

On the beta decay-induced radiation damage

Shengli Chen^{a,b,*}, David Bernard^a

^a CEA, DEN, DER, SPRC, LEPh, F-13108 Saint-Paul-Lez-Durance, France

^b Université Grenoble Alpes, I-MEP2, 38402 Saint Martin d'Hères, France

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ABSTRACT

The present work proposes the methods to calculate beta decay-induced atomic displacement damage, including the emitted electron-induced damage and the residual nucleus-induced damage using three-body kinematics. Compared with the standard Norgett-Robinson-Torrens (NRT) metric of the number of Displacements per Atom (DPA), the modified NRT proposed in the present work based on the definition of threshold displacement energy leads to 36% more DPA induced by the emitted electron of ^{56}Mn beta decay. The example of ^{56}Mn beta decay shows that the emitted electron-induced DPA is fewer than the DPA induced by the residual nucleus by a factor of 14. The residual recoil energy should be taken into account for elements such as iron, nickel, chromium, aluminum, and especially for silicon, whereas the maximum kinetic energy of beta decay residual is below the threshold of atomic displacement for tungsten.

1. Introduction

Radiation damage is one of the most important factors that influence behavior of materials through atomic displacements and the subsequent migration of defects. The conventional quantity to measure atomic displacement damage is the number of Displacements per Atom (DPA), which defines the average displacements of each atom in lattice. DPA is now used as a basic quantity for describing the radiation damage of materials induced by different particles. Because of its importance, many models were developed for DPA computation using the Primary Knock-on Atom (PKA) kinetic energy as a major parameter.

Due to the various sources of irradiation, extensive methods and codes have been developed into studying the displacement damage induced by an incident particle, such as neutron and gamma in nuclear reactors. For example, the neutron-induced PKA spectra can be computed by SPECTRA-PKA [1] and DART [2] codes using Evaluated Nuclear Data Files (ENDF) or SPECTER [3] code which only uses ENDF/B-V library. Using the standard Norgett-Robinson-Torrens (NRT)-DPA metric [4] or other analytical formulae, neutron-induced DPA cross sections can be computed by the processing codes like NJOY [5]. Similarly, the electron [6] and photon-induced [7] DPA cross sections can be calculated for a specific formula of DPA calculation.

However, nuclear disintegrations, which are normally slower than atomic displacement cascade (~ 10 ps [8]), are rarely individually studied for atomic displacement calculation. The three nuclear transitions are alpha decay, beta decay (β^- and β^+), and gamma transition.

The gamma transition is found in all nuclear reactions other than elastic scattering due to the deexcitation of recoil nuclei. Because the emitted gamma is considered in the gamma spectrum, the contribution of gamma transition is partially included in gamma-induced DPA [7]. Alpha decay is a two-body reaction and is conservatively considered in Ref. [9]. For most neutron-induced reactions other than (n,2n), nuclei generally lose more protons than neutrons, such as (n,p), (n,d), (n, ^3He), (n, α), and (n,np). Therefore, the unstable recoil nuclei are mostly in the “south-east” of the line of stability on the N-Z plot. The most possible nuclear transition is the beta decay which emits an electron. Moreover, due to the emission of (anti)neutrino, the beta decay is a three-body reaction, which complicates the calculation of irradiation damage from kinematics. The present work aims to show the calculation and contribution of beta decays to atomic displacement damage.

Gilbert and Sublet took the beta decay into consideration for PKA spectra [9]. Nevertheless, they neglected the energy taken by anti-neutrino (so the two-body kinematics is used) and the energy lost to the photon via deexcitation. Moreover, the displacement induced by the emitted electron is not considered in Ref. [9]. The present work investigates the atomic displacement induced by both residual nuclei and emitted electron of beta decay using the energy distribution of electron. Section 2.1 briefly presents beta decay and the energy distribution of the emitted electron. Section 2.2 shows the methods for computing electron-induced atomic displacement. Section 2.3 points out the method to calculate the residual nucleus-induced atomic displacement

* Corresponding author at: CEA, DEN, DER, SPRC, LEPh, F-13108 Saint-Paul-Lez-Durance, France.

E-mail address: shengli.chen@cea.fr (S. Chen).

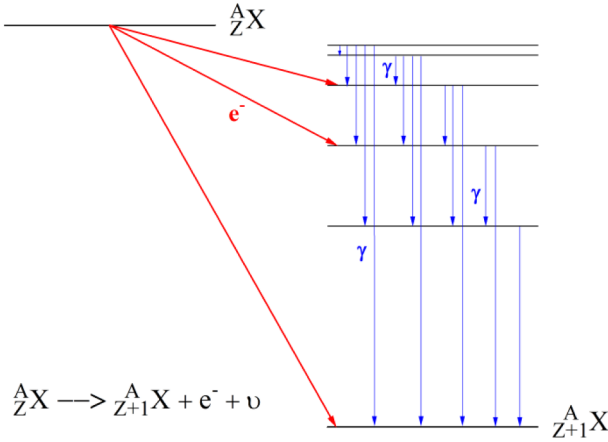


Fig. 1. General energy level schema of a beta decay.

that cannot be considered in particle transport codes. Section 3 gives the results for the beta decay of ^{56}Mn . The examples on ^{56}Mn are shown because it is the product of (n,p) reaction with ^{56}Fe , which is the most abundant isotope in stainless steel. Section 3 also brings general discussion on beta decay-induced DPA. The main conclusions are summarized in Section 4.

