Irradiation Damage Calculation with Angular Distribution

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Abstract

The operating lifetime of a reactor is determined by the irradiation damage which is quantitatively accounted by the number of Displacement per Atom (DPA). The DPA rate is conventionally computed with DPA cross sections in reactor applications. However, the Gauss-Legendre Quadrature (GLQ) method used in current processing codes such as NJOY is shown unable to ensure the convergence of DPA cross sections due to the discontinuity of the damage energy versus the emission angle. The GLQ-based Piecewise Integration (GLQPI) is proposed to ensure the numerical convergence. The integration based on the GLQPI is shown suitable to compute DPA. On the other hand, even if high-order Legendre polynomials are important to describe the anisotropic angular distribution, the DPA cross section is not sensitive to the high-order Legendre polynomials because the former is an angle-integrated quantity. Numerical results of neutron elastic scattering show that 2 orders of Legendre polynomials can give the DPA rates of ⁵⁶Fe within 0.5% overestimation for fission reactors, while 4 orders are required for fusion reactors. In the case of neutron inelastic scatterings-induced DPA, only the first order Legendre polynomial is sufficient for both fission and fusion reactors.

Keywords: DPA, angular distribution, Gauss-Legendre quadrature, ⁵⁶Fe

1. Introduction

The 21st Conference of the Parties to the UN framework convention on climate change (COP21) builds upon the convention of a significant reduction in the emission of greenhouse gases. Nuclear power is and will be one of the most important energies due to its high efficiency and low CO₂ emission. However, the irradiation environment changes the properties of materials. For example, the designed service life of Pressurized Water Reactors (PWRs) and the potential extension of operating lifetime are based on the irradiated performance of the Reactor Pressure Vessel (RPV). The irradiation leads to the decrease of the rupture strain for metals. The investigations of irradiation effect on materials are of significance.

When an atom in a material is knocked-on by a kinematic particle, a vacancy and a corresponding interstitial are formed in the lattice. In addition, the Primary Knock-on
Atom (PKA) can induce a displacement cascade, which leads to more crystallographic defects in the material. The Displacement per Atom (DPA) measures the average displacements of each atom under irradiation. It is one of the key parameters to evaluate the irradiated damage. Many models have been developed to calculate DPA using the energy of PKA as a major parameter, including classical DPA metrics, such as the Norgett-Robinson-Torrens (NRT) formula [1] and the Athermal Recombination-Corrected (ARC) model [2] presented in Section 2.

Thanks to the development of computation capacity, the Molecular Dynamics (MD) is able to calculate the DPA in crystalline using the Newton’s second law. However, it is difficult to do MD simulations for high PKA energies because of the huge computational cost. To overcome this shortcoming, the Cell Molecular Dynamics for Cascades (CMDC) [3] code has been developed to accelerate the MD simulations by treating only the “active box” rather than the whole domain of the simulation. Ortiz proposed another solution that the MD is used at low energy and the Binary Collision Approximation (BCA) is used at high energy [4].

It is widely believed that the MD simulations are more reliable than the DPA metrics. The corresponding PKA spectra can be computed with special codes, such as SPECTER [5], SPECTRA-PKA [6], and DART [7]. However, the DPA metrics, such as the NRT model [1], are more popular in nuclear reactor applications until now. The most important reason is the heavy calculation burden of the MD simulations, while a continuous PKA spectrum requires a large number of MD simulations.

The typical method of DPA calculation applied in nuclear reactors is the generation of DPA cross sections through the processing code NJOY [8]. The DPA rates can be calculated with the DPA cross sections and the spectra of incident particles computed through the transport codes. The Computation of Radiation Damage (CRaD) code [9] is recently developed to calculate DPA cross sections and PKA spectra from nuclear data. The agreement between the CRaD calculations and NJOY is ensured through the examples of $^{56}$Fe [9].

Due to the conservation of energy and momentum, the recoil energy of PKA is conventionally calculated through the angular distribution of the emitted particle. The DPA cross sections are computed with the integral of the damage energy versus the emission angle. The present work investigates the reliability of the method of integral used in the widely used processing code NJOY [8]. Because the numerical method used in NJOY cannot ensure the convergence of the integral with limited points, a new method is proposed to perform the integral over the emission angle in Section 3.

