = Xpos1(NonSel)+aX
Ypos27(14) = Ypos1(NonSel)-by
Zpos27(14) = Zpos1(NonSel)
Xpos27(15) = Xpos1(NonSel)+aX
Ypos27(15) = Ypos1(NonSel)
Zpos27(15) = Zpos1(NonSel)-cZ
Xpos27(16) = Xpos1(NonSel)
Ypos27(16) = Ypos1(NonSel)+bY
Zpos27(16) = Zpos1(NonSel)-cZ
Xpos27(17) = Xpos1(NonSel)-aX
Ypos27(17) = Ypos1(NonSel)+by
Zpos27(17) = Zpos1(NonSel)
Xpos27(18) = Xpos1(NonSel)-aX
Ypos27(18) = Ypos1(NonSel)
Zpos27(18) = Zpos1(NonSel)+cZ
Xpos27(19) = Xpos1(NonSel)
Ypos27(19) = Ypos1(NonSel)-bY
Zpos27(19) = Zpos1(NonSel)+cZ
Xpos27(20) = Xpos1(NonSel)+aX
Ypos27(20) = Ypos1(NonSel)+by
Zpos27(20) = Zpos1(NonSel)+cZ
Xpos27(21) = Xpos1(NonSel)-aX  
Ypos27(21) = Ypos1(NonSel)+bY  
Zpos27(21) = Zpos1(NonSel)+cZ  
Xpos27(22) = Xpos1(NonSel)+aX  
Ypos27(22) = Ypos1(NonSel)-bY  
Zpos27(22) = Zpos1(NonSel)+cZ  
Xpos27(23) = Xpos1(NonSel)+aX  
Ypos27(23) = Ypos1(NonSel)+bY  
Zpos27(23) = Zpos1(NonSel)-cZ  
Xpos27(24) = Xpos1(NonSel)-aX  
Ypos27(24) = Ypos1(NonSel)-bY  
Zpos27(24) = Zpos1(NonSel)+cZ  
Xpos27(25) = Xpos1(NonSel)-aX  
Ypos27(25) = Ypos1(NonSel)+bY  
Zpos27(25) = Zpos1(NonSel)-cZ  
Xpos27(26) = Xpos1(NonSel)+aX  
Ypos27(26) = Ypos1(NonSel)-bY  
Zpos27(26) = Zpos1(NonSel)-cZ  
Xpos27(27) = Xpos1(NonSel)+aX  
Ypos27(27) = Ypos1(NonSel)-bY  
Zpos27(27) = Zpos1(NonSel)-cZ

DO 54 i = 1,27
  xPBC(i) = Xpos27(i)-Xpos1(DefSel)
  yPBC(i) = Ypos27(i)-Ypos1(DefSel)
  zPBC(i) = Zpos27(i)-Zpos1(DefSel)
  PBCDis(i)=SQRT(xPBC(i)**2+yPBC(i)**2+zPBC(i)**2)
 54        CONTINUE

PBC=sqrt(aX**2+bY**2+cZ**2)
DO 55 i = 1,27
IF(PBCDis(i).LT.PBC)THEN
  PBC=PBCDis(i)
iPBC=i
ELSE
  ENDIF

55        CONTINUE
Xpos1(NonSel) = Xpos27(iPBC)
Ypos1(NonSel) = Ypos27(iPBC)
Zpos1(NonSel) = Zpos27(iPBC)
RETURN
END

*-------------------------------------------------------------
Subroutine Sivacancy(a,xSi,ZDefect,x1,y1,z1,z2,Znear)
*-------------------------------------------------------------
* This subroutine is to choose the nearest lattice position
* to a Si-vacancy. This determines the direction of the migration.

198
character*80 string, line
dimension xSi(3,8),a(3,3)
REAL ZDefect,Zb,a
Zb = ABS(ZDefect/a(3,3) - INT(ZDefect/a(3,3)))
ZAtom = 1.
Do 200 i1 = 1,8
ZAtom1 = ABS(Zb - xSi(3,i1))
IF(ZAtom1.LT.ZAtom)THEN
ZAtom = ZAtom1
Znear = xSi(3,i1)
ELSE
END IF
200 CONTINUE
IF(Znear.EQ.xSi(3,1).OR.Znear.EQ.xSi(3,2))THEN
z2 = -(2.50146+2.52154)/2
z1 = (2.50146+2.52154)/2
ELSEIF(Znear.EQ.xSi(3,3).OR.Znear.EQ.xSi(3,4))THEN
z2 = (2.50146+2.52154)/2
z1 = -(2.50146+2.52154)/2
ELSEIF(Znear.EQ.xSi(3,5).OR.Znear.EQ.xSi(3,6))THEN
z2 = -(2.50146+2.52154)/2
z1 = (2.50146+2.52154)/2
ELSEIF(Znear.EQ.xSi(3,7).OR.Znear.EQ.xSi(3,8))THEN
z2 = (2.50146+2.52154)/2
z1 = -(2.50146+2.52154)/2
ELSE
END IF
x1 = 1.539002
y1 = 0.888543
RETURN
END