2. Methods

2.1. Beta decay

The beta decay of a nucleus $^A_Z X$ (where A and Z are respectively the mass number and the atomic number of the nucleus) can be expressed by:

$$^A_Z X \rightarrow ^A_{Z+1} X + e^- + \bar{\nu}, \quad (1)$$

where $\bar{\nu}$ represents antineutrino. The electronic antineutrino is conventionally denoted by $\bar{\nu}_e$. For the sake of convenience, the present work uses the simple notation $\bar{\nu}$. Fig. 1 illustrates the corresponding schema of the beta decay for the nucleus $^A_Z X$. After the beta decay, the excited nucleus will deexcite via a cascade of gamma emissions. The probability of different branch of gamma transitions can be determined by Fermi's Golden Rule [10]:

$$P = \frac{2\pi}{\hbar} |H_{fi}|^2 \rho(E_f) \quad (2)$$

where $\rho(E_f)$ is the density of final state, H_{fi} is the Hamiltonian describing the interaction between the initial state and the final state. Fig. 2 shows (in red) the intensity (or relative probability) of beta decay of ^{56}Mn with data from the latest Evaluated Nuclear Structure Data File (ENSDF) evaluation [11].

Since the beta decay is always accompanied by an antineutrino, kinetic energy of the emitted electron is not the total energy release of the beta decay. For each level i beta decay, the electron spectrum can be approximately calculated by [10]:

$$\chi_i(p) \propto p^2 (Q_i - E_e)^2 F(Z+1, p) |M_{fi}|^2 S(p, q) \quad (3)$$

where p and q respectively represent the momenta of the electron and the antineutrino, Q_i is the Q -value of transition i , E_e is the kinetic energy of the electron, $F(Z+1, p)$ is Fermi's function accounting the Coulomb field, $|M_{fi}|^2$ is the nuclear matrix element [12], and $S(p, q)$ is an additional electron and antineutrino momentum dependence.

Taking all transition channels into account, the electron spectrum of a beta decay is:

$$\chi(p) = \sum_i \tilde{P}_i \chi_i(p), \quad (4)$$

where $\tilde{P}_i$ is the intensity (or relative probability) of the i -level beta

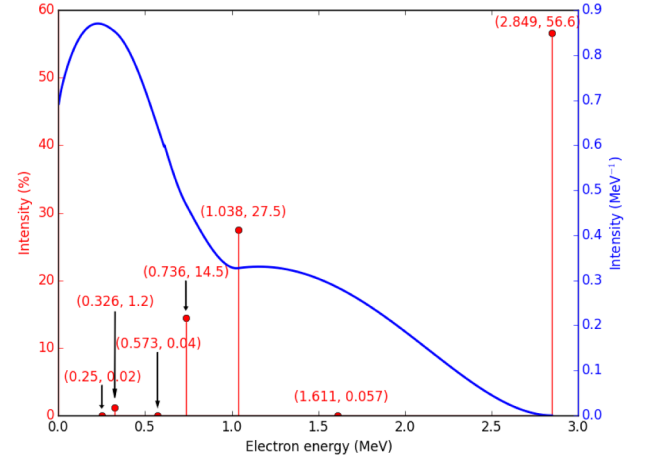


Fig. 2. Intensity of ^{56}Mn beta emission (from ENSDF [11]) and the corresponding energy distribution of the emitted electrons (calculated via Eqs. (3) and (4)).

decay. Fig. 2 illustrates (in blue) the energy distribution of the emitted electron from the beta decay of ^{56}Mn [11]. The form of the electron spectrum shown in Fig. 2 is in good agreement with those produced by JANIS [13]. The electron spectrum can be used to determine the number of DPA using the corresponding electron-induced DPA cross section.

2.2. Electron-induced displacement damage

The electron-induced DPA cross section is calculated by:

$$\sigma(E) = \int_0^{T_m} \nu(T) \frac{d\sigma}{dT} dT \quad (5)$$

where $d\sigma/dT$ is the differential scattering cross section of an electron, $\nu(T)$ is the number of displaced atoms induced by the target of which the kinetic energy is T , T_m is the maximum energy of the target:

$$T_m(E) = \frac{2E}{Mc^2} (E + 2mc^2) \quad (6)$$

where mc^2 and Mc^2 are respectively the rest energy of an electron and that of the knock-on atom. $d\sigma/dT$ can be calculated by Mott cross section [14] or the McKinley-Feshbach analytic approach (MF) [15].