The influence of the anisotropic angular distribution on PKA energy was shown in Ref. [10]. Jouanne showed that the first order Legendre polynomial of the angular distribution of $^{56}$Fe is almost sufficient to determine the neutron fluence on the iron bulk from 5 cm to 1.2 m [11]. The present work evaluates the importance of high-order Legendre polynomials of angular distribution for DPA calculations. The Stainless Steel (SS) is used in RPV in PWR, fuel cladding in Fast Reactor (FR), and candidate fuel cladding in Accident Tolerant Fuel (ATF) [12]. $^{56}$Fe has more than 90% abundance among all Fe isotopes in natural iron, which is the most concentrated element in the SS. The examples on $^{56}$Fe are taken to show the numerical results.
2. DPA Metrics

Many models and empirical formulae have been developed to calculate the DPA in materials. Kinchin and Pease proposed a formula (KP) to calculate the number of displaced atoms induced by a PKA in 1955 [13]. In this model, the PKA cannot produce any atomic displacement if the PKA energy $E_{PKA} < E_d$, where $E_d$ is the averaged threshold energy of atomic displacement. Different definitions of the threshold energy and corresponding values for Fe can be found in the Nordlund’s work [14]. The mostly used average threshold energy and the value proposed by the ASTM for the iron is 40 eV [15]. When $E_d < E_{PKA} < 2E_d$, the PKA displaces 1 atom in the lattice. Once the PKA energy is higher than the ionization energy of the target atom ($E_i$), the exceed PKA energy is transformed to electrons. The kinetic energy of PKA is thus equal to $E_i$. The KP formula is mathematically expressed as:

$$N(E_{PKA}) = \begin{cases} 
0, & 0 < E_{PKA} < E_d \\
1, & E_d < E_{PKA} < 2E_d \\
\frac{E_{PKA}}{2E_d}, & 2E_d < E_{PKA} < E_i \\
\frac{E_i}{2E_d}, & E_i < E_{PKA} < \infty
\end{cases} \quad (1)$$

By modifying the KP formula, Norgett, Robinson, and Torrens proposed the NRT model in 1975 [1]. The NRT formula is based on Robinson’s partition function [16], which is deduced from Lindhard’s numerical results of damage energy [17]. The NRT formula is given by:

$$N(E_a) = \begin{cases} 
0, & 0 < E_a < E_d \\
1, & E_d < E_a < 2E_d/0.8 \\
\frac{0.8E_d}{2E_d}, & 2E_d/0.8 < E_a < \infty
\end{cases} \quad (2)$$

where $E_a$ is the energy available to create displacement of atoms by collision, called as damage energy, 0.8 is the displacement efficiency obtained by the BCA by Robinson and Torrens [18]. $E_a = E_{PKA} \times P(E_{PKA}/E_L)$, where $P$ is the partition function which describes the fraction of $E_{PKA}$ left in atomic motion [16]:

$$P(\varepsilon) = 1/[1 + k(3.4008\varepsilon^{1/6} + 0.40244\varepsilon^{3/4} + \varepsilon)], \quad (3)$$

where $\varepsilon = E_{PKA}/E_L$ with $E_L = 86.931Z^{7/3}$ eV, $k = 0.133745Z^{2/3}A^{-1/2}$, $Z$ and $A$ are atomic number and atomic mass number, respectively. In the KP formula, the saturation of DPA is evident. The saturation exists also in NRT due to the inverse proportionality to the PKA energy of the partition function at high energy [17].

However, the overestimation of DPA in the NRT model is found in 1977 with experimental data for copper and silver [19]. One of the issues in the NRT model is that the in-cascade recombination of displaced atoms is neglected. Taking this effect into account, the ARC-DPA is proposed by Nordlund et al. [2]. The relative damage efficiency $\xi$ defines the ratio of the “true” number of Frenkel Pairs (FP) to the number of FP calculated with NRT formula. Its expression is based on the fact that the number of FP $N_{FP}$ tends to $a'E_a$ when $E_a$ tends to infinity and $N_{FP}$ tends to $c'E_a^{0.8}$ at low energy. Therefore, the ARC-DPA formula is given by:
\[ N(E_a) = \begin{cases} 
0, & 0 < E_a < E_d \\
1, & E_d < E_a < 2E_d/0.8 \\
\frac{0.8E_a}{2E_d} \xi(E_a), & 2E_d/0.8 < E_a < \infty 
\end{cases}, \quad (4) \]

where
\[ \xi(E_a) = (1 - c) \times \left[ 0.8 \frac{E_a}{2E_d} \right]^b + c. \quad (5) \]

The coefficients \( b \) and \( c \) are determined by fitting experimental data or molecular dynamics simulation results. For Fe isotopes, \( b = -0.568 \) and \( c = -0.286 \) [2].

