Chapter 12 Radiation Damage

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12.1 Introduction and Historical Background

While in service, reactor materials are exposed to intense fast neutron and gamma fluxes originating from the fission reactions taking place in the fuel. The interaction of these energetic particles with the atoms of the metallic structures displaces the atoms from their stable positions in the crystalline lattice, thus creating lattice defects. The exact nature and density of such defects is at the root of the microstructure changes suffered by these materials during irradiation. These characteristics are determined by the radiation damage process, which is the subject of this chapter.

After the Second World War, civilian applications of nuclear power were at the forefront of technological development in society. In that context, it was recognized that radiation damage to materials used in nuclear reactors would play a large role in determining the suitability of such materials for service. E. Wigner’s predicted in 1946 that radiation damage would degrade material properties [1], so the term “Wigner disease” was coined to encompass the deleterious changes in material properties when exposed to irradiation by energetic particles.

Intense scientific efforts started around the world to characterize radiation damage in materials of interest for nuclear applications, such as metallic uranium, graphite, uranium dioxide, steels, and zirconium alloys, at first in secret research programs. With the advent of the Atoms for Peace initiative in 1954, this information started to be shared, principally in the International Conferences for the Peaceful uses of Nuclear Energy. In parallel with these technological applications of nuclear power, physicists recognized that energetic particles could be used to produce controlled concentrations of point defects in solids. This spawned a significant effort to study the properties of these defects by techniques such as resistivity changes and positron annihilation spectroscopy. In the last two decades these efforts have been converging, as physicists tackle more and more complex technological problems and as engineers seek to understand the underlying physical mechanisms for radiation degradation in increasingly greater detail.

12.2 Particle-Solid Interactions

It is useful to divide the effect of an external flux of energetic particles in a metal into two components: (i) creation of primary knock-on atoms and (ii) creation of transmuted atoms. Both of these result from the interaction of the particles with the atoms in the solid, as shown in Figure 12.1:
where \( \phi_i(E_i) \) represents all particle fluxes \( i \) incident on the solid \((i=\text{neutron, gamma, ions, ...})\), while \( \Sigma_\kappa(E_i,E) \) represents the probability of interaction of all relevant particle-solid reactions \( \kappa \), transferring energy \( E \) to the atoms in the solid (see box 12.1). The product of interaction of the flux of energetic particles (represented by \( \phi \)) and the atoms in the solid (represented by \( \Sigma \)) is the creation of \( N_{\text{PKA}}(E) \) self-atom recoils called primary knock-on atoms \( \text{(PKAs)} \) and a concentration of transmutation atoms \( C_k \), where \( k \) represents the atomic species created.

Many processes cause atomic displacements in solids under the flux of energetic particles, and some of these are discussed in this chapter. However, the largest contributor to displacement damage of structural components in reactor cores is a fast neutron flux (in which case \( \phi_i(E_i) = \phi_n(E_n) \)) interacting by elastic scattering (and so \( \Sigma_\kappa = \Sigma_s \)) with the atoms in the solid, creating a distribution of primary recoils \( N_{\text{PKA}}(E) \), which in turn displace other atoms. This is the case discussed in greatest detail in this chapter.

**Box 12.1: Cross-Section**

The probability of occurrence of a particular reaction between the atoms in the solid and the incident particle flux is commonly represented in terms of the cross-section for the reaction. The concept of the microscopic cross-section is illustrated in figure 12.2. It derives from the experimental measurement of the reaction rates and consists of the attribution of an apparent size to the atoms in the solid, depending on whether the reaction rate is high or low. That is, given a particle flux into a solid of a given atomic density, the probability of reaction increases with the apparent particle size. This is illustrated in Figure 12.2. Two types of atoms are present in the solid: atom A has a greater reaction rate for reaction 1 than atom B, and thus these atoms appear very large when reaction 1 is considered. In contrast, for reaction 2, atom B has a much larger cross section and consequently these atoms appear much bigger when reaction 2 is considered.
If for example Reaction 1 is taken to be nuclear fission and Reaction 2 the \((n, \alpha)\) reaction (absorption of neutron and emission of an alpha particle), with atom A (light atoms) being uranium-235 and atom B (dark atoms) being boron-10. When submitted to a thermal neutron flux the cross sections for reactions 1 and 2 would qualitatively appear as in figure 12.2. The microscopic cross-section is given in units of barn \((10^{-24} \text{ cm}^2)\). The macroscopic cross-section \(\Sigma\) \((\text{cm}^{-1})\) is simply the product of the microscopic cross-section and the atomic density \((\text{cm}^{-3})\). The usefulness of the cross section concept comes from the fact that when multiplied by a particle flux \((\text{particle.s}^{-1}\text{.cm}^{-2})\), the reaction rate \(RR = \phi \Sigma\) \((\text{reactions.s}^{-1}\text{.cm}^{-3})\) is obtained.