Many formulae were developed to compute the number of atomic displacements using the PKA energy and the average threshold displacement energy E_d [4,16–20]. E_d defines the “equivalent” minimum energy that an atom can be permanently displaced [16]. In the current international standard NRT model [4], it is conventionally assumed that no atom can be displaced if the damage energy is lower than the average threshold displacement energy E_d [19] (not explicitly declared in Ref. [4]). Nevertheless, according to the definition of threshold displacement energy, a PKA with kinetic energy higher than E_d is able to induce 1 atomic displacement (energy lost to inelastic collision is after the displacement of PKA). Therefore, the present work proposes to use a modified NRT (mNRT) as:

$$\nu(T) = \begin{cases} 0, & T < E_d \\ 1, & (E_d < T) \& (T_d(T) < 2.5E_d) \\ 0.8T_d/2E_d, & T_d(T) > 2.5E_d \end{cases} \quad (7)$$

where T_d is the damage energy [21]. The difference between NRT and mNRT is quite small for most cases where the atomic displacements are mainly induced by high damage energy. However, for the study of electron-induced damage, the use of NRT or mNRT leads to large differences (c.f. Section 3). Fig. 3 shows the electron-induced DPA cross sections of iron for NRT and mNRT formulae using the MF approach and Mott series.

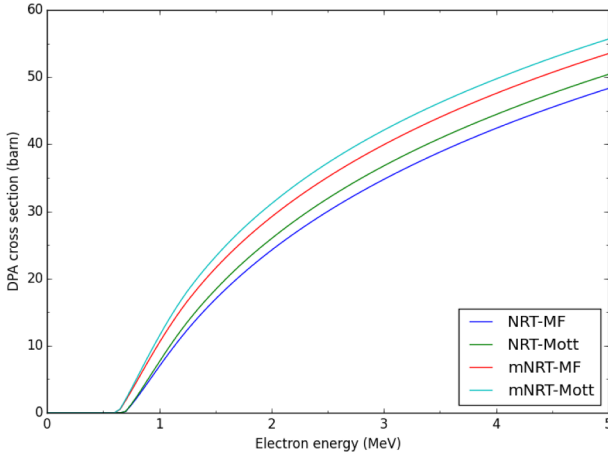


Fig. 3. Electron-induced DPA cross sections for iron.

In a specific material, the average number of atomic displacements induced by a kinematic electron is computed with:

$$n(E) = N_V \int_0^E \frac{\sigma(T)}{S(T)} dT \quad (8)$$

where N_V denotes the atomic density of the target, S stands for the stopping power [22], and σ is the electron-induced DPA cross section. Fig. 4 illustrates the examples of $n(E)$ calculated with the DPA cross sections shown in Fig. 3. Using the spectrum of the electron and $n(E)$, the number of DPA can be determined by:

$$DPA = \int_0^\infty n(E) \phi(E) dE \quad (9)$$

where ϕ refers to the electron flux spectrum (such as the smooth blue curve shown in Fig. 2).

2.3. Atomic displacement induced by residual atom

Section 2.2 shows the method for the calculation of the emitted electron-induced atomic displacement. For general studies of beta decay, the recoil kinetic energy of the residual nucleus is negligible in comparison with the energies of electrons and antineutrinos [23]. However, since the threshold energy of atomic displacement is generally below 100 eV, the residual nucleus of a beta decay is also able to induce atomic displacement.

Fig. 5 illustrates the kinematics of the three particles after a beta decay. The conservation of momenta implies:

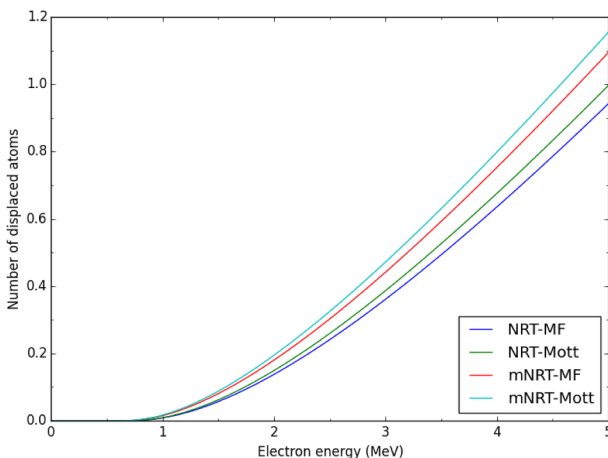


Fig. 4. Total displaced atoms per incident electron.

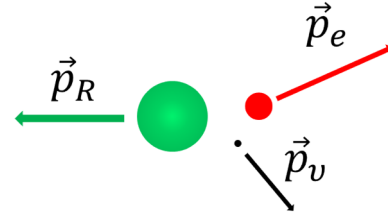


Fig. 5. Schematic of kinematics of a beta decay. R , e , and ν represent the residual atom, the emitted electron, and the antineutrino, respectively.