### 3. DPA and Angular Distribution

3.1 From nuclear data to DPA cross sections

As mentioned in Section 1, the recoil energy of PKA is normally calculated with the angular distribution of the outgoing particle. Figure 1 shows the schemas of the collision in the Laboratory (Lab) and Center of Mass (CM) frames. The incident and emitted kinetic energies are referred to \( E \) and \( E' \) in the Lab frame, respectively. \( E_R \) stands for the recoil energy of the target in the Lab frame. \( m \) and \( v_1 \) (\( m' \) and \( u_1 \)) are the mass and velocity of incident (outgoing) particle in the CM frame, respectively. \( M \) and \( v_2 \) (\( M' \) and \( u_2 \)) are the mass and velocity of target particle before (after) the collision in the CM frame, respectively.

![Figure 1. Schemes of the collision in the Laboratory (upper) and Center of Mass (lower) frames](image)

The relativistic effect is negligible for DPA calculations with incident energy lower than 20 MeV [20]. The following studies are based on classical mechanism. The conservation of energy before and after the collision in the CM frame conducts to:

\[ m'c^2 + M'c^2 + \frac{1}{2} m'u_1^2 + \frac{1}{2} M'u_2^2 + Q' = mc^2 + Mc^2 + \frac{1}{2} m v_1^2 + \frac{1}{2} M v_2^2, \quad (6) \]

where \( v_1 = v_0 - v_{CM} \) and \( v_2 = v_{CM} \) because the target is static in the Lab frame.
before the collision. $Q'$ is the reaction energy. The total energy loss during the collision
is $Q = Q' + [(m' + M') - (m + M)]c^2$, which is then transferred into the excitation
energy of the recoil nucleus. Transforming the recoil velocity from the CM to the Lab frame:

$$v_R^2 = u_2^2 + v_{CM}^2 - 2u_2 v_{CM} \cos \theta,$$

where $\theta$ is the scattering angle of the emitted particle in the CM frame.

The conservation of momentum points out:

$$(m + M)v_{CM} = mv_0,$$

where $v_0$ and $v_{CM}$ are the initial velocity of the incident particle and the velocity of
the Center of Mass in the Lab frame, respectively. The momentum in the CM frame is
always null. Hence,

$$m'u_1 = M'u_2.$$

As a matter of fact, $(m' + M')/(m + M) = 1$ is numerically valid even though quite
small percentage of the mass is reduced during the nuclear reactions. Defining the
“effective mass” $R(E)$ as:

$$R(E) = \sqrt{1 - \frac{(m+M)Q}{ME}}.$$

One obtains:

$$E_R = \frac{m' ME}{(m+M)^2} \frac{m' M}{m^2 M} - 2R(E)\sqrt{\frac{m' M}{m^2 M}} \mu + R(E)^2],$$

where $\mu = \cos \theta$.

Because only the ratios of mass are present in Eq. (11), all masses can be replaced
by the relative masses to the neutron mass. The relative masses are evaluated and stored
in the ENDF files, such as 55.4544 for $^{56}$Fe. The recoil energy $E_R$ of the elastic or
discrete inelastic scatterings is expressed by:

$$E_R(\mu, E) = \frac{m' ME}{(m+M)^2} [1 - 2R(E)\mu + R(E)^2].$$

With $Q = 0$ ($R(E) = 1$) for elastic scattering.