Subroutine Cvacancy(a,xC,ZDefect,x1,y1,z1,z2,Znear)
*-------------------------------------------------------------
* This subroutine is to choose the nearest lattice position
* to a C-vacancy. This determines the direction of the migration.
*-------------------------------------------------------------
character*80 string, line
dimension xC(3,8),a(3,3)
REAL ZDefect,Zb,a
Zb = ABS(ZDefect/a(3,3) - INT(ZDefect/a(3,3)))
ZAtom = 1.
Do 200 i1 = 1,8
ZAtom1 = ABS(Zb - xC(3,i1))
IF(ZAtom1.LT.ZAtom)THEN
ZAtom = ZAtom1
Znear = xC(3,i1)
ELSE
END IF
200 CONTINUE
IF(Znear.EQ.xC(3,1).OR.Znear.EQ.xC(3,2))THEN
z2 = -(2.50146+2.52154)/2
z1 = (2.50146+2.52154)/2
ELSEIF(Znear.EQ.xC(3,3).OR.Znear.EQ.xC(3,4))THEN
z2 = (2.50146+2.52154)/2
z1 = -(2.50146+2.52154)/2
ELSEIF(Znear.EQ.xC(3,5).OR.Znear.EQ.xC(3,6))THEN
z2 = -(2.50146+2.52154)/2
z1 = (2.50146+2.52154)/2
ELSEIF(Znear.EQ.xC(3,7).OR.Znear.EQ.xC(3,8))THEN
z2 = (2.50146+2.52154)/2
z1 = -(2.50146+2.52154)/2
ELSE
END IF
x1 = 1.539002
y1 = 0.888543
RETURN
END
Znear = xC(3,i1)
ELSE
END IF
200       CONTINUE
IF(Znear.EQ.xC(3,1).OR.Znear.EQ.xC(3,2))THEN
z1 = -(2.50146+2.52154)/2
z2 =  (2.50146+2.52154)/2
ELSEIF(Znear.EQ.xC(3,3).OR.Znear.EQ.xC(3,4))THEN
z1 =  (2.50146+2.52154)/2
z2 = -(2.50146+2.52154)/2
ELSEIF(Znear.EQ.xC(3,5).OR.Znear.EQ.xC(3,6))THEN
z1 = -(2.50146+2.52154)/2
z2 =  (2.50146+2.52154)/2
ELSEIF(Znear.EQ.xC(3,7).OR.Znear.EQ.xC(3,8))THEN
z1 =  (2.50146+2.52154)/2
z2 = -(2.50146+2.52154)/2
ELSE
END IF
x1 = 1.539002
y1 = 0.888543
RETURN
END

*-------------------------------------------------------------
Subroutine Interstitial(a,xC,xSi,ZDefect,x1,y1,z1,z2,Znear)
*-------------------------------------------------------------

*         This subroutine is to choose the nearest lattice position*
*         to an Interstitial. This determines the direction of the migration.*
* character*80 string, line
* dimension xC(3,8),xSi(3,8),a(3,3)
REAL ZDefect,Zb,a
Zb = ABS(ZDefect/a(3,3) - INT(ZDefect/a(3,3)))
ZAtom = 1.
Do 201 i1 = 1,8
ZAtom1 = ABS(Zb - xC(3,i1))
IF(ZAtom1.LT.ZAtom)THEN
ZAtom = ZAtom1
Znear = xC(3,i1)
ELSE
END IF
201       CONTINUE
Do 202 i2 = 1,8
ZAtom1 = ABS(Zb - xSi(3,i2))
IF(ZAtom1.LT.ZAtom)THEN
ZAtom = ZAtom1
Znear = xSi(3,i2)
202
ELSE
END IF
202 CONTINUE
IF(Znear.EQ.xC(3,1).OR.Znear.EQ.xC(3,2))THEN
  z1 = -(2.50146+2.52154)/2
  z2 = (2.50146+2.52154)/2
ELSEIF(Znear.EQ.xC(3,3).OR.Znear.EQ.xC(3,4))THEN
  z1 = (2.50146+2.52154)/2
  z2 = -(2.50146+2.52154)/2
ELSEIF(Znear.EQ.xC(3,5).OR.Znear.EQ.xC(3,6))THEN
  z1 = -(2.50146+2.52154)/2
  z2 = (2.50146+2.52154)/2
ELSEIF(Znear.EQ.xC(3,7).OR.Znear.EQ.xC(3,8))THEN
  z1 = (2.50146+2.52154)/2
  z2 = -(2.50146+2.52154)/2
ELSEIF(Znear.EQ.xSi(3,1).OR.Znear.EQ.xSi(3,2))THEN
  z2 = -(2.50146+2.52154)/2
  z1 = (2.50146+2.52154)/2
ELSEIF(Znear.EQ.xSi(3,3).OR.Znear.EQ.xSi(3,4))THEN
  z2 = (2.50146+2.52154)/2
  z1 = -(2.50146+2.52154)/2
ELSEIF(Znear.EQ.xSi(3,5).OR.Znear.EQ.xSi(3,6))THEN
  z2 = -(2.50146+2.52154)/2
  z1 = (2.50146+2.52154)/2
ELSEIF(Znear.EQ.xSi(3,7).OR.Znear.EQ.xSi(3,8))THEN
  z2 = (2.50146+2.52154)/2
  z1 = -(2.50146+2.52154)/2
ELSE
  END IF
  x1 = 1.539002
  y1 = 0.888543
  RETURN
END

*-------------------------------------------------------------
DOUBLE PRECISION function ran0(seed)
*-------------------------------------------------------------
INTEGER*4 A,P,seed,B15,B16,XHI,XALO,LEFTLO,FHI,K
PARAMETER (A=16807)
PARAMETER (B15=32768)
PARAMETER (B16=65536)
PARAMETER (P=2147483647)
XHI=seed/B16
XALO=(seed-XHI*B16)*A
LEFTLO=XALO/B16
FHI=XHI*A+LEFTLO
K=FHI/B15
seed=((XALO-LEFTLO*B16)-P)+(FHI-K*B15)*B16)+K
IF(seed.LT.0) seed=seed+P
RAN0=REAL(seed)*4.65661287D-10
RETURN
END