$$\vec{p}_R + \vec{p}_e + \vec{p}_\nu = \vec{0} \quad (10)$$

where the subscripts R , e , and ν represent the residual atom, emitted electron, and the antineutrino, respectively. The norm of the momentum of the residual nucleus is thus:

$$\|\vec{p}_R\| = \|\vec{p}_e + \vec{p}_\nu\| \quad (11)$$

For the sake of convenience, one denotes the norm of a vector by the same notation without an arrow. Accordingly,

$$p_R^2 = p_e^2 + p_\nu^2 + 2\vec{p}_e \cdot \vec{p}_\nu \quad (12)$$

Supposing isotropic distribution of the angle between the directions of electron emission and antineutrino emission, one has:

$$\int \vec{p}_e \cdot \vec{p}_\nu d\Omega = 0 \quad (13)$$

where Ω is the solid angle. Therefore, averaging over the angular distribution, one has:

$$p_R^2 = p_e^2 + p_\nu^2 \quad (14)$$

According to the relationship between momentum and energy, the kinetic energy of the residual nucleus is expressed by:

$$E_R = \sqrt{p_R^2 c^2 + M^2 c^4} - M c^2 \quad (15)$$

where c is the speed of light and M is the rest mass of the residual nucleus:

$$M = M_0 + E^*/c^2 \quad (16)$$

where M_0 is the mass in ground state, E^* is the excitation energy. In general, the excitation energy is negligible in comparison with the rest mass. The approximation $M \cong M_0$ can be thus used in most cases, including the beta decay. It is noteworthy that nonrelativistic treatment can be directly used for the residual nucleus because $E_R \ll M c^2$ [24]. On the other hand, Eq. (14) shows that $p_R \geq p_e$. Consequently,

$$E_R \geq E_R^- \equiv \sqrt{E_e(E_e + 2mc^2) + M^2 c^4} - M c^2 \quad (17)$$

where E_e represents the kinetic energy of the emitted electron. This lower boundary is emphasized because the spectrum of E_R^- can be directly determined using the spectrum of E_e as the example shown in Fig. 2.

Since the kinetic energy of the residual nucleus is generally much smaller than those of emitted electron and antineutrino, the energy of antineutrino is approximately:

$$E_\nu = Q - E_e \quad (18)$$

where Q is the total energy release in the beta decay. On the other hand, due to the negligible mass of antineutrino, one has directly:

$$p_\nu = E_\nu/c \quad (19)$$

Therefore, for each level of the beta decay, the recoil energy of the residual nucleus is:

$$E_R = \sqrt{E_e(E_e + 2mc^2) + (Q - E_e)^2 + M^2 c^4} - M c^2 \quad (20)$$

The spectrum of E_R is calculated during the calculation of the one of E_e .

Similar to E_R^- defined in Eq. (17), one can have an upper limit of recoil energy:

$$\begin{aligned} E_R &\leq E_R^+ \equiv \sqrt{E_e(E_e + 2mc^2) + (Q_{\max} - E_e)^2 + M^2c^4} - Mc^2 \\ &\leq E_R^{+b} \equiv \sqrt{E_e(E_e + 2mc^2) + Q_{\max}^2 + M^2c^4} - Mc^2 \end{aligned} \quad (21)$$

where $Q_{\max}$ is the maximum energy release (e.g. 2.85 MeV for the beta decay of ^{56}Mn). E_R^+ (or E_R^{+b}) can also be directly determined via the spectrum of E_e . Using E_R^- and E_R^+ , one can obtain the range of DPA numbers induced by the residual nucleus without calculating the spectrum of E_R . It is noteworthy that $E_R \leq E_R^{+b}$ given Eq. (21) shows that the two-body treatment in Ref. [9] can give a conservative value for the residual nucleus-induced DPA of a beta decay.

3. Results and discussion

The numerical results shown in this section are based on ^{56}Mn because it is the product of (n,p) reaction with ^{56}Fe (the most abundant isotope in stainless steel). One can treat any isotope using the methods presented in Section 2.

3.1. Atomic displacement induced by the emitted electron

As mentioned in Section 2.2, both the MF approach and Mott series are used to compute the electron-induced DPA cross sections. Even if the latter is more accurate, the former is more widely used because of the analytic formula. Our recent work shows the relative difference on DPA cross section of ^{56}Fe computed with the two scattering cross sections decreases from 10% to 1% for incident electron energy increases from 2 MeV to 100 MeV [7]. Since the electron energy from beta decay is mostly of several MeV or even lower, the present work compares the number of electron-induced DPA using the two methods.

Moreover, as explained in Section 2.2, since the kinetic energy of PKA knocked-on by a beta decay electron is generally lower than several hundred eV, the use of kinetic energy or damage energy to compute the number of displacements close to the threshold energy is important. Therefore, we compare the number of DPA using the standard NRT and the mNRT.

Table 1 summarizes the number of Displaced Atoms (DA) induced by an electron from ^{56}Mn beta decay in pure ^{56}Fe . Taking the widely used MF approach of electron scattering cross section as the reference, the use of Mott's series leads to additional 8% DPA. This value is in good agreement with the data shown in Ref. [7]. Compared with the standard NRT formula, the mNRT-based DPA should be increased by 36%. It is observed that the mNRT and Mott's series can yield 47% more DPA than the standard NRT and the widely used MF approach for ^{56}Mn beta decay electron-induced atomic displacement in pure ^{56}Fe . Therefore, the use of Mott's series and the mNRT is of importance for computing the atomic displacement induced by beta decay electrons.