The Robinson’s damage energy is given by:

$$E_d(\mu, E) = E_R(\mu, E)P(E_R(\mu, E)/E_L).$$

The angular integrated DPA cross section is obtained by:

$$\sigma_{DPA}(E) = \sigma(E) \int_{-1}^{1} f(\mu, E)E_d(\mu, E)\xi(E_{\alpha})d\mu,$$

where $\sigma(E)$ is the corresponding cross section. $\xi(E_{\alpha})$ is the efficiency of displacement
based on the NRT metric, it is unity for the NRT and Eq. (5) for the ARC model.
$f(\mu, E)$ is the probability density of angular distribution for the incident energy $E$
versus the cosine of the emission angle in the CM frame $\mu$. $f(\mu, E)$ is conventionally
as a sum of Legendre polynomials:

$$f(\mu, E) = \sum_{l=0}^{l_{\max}} \frac{2l+1}{2} a_l(E)P_l(\mu).$$
where \( P_l \) is the \( l \)-th Legendre polynomial and \( a_i \) is the corresponding Legendre coefficient given in the Evaluated Nuclear Data Files (ENDF).

### 3.2 Improvement of DPA calculations

The DPA cross section in Eq. (14) is based on the formula \( DPA(E_a) = 0.8E_a/2E_d \xi(E_a) \). The latter is available only for \( E_a > 2E_d/0.8 \) according to the DPA metrics given in Eqs. (2) and (4). In order to use the same expression of DPA in whole domain, one generalizes the damage energy in the interval \([0, 2E_d/0.8]\) as:

\[
E_a(\mu, E) = \begin{cases} 
0, & 0 < E_a < E_d \\
2E_d/0.8, & E_d < E_a < 2E_d/0.8 \\
E_a(\mu, E), & 2E_d/0.8 < E_a < \infty
\end{cases} \tag{16}
\]

Eq. (14) is available for any physical value of \( E \) or \( \mu \) by using the generalized damage energy. The computation of DPA cross section is simplified due to the same expression in whole domain. This strategy is used in most processing codes for the computation DPA. It is noticeable that the second “stair” is not accounted in the widely used code NJOY2016 [21]. Users should add this interval in the partition function in the HEATR module. To simplify the notation, the generalized damage energy in Eq. (16) is also called as the damage energy hereinafter. Figure 2 illustrates the damage energy of a 5 keV neutron elastic scattering on \( ^{56}\text{Fe} \).

![Figure 2. Damage energy of \( ^{56}\text{Fe} \) versus the cosine in CM for 5 keV neutron elastic scattering](image)

To calculate the integral in Eq. (14), a 64-point Gauss-Legendre Quadrature (GLQ) method is used in NJOY2016 (20-point in the manual) [21]. However, the damage energy is not a continuous function of the cosine of the emission angle (Eq. (16)), so neither the product with the angular distribution is. 64-point GLQ cannot necessarily ensure the accuracy of the integral. As the standard metric, the NRT formula is used in numerical examples in the following studies. Figure 3 indicates the neutron elastic DPA cross sections of \( ^{56}\text{Fe} \) computed with different numbers of points in the GLQ. The DPA
cross section does not converge for the 150-point GLQ at neutron energy below 10 keV because of the large contribution of damage energy in [0, \(2E_d/0.8\)]. The integral converges at high incident energy because the damage energy lower than \(2E_d/0.8\) is less important.

In order to compute the DPA cross sections without using several hundred or even more points in the GLQ, we propose to compute the integral in three intervals according to the damage energy. The two critical points to connect the three intervals are obtained with:

\[
E_a(\mu_1, E) = E_d, \quad (17)
\]

\[
E_a(\mu_2, E) = 2E_d/0.8. \quad (18)
\]

According to Eq. (16), the damage energy is in the \(E_a > 2E_d/0.8\) range for \(\mu\) in the interval \([-1, \mu_2]\). \(\mu\) in \([\mu_2, \mu_1]\) is equivalent to damage energy in \([E_d, 2E_d/0.8]\), so the damage energy is \(2E_d/0.8\). For \(\mu > \mu_1\), the damage energy is zero.