Considering a solid containing \(N\) targets per unit volume through which passes a single particle of energy \(E_i\), the differential probability \(dP\) that this particle will interact with one of the target atoms in an element of small thickness \(dx\) is given by:

\[
dP = N\sigma(E_i)dx = \Sigma dx
\]  

\textit{(12.1)}

Equation 12.1 is valid for any reaction (absorption, fission, scattering, etc.). If \(\sigma(E_0)\) is an elastic scattering cross section, then the result of such an interaction is a transfer of energy \(T\) from the energetic particle to the struck atom, which then becomes an energetic recoil atom, called the primary knock-on atom (PKA). The PKA energy distribution is the primary means of characterizing the damage caused by irradiation.
The creation of foreign atoms will be considered elsewhere in this book. We will consider in this chapter the displacement damage caused by the interaction of the energetic particles with the solid. When a neutron flux passes through a solid, fast neutrons can scatter elastically or inelastically, and thermal neutrons can induce nuclear reactions, all of which can deposit energy onto the material. In any case, the result of a neutron-atom interaction is the formation of a Primary Knock-on Atom (PKA). We use the following notation for the energies of the particles concerned:

\[
\begin{align*}
E_n & \Rightarrow E \\
\text{Neutron} & \Rightarrow \text{PKA} \\
& \Rightarrow \text{Secondary Recoils}
\end{align*}
\]

The problem of calculating the displacement damage can be divided into the tasks of (i) finding the energy spectrum of the PKA created by interaction of the neutrons with the solid and (ii) calculating how much damage a PKA of a given energy can produce. We address the second question in the next few sections and later in the chapter we consider the first.

12.3. Primary Knock on Atom (PKA) Energy Loss Mechanisms

Given a PKA of energy \( E \), the total rate of energy loss while moving through a solid can be separated into three different components:

\[
\frac{dE}{dx}_{\text{TOTAL}} = \frac{dE}{dx}_E + \frac{dE}{dx}_N + \frac{dE}{dx}_I
\]

(12.2)

where the three terms on the RHS of equation 12.2 refer to electronic energy loss (E), nuclear elastic scattering (N) and nuclear inelastic scattering (nuclear reactions) (I). Because the typical PKA energies are considerably lower than the typical energy values required for inelastic scattering, the first two processes dominate energy loss in most materials of interest. In metals, because the electrons are shared by all atoms in the lattice, the collisions with electrons have little permanent consequence to the solid; the energy of high-speed electrons is degraded into heat. In insulators or electronic materials, however, electronic damage can be significant. Nuclear elastic scattering can cause permanent damage in the form of atomic displacements. The partition between these two forms of energy loss determines the amount of radiation damage and the subsequent radiation effects observed. We now consider these processes in turn.
Box 12.2

Binary Elastic Collision Dynamics

We derive here the energy transfer between two hard spheres that collide. Figure 12.3 shows such a process in the laboratory frame of reference. An atom mass $M_1$ and velocity $v_{10}$ strikes a stationary atom mass $M_2$. After the collision, they scatter at angles $\varphi_1$ and $\varphi_2$ and velocities $v_{1F}$ and $v_{2F}$.

![Figure 12.3: Schematic depiction of the elastic scattering process in the laboratory frame of reference.](image)

In the center of mass system, the above collision is shown as:

![Figure 12.4: Schematic depiction of the elastic scattering process in the center of mass frame of reference.](image)

The center of mass has the equivalent mass of the system $(M_1+M_2)$ and from conservation of momentum from one frame of reference to another we obtain the center of mass velocity $v_{CM}$

$$v_{CM} = \frac{M_1}{(M_1 + M_2)} v_{10} \quad (12.3)$$
If we take two instants, the first well before the collision and the second well after the collision, and apply conservation of kinetic energy and momentum, we can write the following equations in the center of mass system:

\[ M_1u_{10} = M_2u_{20} \]  \hspace{1cm} (12.4)

\[ M_1u_{1F} = M_2u_{2F} \]  \hspace{1cm} (12.5)

\[ \frac{1}{2} M_1u_{10}^2 + \frac{1}{2} M_2u_{20}^2 = \frac{1}{2} M_1u_{1F}^2 + \frac{1}{2} M_2u_{2F}^2 \] \hspace{1cm} (12.6)

where \( u_{10} = v_{10} - v_{CM} \) and \( u_{20} = -v_{CM} \)

Substituting equation 12.3 and 12.4 into 12.5 we obtain \( u_{1F} = u_0 \) for both particles, and thus \( u_{2F} = v_{CM} \). From the definition of the center of mass velocities and noting that \( u_{1F} \) and \( u_{2F} \) have the same orientation but opposite directions, the following vectorial relationship exists for the velocities:

![Figure 12.5 Relationship between velocities in the center of mass and laboratory frame of reference.](figure)