3.2. DPA induced by the residual nucleus

Section 3.1 shows the electron spectrum averaged DA in the calculation of beta decay-induced atomic displacement. Nevertheless, as explained in Section 2.3, even if the kinetic recoil energy of the residual nucleus is negligible for general studies on beta decay, this part should be considered for the computation of atomic displacement. Since the spectrum of the residual nucleus is often neglected in nuclear physics,

Table 1

Number of ^{56}Fe DA induced by an electron from ^{56}Mn beta decay.

	NRT_MF	NRT_Mott	mNRT_MF	mNRT_Mott
10^{-3}DA	27.97	30.39	38.03	41.21
Ratio to NRT_MF	1.000	1.086	1.359	1.472

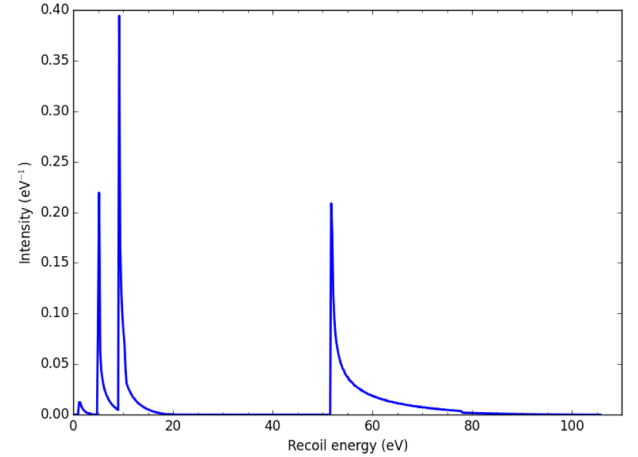


Fig. 6. Spectrum of recoil energy from ^{56}Mn beta decay.

the present work proposes the lower and upper boundaries E_R^- and E_R^+ (defined in Eq. (21)), of which the spectra can be directly determined by means of the electron spectrum. This section compares the DPA calculated with E_R^- , E_R^+ , and E_R given in Eq. (20). The spectrum of E_R from ^{56}Mn beta decay is shown in Fig. 6. The maximum kinetic energy of the residual nucleus ^{56}Fe is 106 eV, which verifies the hypothesis that E_R is negligible in comparison with kinetic energy of the emitted electron or antineutrino. It is noticeable that the recoil energy calculated by Eq. (5) in Ref. [9] is 167.3 eV. This further verifies that neglecting antineutrino and excitation of the residual nucleus in Ref. [9] is a conservative estimate of the beta decay-induced damage.

Table 2 gives the number of DA induced by the kinetic energy of the residual nucleus from ^{56}Mn beta decay in pure ^{56}Fe . The data in Table 2 are calculated by the lower boundary E_R^- , two upper boundaries E_R^+ and E_R^{+b} , and the spectrum of recoil energy illustrated in Fig. 6. As expected, using E_R^- and E_R^+ (or E_R^{+b}) and the emitted electron spectrum can give the range of real DPA. Therefore, in the case where the beta decay-induced DPA is not so important, one can directly use E_R^+ to obtain a conservative value. On the other hand, one can take the average of two values calculated with E_R^- and E_R^+ for a reasonably approximative value. In the case of ^{56}Mn beta decay, the average DPA calculated based on E_R^- and E_R^+ is 0.5798, which is quite close to the reference calculation 0.5665.

Using the method in Ref. [9], the residual nucleus-induced DPA in ^{56}Mn beta decay is 1.43. Therefore, compared with the methods proposed in the present work, Ref. [9] overestimates the residual kinetic energy-induced atomic displacement by a factor of 2.5 in ^{56}Mn beta decay. It is noteworthy that Ref. [9] proposes the use of the mass difference, which is 3695.64 keV for ^{56}Mn beta decay. However, $Q_{\max} = 2848.86$ keV because the β^- emission of ^{56}Mn leads to ^{56}Fe at excited level with excitation energy higher than 846.776 keV [11]. If we replace the mass difference by $Q_{\max}$, the recoil energy proposed by Ref. [9] becomes 83.8 eV, which implies 1 DPA if the NRT or the mNRT formula is applied.

Comparing data from Tables 1 and 2, the number of DPA induced by the recoil energy of the residual nucleus is larger than that induced by

Table 2

Number of ^{56}Fe DA induced by the residual nucleus from ^{56}Mn beta decay with different approximations of recoil energy using mNRT.

Recoil energy	E_R^-	E_R^+	E_R^{+b}	Average ^a	E_R (Fig. 6)	Ref. [9] ^b
DA	0.1596	1.0000	1.0251	0.5798	0.5665	1.4313

^a The averaged value of DA computed by E_R^- and E_R^+ : $(0.1596 + 1.0000)/2$.

^b Damage energy is 143.13 eV, both NRT and mNRT imply thus the same value.