In fact, by definition of the threshold energy, a PKA with energy higher than \(E_d\) should be displaced. In addition, lower than \(2E_d\) (\(2E_d/0.8\) by accounting the efficiency) PKA energy cannot induce a second vacancy. The energy transferred to the excitation energy of electrons during and after collision has no influence on DPA in this range. It is better to use the PKA energy rather than the damage energy in the interval [0, \(2E_d/0.8\)]. Eqs. (17) and (18) become:

\[
E_R(\mu_1, E) = E_d, \quad (19)
\]

\[
E_R(\mu_2, E) = 2E_d/0.8. \quad (20)
\]

Taking the limits of the cosine into account, the boundaries are:

\[
\mu_1(E) = p_{[-1,1]} \left( \left[ \frac{mM'}{m'M} + R(E)^2 \frac{(m+M)^2}{m'M^2} E_d \right] / \left[ 2R(E) \sqrt{\frac{mM'}{m'M}} \right] \right), \quad (21)
\]

\[
\mu_2(E) = p_{[-1,1]} \left( \left[ \frac{mM'}{m'M} + R(E)^2 \frac{2(m+M)^2}{0.8m'M^2} E_d \right] / \left[ 2R(E) \sqrt{\frac{mM'}{m'M}} \right] \right), \quad (22)
\]

where \(p_{[-1,1]}\) is the projection on [-1,1]. It is defined by:

\[
p_{[-1,1]}(x) = \begin{cases} 
-1, & x < -1 \\
\frac{x}{2}, & -1 \leq x \leq 1 \\
1, & x > 1 
\end{cases}. \quad (23)
\]
Figure 3. Neutron elastic scattering DPA cross sections of $^{56}$Fe performed with 20, 64, 100, and 150 points Gauss-Legendre quadrature (upper) and the corresponding ratios to the 200-point Gauss-Legendre quadrature calculation (lower).

According to Eq. (16), the NRT-DPA cross sections are computed with:

$$
\sigma_{DPA}(E) = \sigma(E)\int_{-1}^{1} f(\mu, E) E_R(\mu, E) P\left(\frac{E_R(\mu, E)}{E_L}\right) d\mu + \frac{2E_d}{0.8} \mu_2^{1/4} f(\mu, E) d\mu.
$$

(24)

The ARC-DPA cross sections are calculated with Eq. (24) by inserting the efficiency $\xi(E_R(\mu, E)P(E_R(\mu, E)/E_L))$ in the first integral.

$f(\mu, E)$ is polynomial with order of Lmax. The $N$-point GLQ compute the exact value of integral for the $(2N-1)$ order polynomials. $[\text{Lmax}/2+1]$-point GLQ is sufficient to perform numerically the second integration in Eq. (3). $[\text{Lmax}/2+1] = 10$ for $\text{Lmax} = 19$, which is the case in JEFF-3.1.1, reveals that 10-point GLQ is sufficient to compute the second integration. Because the integrand in the first integration in Eq. (24) is the product of a 20-order polynomial and a smooth but not polynomials form function, 20-
point GLQ is suggested. This GLQ method applied in DPA calculations is referred to the GLQ based Piecewise Integration (GLQPI) hereinafter. Figure 4 indicates the DPA cross sections with 20 points and 200 points GLQPI. The excellent agreement between the DPA cross sections performed with 20-point GLQPI and 200-point GLQPI points out the convergence of the integral. In addition, 20 points are sufficient to perform the integrals in Eq. (24).

![Graph showing DPA cross sections with 20 and 200 points.]

Figure 4. Neutron elastic scattering DPA cross sections of $^{56}$Fe performed with 20 and 200 points Gauss-Legendre Quadrature based Piecewise Integration (GLQPI).

4. Role of High-Order Legendre Polynomials

4.1 DPA cross sections and Legendre orders

The angular distribution is conventionally presented in the form of Legendre polynomials of the emission angle. Jouanne showed that the first order Legendre polynomial of $^{56}$Fe is sufficient to determine the neutron fluence with energy higher than 40 keV on the capsule in a Pressurized Water Reactor (PWR) [11]. However, the high-order Legendre polynomials play an important role in describing the anisotropy of angular distribution. Taking the neutron elastic scattering of $^{56}$Fe in JEFF-3.1.1 [22] as an example, as shown in Figure 5, 0th up to 19th order Legendre polynomials are required to describe the angular distribution for incident energies higher than 17.5 MeV, while only up to 4th order are sufficient at incident energies below 1.4 MeV. It is of interest to investigate the influence of high-order Legendre polynomials on DPA calculations.
Figure 5. Angular distributions of the neutron elastic scattering reaction of $^{56}$Fe in JEFF-3.1.1 [22] with the incident energies in the inverval [200 keV, 1 MeV] (upper) and [4 MeV, 20 MeV] (lower).