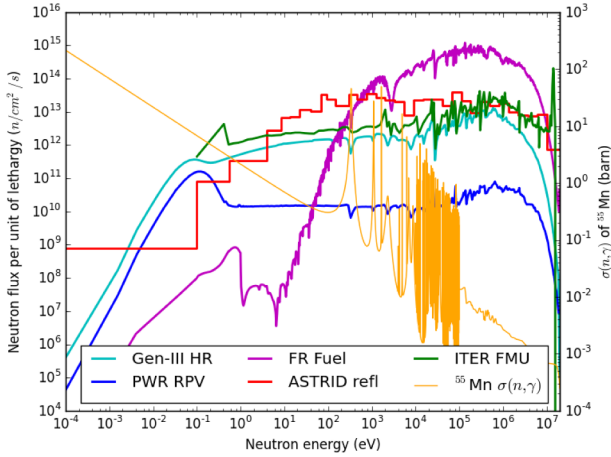


Fig. 7. Neutron flux in different nuclear facilities and the neutron capture cross section of ^{55}Mn .

the emitted electron by a factor of 13.5 (20 if the standard NRT formula and the MF approach are used). Consequently, for the calculation of beta decay-induced atomic displacement, the kinetic energy of the residual nucleus has to be taken into account. In other words, only the consideration of electron is not sufficient to compute the beta decay-induced atomic displacements.

3.3. Beta decay-induced DPA in nuclear facilities

In pure ^{56}Fe , ^{56}Mn is the product of (n,p) reaction. In equilibrium, the production rate and the decay rate of ^{56}Mn are equal. Therefore, the decay rate of ^{56}Mn is equivalent to the (n,p) reaction rate of ^{56}Fe . The present work computes the DPA rate induced by ^{56}Mn beta decay in ^{56}Fe using the neutron flux shown in Fig. 7, including the flux in a Gen-III Heavy Reflector (HR) [25], Reactor Pressure Vessel (RPV) of a 900 MW Pressurized Water Reactor (PWR) [26], Fast Reactor fuel cladding, ASTRID Reactor reflector [27], ITER First Mirror Unit (FMU) [26]. The corresponding DPA rates induced by ^{56}Mn beta decay are given in Table 3.

For comparison, Table 3 points out the total DPA rate (approximately equal to neutron-induced one) in the last column. We can find that beta decay-induced DPA is quite negligible in comparison with the incident neutron-induced atomic displacement. The main reason is that (i) (n,p) reaction cross section of ^{56}Fe is quite small compared with other cross sections and (ii) the kinetic energy of lattice atoms from beta decay is much smaller than the energy transfer in neutron-induced kinematic collisions. The second point is almost general for all beta decays, while the first one depends on nucleus. Since ^{56}Mn is the product of neutron radiative capture reaction of ^{55}Mn and ^{55}Mn (100% abundance in natural Mn) is also an element in RPV steel, we introduce 1% ^{55}Mn into ^{56}Fe to evaluate the importance of ^{55}Mn in the beta decay-induced DPA.

Table 4 shows the beta decay-induced DPA rate by 1% ^{55}Mn incorporation and the total beta decay induced DPA rate in 1% ^{55}Mn - ^{56}Fe . Because of much larger ^{55}Mn neutron capture reaction rate than the

^{56}Fe (n,p) reaction rate, 1% ^{55}Mn in iron can largely increase the ^{56}Mn beta-decay induced DPA. As shown in Fig. 7, the neutron capture cross section of ^{55}Mn largely decreases with the neutron energy when incident energy is below 100 eV. Therefore, the increase of beta decay-induced DPA rate owing to the ^{55}Mn is more important for neutron spectrum having higher relative flux at low energy. In PWR RPV, the effect of 1% ^{55}Mn is enormous. Taking the 1.39% Mn in RPV [28] into account, 5.8×10^{-7} DPA/year is induced by the beta decay of ^{56}Mn . Nevertheless, this value is still quite negligible in comparison with atomic displacement induced by kinematic neutrons.

The present work compares only the beta decay-induced atomic displacements with the neutron and photon-induced one in operating reactors, where high density neutron and photon are produced. It is noteworthy that the beta decay-induced a few atomic displacements may be important for semiconductors and detectors, where the neutron and photon flux are quite low. In addition, beta decay-induced damage may also of importance for shutdown reactors and the cladding of spent fuels.

In the case of stop of neutron source such as shutdown reactors or even retired reactors, the beta decay becomes one of the most important irradiation sources for atomic displacement. For radioactive nucleus i , the isotopic concentration follows Bateman equation:

$$\frac{dN_i}{dt} = \sum_{j \neq i} N_j \sigma_{j \rightarrow i} \phi - \left(\sum_{j \neq i} \sigma_{i \rightarrow j} \right) N_i \phi - \lambda_i N_i + \sum_{j \neq i} \lambda_{j \rightarrow i} N_j \quad (22)$$

where $\sigma_{j \rightarrow i}$ represents the microscopic cross section of isotope j producing i , ϕ is the neutron flux, $\lambda_i = \ln(2)/T_{1/2}^i$ where $T_{1/2}^i$ refers to the half-life of isotope i . In equilibrium, $dN_i/dt = 0$ leads to:

$$N_i = \frac{\sum_{j \neq i} N_j \sigma_{j \rightarrow i} \phi + \sum_{j \neq i} \lambda_{j \rightarrow i} N_j}{\left(\sum_{j \neq i} \sigma_{i \rightarrow j} \right) \phi + \lambda_i} \quad (23)$$

This quantity will be the source of all beta decays of isotope i . If one neglects the radioactive decay of which the daughter nucleus is isotope i after the stop of neutron source, the number of atomic displacements induced by the beta decay is proportional to the DPA rate in equilibrium by a factor of $1/\left(\left(\sum_{j \neq i} \sigma_{i \rightarrow j} \right) \phi + \lambda_i \right)$, which is equivalent to $1/\lambda_i$ if the disappearance reaction rate in equilibrium is negligible in comparison with radioactive decay.

3.4. Discussion on general beta decay-induced DPA

Due to the large difference between the masses of an electron and a nucleon, the threshold energy of atomic displacement corresponds to quite large energy release in the beta decay. According to Eq. (12), one has:

$$\begin{aligned} P_R &\leq \frac{P_e + P_\nu}{(\sqrt{E_e(E_e + 2mc^2)} + (Q - E_e))/c} \\ &\leq \sqrt{Q(Q + 2mc^2)}/c \end{aligned} \quad (24)$$

As remarked in Section 2.3 and the example shown in Section 3.2, nonrelativistic treatment is suitable for the residual nucleus. Accordingly,

$$E_R \leq E_R^m \equiv \frac{Q(Q + 2mc^2)}{2Mc^2} \quad (25)$$

By consequence, for beta decay that $E_R^m \leq E_d$, the residual nucleus has no effect on atomic displacement.

Table 5 points out the value of E_R^m for some isotopes. Ta isotopes are (n,p) reaction products of W, which can be used in fusion reactor [29]. Fe, Ni, and Cr are main elements in stainless steel. Al is used in accident tolerant fuel cladding FeCrAl [30–32]. Si is one of the most important elements for semiconductor and the candidate cladding material SiC. E_R^m values are smaller than the corresponding E_d for W and Re isotopes. For the stable isotopes of Fe, Ni, Cr, Si, and Al shown in Table 5, the

Table 3
 ^{56}Mn beta decay-induced DPA rate (DPA/year) in different facilities.

	Electron	Residual	Beta decay	Neutron
Gen-III HR	4.75E-09	6.53E-08	7.01E-08	0.306 (8E-5) ^a
PWR RPV	1.63E-10	2.25E-09	2.41E-09	0.003
FR Cladding	5.28E-07	7.26E-06	7.78E-06	25.300
ASTRID	6.55E-07	9.01E-06	9.67E-06	0.568
ITER FMU	2.49E-06	3.42E-05	3.67E-05	2.389

^a The value in parenthesis is the gamma-induced DPA rate [7].

Table 4⁵⁶Mn beta decay-induced DPA rate (DPA/year) by 1%⁵⁵Mn in ⁵⁶Fe in different facilities.

	Electron	Residual	Beta decay	Ratio to Table 3
Gen-III HR	2.26E-07 (2.30E-07) ^a	3.10E-06 (3.17E-06)	3.33E-06 (3.40E-06)	47.5 (48.5)
PWR RPV	2.83E-08 (2.85E-08)	3.89E-07 (3.92E-07)	4.18E-07 (4.20E-07)	173.3 (174.3)
FR Cladding	1.69E-06 (2.21E-06)	2.32E-05 (3.04E-05)	2.49E-05 (3.26E-05)	3.20 (4.20)
ASTRID	3.89E-09 (6.53E-07)	5.35E-08 (8.97E-06)	5.74E-08 (9.63E-06)	0.006 (0.996)
ITER FMU	2.62E-06 (5.09E-06)	3.61E-05 (7.00E-05)	3.87E-05 (7.50E-05)	1.05 (2.04)

^a Values in parenthesis are beta decay-induced DPA rate in 1%⁵⁵Mn-⁵⁶Fe.

maximum kinetic recoil energies of the residual nuclei are larger than the corresponding average atomic displacement threshold. Therefore, the kinetic recoil of the residual nucleus should be taken into account for these daughter nuclei. An exception is ⁶⁰Co beta decay, of which E_R^m is slightly larger than E_d . However, the intensity of ⁶⁰Co beta decay branch having $E_R^m > E_d$ is only 0.22%, whereas the rest 99.88% cannot displace the residual ⁶⁰Ni. It is noteworthy that for the cases where the recoil energy is comparable with E_d , the direction-dependence of E_d should also be considered.

E_R^m are more than 7 times larger than the threshold displacement energies for the residual nuclei from ^{62,64}Co and ^{28,29,30}Al beta decays (shown in boldface in Table 5). Using E_R^m for a conservative estimate, the ^{28,29,30}Si residual nuclei from ^{28,29,30}Al beta decays respectively lead to 3.6, 2.6, and 13.8 atomic displacements based on the NRT formula. These values show that the beta decay-induced primary radiation damage may be important for silicon-based semiconductors and detectors.