Figure 6 shows the neutron elastic scattering DPA cross sections of $^{56}$Fe computed with different maximum Legendre (Lmax) polynomials. Lmax = 0 is equivalent to the isotropic angular distribution. As shown in Figure 5, at high incident energies, the forward-oriented distribution of the emitted neutron is more probable than other directions. Eq. (12) indicates the decrease of the recoil energy with the cosine in the CM frame. Therefore, the anisotropic angular distribution has a negative contribution on DPA cross sections. This result is in accordance with the DPA cross sections of $^{58}$Ni studied in Ref. [10]. The first order Legendre polynomial (L1) can describe somewhat the forward-oriented anisotropy. Nevertheless, L1 is not sufficient to reveal the anisotropy for high incident energies. For example, at an incident neutron energy of 20
MeV, L1 contributes 1.23 (6.15%) to the value of probability density $f$ at $\mu = 1$, while the probability density is $f(1, 20 \text{ MeV}) = 20$. In other words, the probability density calculated with L0 and L1 at $\mu = 1$ is only 11% of the value in JEFF-3.1.1.

![Figure 6. Neutron elastic scattering DPA cross sections of $^{56}$Fe performed with different maximum Legendre (Lmax) polynomials.](image)

High-order Legendre polynomials play an important role in the anisotropic distribution of the emitted particle. The DPA cross section is an angle-integrated quantity. High-order Legendre polynomials may be of less importance for the DPA cross sections. The example shown in Figure 6 points out that Lmax = 3 is sufficient for the neutron elastic scattering DPA cross sections of $^{56}$Fe.

![Figure 7. Angular distributions of the neutron first level inelastic scattering reaction (MT51) of $^{56}$Fe in JEFF-3.1.1 [22] with the incident energies from 2 MeV up to 20 MeV](image)
Lower Legendre polynomials should be used for inelastic scatterings because of the more isotropic angular distribution, as the example shown in Figure 7. The elastic scattering is more forward-oriented than the discrete inelastic scatterings due to the contribution of the potential scattering. Figure 8 shows the example of the first level inelastic scattering DPA cross sections. The first order Legendre polynomial can provide enough information on the calculations of DPA cross sections.

4.2 Results and discussion

Section 4.1 reveals that the high-order Legendre polynomials are not necessary for DPA cross sections computation because the latter are the angle-integrated values. In order to evaluate the corresponding effect on DPA rates, the examples of the fuel cladding in the Sodium Fast Reactor (SFR) Phenix and the inner surface of RPV in a typical PWR are shown because the DPA of the fuel cladding (RPV) in fast reactors (thermal reactors) is the most important factor concerning the service life of reactors. In addition, the DPA rates in a diagnostic mirror, which is just after the first-wall facing the plasma, are investigated to evaluate the influence on fusion reactors.

The nuclear data library JEFF-3.1.1 [22] is used to determine the neutron flux. The neutron flux in the fuel cladding of Phenix is calculated with ERANOS [23] code. Due to the penetration in the iron, the neutron flux decreases with the depths in RPV. The maximum DPA in RPV is found in the inner surface. The neutron spectrum in the inner surface of RPV in a typical PWR is computed with the stochastic code TRIPOLI-4® [24]. The corresponding neutron spectra are shown in Figure 9.
Figure 9. Neutron spectra in the fuel cladding of Phenix reactor, in the inner surface of RPV in a typical PWR, and in the diagnostic mirror of a fusion reactor.

Table I. Relative DPA rates of $^{56}$Fe with different maximum orders of Legendre polynomials (Lmax) in the fuel cladding of Phenix, in the inner surface of RPV in PWR, and just after the first wall of a fusion reactor. MT2, MT51, and MT52 refer to the elastic, the first inelastic level, and the second inelastic level scatterings, respectively. The DPA rates are normalized by those calculated with all orders of Legendre polynomials in JEFF-3.1.1. The numerical results indicate that Lmax = 2 for the elastic scattering can ensure the DPA rates.

|     | Lmax | 0   | 1   | 2   | 3   | 4   | 19  |
|-----|------|-----|-----|-----|-----|-----|-----|
| Phenix | MT2  | 1.405 | 1.022 | 1.002 | 1.000 | 1.000 | 1.000 |
|      | MT51 | 1.023 | 1.002 | 1.001 | 1.001 | 1.000 | 1.000 |
|      | MT52 | 1.009 | 1.001 | 1.001 | 1.001 | 1.000 | 1.000 |
| PWR  | MT2  | 1.577 | 1.036 | 1.004 | 1.001 | 1.000 | 1.000 |
|      | MT51 | 1.026 | 1.002 | 1.001 | 1.001 | 1.000 | 1.000 |
|      | MT52 | 1.011 | 1.000 | 1.001 | 1.001 | 1.000 | 1.000 |
| 14 MeV | MT2 | 2.425 | 1.192 | 1.036 | 1.009 | 1.003 | 1.000 |
|      | MT51 | 1.125 | 1.008 | 1.000 | 1.000 | 1.000 | 1.000 |
|      | MT52 | 1.084 | 1.002 | 1.000 | 1.000 | 1.000 | 1.000 |

The DPA rate induced by particles with continuous spectrum is calculated by:

$$DPA = \frac{0.8}{2E_d} \int_0^\infty \sigma_{DPA}(E)\phi(E)dE,$$

where $\phi(E)$ is the flux of the incident particle. Table I lists the relative DPA rates of $^{56}$Fe with different maximum orders of Legendre polynomials (Lmax) in the fuel cladding of Phenix, in the inner surface of RPV in PWR, and just after the first-wall of a fusion reactor. MT2, MT51, and MT52 refer to the elastic, the first inelastic level, and the second inelastic level scatterings, respectively. The DPA rates are normalized by those calculated with all orders of Legendre polynomials provided in JEFF-3.1.1. The numerical results indicate that Lmax = 2 for the elastic scattering can ensure the DPA rates.
rates within 0.5% overestimation for fission reactors, while the uncertainties of the neutron elastic scattering are about 5%. For fusion reactors, up to 4th order Legendre polynomials are required to calculate neutron elastic scattering DPA rate. Due to the more isotropic angular distribution as explained in Section 4.1, only the first order Legendre polynomial is necessary to ensure the DPA rates of the discrete inelastic scatterings for both fission and fusion reactors. Important correlations are recently shown between high-order Legendre coefficients and reaction cross sections (and also low-order Legendre coefficient) [25]. The uncertainty quantification in DPA calculations can be largely simplified due to the negligible role of high-order Legendre polynomials.

5. Conclusions

The elastic and discrete inelastic scatterings-induced DPA cross sections are computed by integration over the emission angle. The widely used processing code NJOY [21] uses the Gauss-Legendre Quadrature (GLQ) to numerically calculate the integral. However, the usage of GLQ in the full range of [-1,1] cannot ensure the convergence of the DPA cross sections due to the discontinuity of the damage energy versus the emission angle. The GLQ-based Piecewise Integration (GLQPI) method is proposed in the present work to ensure the convergence of numerical calculations. The GLQPI method uses the GLQ in each piecewise interval, on which the integrand is a smooth function. The convergence of the integral is ensured by the 20-point GLQPI, while the 150-point GLQ calculation does not converge.

The high-order Legendre polynomials are of importance to describe the anisotropy of angular distributions. Nevertheless, the high-order Legendre polynomials is shown not important for DPA calculations because DPA cross section is an angle-integrated quantity. The DPA cross sections computed with isotropic angular distribution are higher than those calculated with the anisotropic emission angle due to the forward-oriented angular distributions, while the damage energy decreases with the cosine of the emission angle. Comparing with inelastic scatterings, higher maximum order of Legendre polynomials is required for the elastic scattering because the emission angle is more forward-oriented due to the contribution of the potential scattering.

The operating lifetime of a fast reactor is determined by the damage of the fuel cladding, while for a thermal reactor it is the damage on the RPV. The calculations of DPA in fission reactors are performed with the fuel cladding of a fast reactor, the inner surface of the RPV of a PWR, and the diagnostic mirror of a fusion reactor. Numerical results of neutron elastic scattering show that 2 orders of Legendre polynomials give DPA rates of $^{56}$Fe within 0.5% overestimation for fission reactors, while 4 orders are required for fusion reactors. For neutron inelastic scatterings, only the first order Legendre polynomial is sufficient to compute DPA rate for both fission and fusion reactors.
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