For emitted electron-induced atomic displacement, one can use the electron-induced DPA cross section and the corresponding electron spectrum. It is noteworthy that the maximum electronic collision-induced recoil energy is:

$$E_{R,e}^m = \frac{4mM_T Q}{(m + M_T)^2} \quad (26)$$

where M_T is the mass of the target particle. The values of $E_{R,e}^m$ using $M_T \approx M$ are also given in Table 5. These values are representative for materials where the atomic masses are close. It is also found that the electrons from beta decay cannot induce atomic displacement damage in tungsten, while these electrons are able to displace atoms in steels.

4. Conclusions

Since most unstable nuclei from neutron-induced nuclear reactions are beta emitters and the beta decay is a three-body reaction, the present work investigates the beta decay-induced atomic displacement damage. The atomic displacement induced by the emitted electron of a beta decay can be directly calculated with the corresponding electron spectrum and electron-induced damage cross section. For electron-induced displacement damage, this paper proposes a modified NRT formula (mNRT) according to the definition of the threshold atomic displacement energy. The example of ⁵⁶Mn beta decay shows that the use of mNRT leads to 36% more DPA than the standard NRT. Moreover, if

Table 5

Maximum recoil energy from beta decay.

Mother	Q_{max} (MeV)	Daughter	E_R^m (eV)	$E_{R,e}^m$ (eV)	E_d (eV)
¹⁸² Ta	1.714	¹⁸² W	14	21	90 [33]
¹⁸³ Ta	0.659	¹⁸³ W	3	8	
¹⁸⁴ Ta	1.585	¹⁸⁴ W	12	19	
¹⁸⁵ Ta	1.820	¹⁸⁵ W	15	22	
¹⁸⁶ Ta	3.778	¹⁸⁶ W	52	45	
¹⁸⁵ W	0.433	¹⁸⁵ Re	2	5	60 [34]
¹⁸⁷ W	1.311	¹⁸⁷ Re	9	15	
⁵⁶ Mn	2.849	⁵⁶ Fe	106 ^b	112	40 [33]
⁵⁷ Mn	2.679	⁵⁷ Fe	93	103	
⁶⁰ Co ^a	0.318	⁶⁰ Ni	4	12	33 [33,34]
	1.491		34	55	
⁶² Co	5.315	⁶² Ni	292 ^c	188	
⁶⁴ Co	7.307	⁶⁴ Ni	511	251	
⁵² V	2.542	⁵² Cr	94	107	40 [33]
⁵³ V	2.430	⁵³ Cr	85	101	
²⁸ Al	2.863	²⁸ Si	213	225	20.5 [35]
²⁹ Al	2.406	²⁹ Si	153	182	
³⁰ Al	6.326	³⁰ Si	832	463	
²⁷ Mg	1.766	²⁷ Al	98	144	27 [33,34]

(See above-mentioned references for further information.)

^a Q_{max} of ⁶⁰Co beta decay is 1.491 MeV but the branch ratio is 0.12%, 99.88% beta decay has 0.318 MeV Q -value.^bData in red have influence on atomic displacement by kinetic recoil of the residual nucleus because $E_R^m > E_d$.^cData in boldface are $E_R^m > 7E_d$.

the mNRT and Mott's series are used rather than the NRT and McKinley-Feshbach approach, the electron-induced DPA will be increased by a factor of 1.5 for the emitted electron of ^{56}Mn beta decay.

The recoil energy of residual nucleus due to nuclear decay is not considered in particle transport codes. However, this part can be important for atomic displacement calculation of beta decay. The present work illustrates the method to calculate the spectrum of recoil energy in a beta decay according to the energy distribution of electron. For ^{56}Mn beta decay, the residual nucleus-induced DPA is larger than that induced by the emitted electron by a factor of 13.5 (and 20 if the NRT and McKinley-Feshbach approach are used). However, if the method proposed in Ref. [9] is used, the residual nucleus-induced atomic displacement would be overestimated by a factor of 2.5.

Because the kinetic energy of the residual nucleus is quasi-inversely proportional to its mass, the recoil energy is almost unable to displace atoms for heavy isotopes such as tungsten. However, the recoil energy of residual nucleus in beta decay is higher than the atomic displacement threshold for elements in stainless steel. Therefore, the accurate calculation or the reasonable estimate proposed in the present work should be used to compute the beta decay-induced atomic displacement. It is remarkable that the method used in SPECTRA-PKA [9] gives a conservative result (verified by Eq. (21)) for beta decay because it neglects the energy lost to antineutrino and gamma cascade.

CRediT authorship contribution statement

Shengli Chen: Conceptualization, Data curation, Formal analysis, Investigation, Methodology, Software, Validation, Visualization, Writing - original draft. **David Bernard:** Formal analysis, Investigation, Methodology, Supervision, Validation, Visualization, Writing - original draft.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Appendix A. Supplementary data

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.nimb.2020.01.017>.

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