Using the law of cosines:

\[ v_{2F}^2 = v_{CM}^2 + u_{2F}^2 - 2v_{CM}u_{2F}\cos\theta \] \hspace{1cm} (12.7)

but since \( v_{CM} = u_{2F} \)

\[ v_{2F}^2 = 2v_{CM}^2(1 - \cos\theta) \] \hspace{1cm} (12.8)

multiplying by \( M_2/2 \), and substituting for \( v_{CM} \) we obtain

\[ E_{2f} = \frac{M_2}{2}v_{2F}^2 = \frac{M_2}{2} \left( \frac{M_1}{M_1 + M_2} \right)^2 v_{10}^2(1 - \cos\theta) = \frac{1}{2} \left( \frac{4M_1M_2}{(M_1 + M_2)^2} \right) (E_{10})(1 - \cos\theta) \]
Equation 12.9 describes the energy $E_{2f}$ transferred to an atom of mass $M_2$ by an energetic particle energy $E_{10}$ and mass $M_1$ as a function of the scattering angle in the center of mass system

$$\Lambda_{M_1M_2} = \frac{4M_1M_2}{(M_1 + M_2)^2}$$

(12.10)

Noting that the initial kinetic energy of particle 1 is $E = \frac{1}{2}M_1v_{10}^2$, we obtain

$$E_{2f} = \frac{1}{2} \Lambda E_{10}(1 - \cos \theta) \quad \text{or if } E_{2f} = T \text{ and } E_{10} = E$$

(12.11)

The maximum amount of energy transferred occurs for a head-on collision in which $\theta = \pi$ and

$$T = \frac{1}{2} \Lambda E(1 - \cos \theta)$$

(12.11)

The amount of energy transferred changes with the mass ratio between the energetic particle and the struck atom. For atoms of equal mass $\Lambda = 1$, that is, in a head-on elastic collision the incoming atom transfers all of its energy to the struck atom. As the masses become more different, the maximum transferred energy decreases.

For example, in a steel (Fe-C) under 1 MeV neutron irradiation the maximum energy transfer from the neutron to the carbon atom is $E_{n,c} = 0.28$ $E_n$ (280 keV) and $E_{n,Fe} = 0.07$ $E_n$ (70 keV). Thus a 1 MeV neutron can only transfer 70 keV in an elastic collision with an iron atom. The 280 keV C primary knock-on atom could then transfer up to 100% of its energy to another C atom but only $T_{C,Fe} = 0.58$ $E_{n,C}$ (162 keV) to an Fe atom. The 70 keV Fe primary knock-on atom in turn could transfer up to 100% of its energy to another Fe recoil atom but only $T_{Fe,C} = 0.58$ $E_{n,Fe}$ (40.6 keV) to a C atom.

Close box 12.2

12.3.1. The limit between nuclear and electronic stopping

Because the electronic density in the material is far greater than the atom density, as long as the energetic particles can transfer energy to the electrons, they preferentially do so. The limiting factor is that in order for the electrons to be able to accept the energy given by the atoms, they need to receive an energy amount equal to or greater than their ionization energy. For metals, since the average kinetic energy of the conduction electrons is about $3/5$ of the Fermi energy $\varepsilon_F$, the ionization energy is approximately

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equal to $2/5 \varepsilon_F$. A simple way to estimate the energy transferred in a collision between an atom mass $M$, energy $E$ and an electron is to use equation 12.11 above:

$$T_{EL}^{\text{max}} = \Lambda_{M-e} E \approx \frac{4m_e}{M} E$$  \hspace{1cm} (12.12)

Setting $T_{EL}^{\text{max}} = I$ (ionization energy) we obtain the minimum PKA energy for electronic energy transfer

$$E > E^* = \frac{M}{4m_e} I$$  \hspace{1cm} (12.13)

The value of 5 eV is a good approximation of the Fermi energy in metals and thus $I \sim 2$ eV; if we take $m_e = \frac{1}{1840} \text{amu} \approx \frac{1}{2000} \text{amu}$, then we obtain a convenient formula for the cutoff energy:

$$E^* \approx 1000 \times M_i [eV] = \mathcal{M}(keV)$$  \hspace{1cm} (12.14)

Thus, the cutoff energy for electronic energy loss $E^*$ is numerically equal to the atomic mass $\mathcal{M}$, expressed in units of keV. For example, according to the model above a $^{56}_{26}Fe$ atom traveling through a solid, starts losing energy to nuclei below 56 keV, approximately.

Clearly, electronic energy loss continues to occur to some extent below $E_{\text{min}}$, in parallel with nuclear stopping, but it is difficult to evaluate its contribution analytically. It is possible, however, to evaluate this energy partitioning by Monte Carlo computer simulation. The computer programs TRIM (TRansport of Ions in Matter) and SRIM (Stopping and Range of Ions in Matter), [2], (described in section 12.8) are Monte Carlo programs that use specially developed interatomic potentials to calculate the energy deposition of energetic atoms in solids. Such programs take into account both electronic and nuclear stopping simultaneously to achieve a more realistic energy partition (see box 12.3 at the end of this chapter.)

12.3.2. Electronic Stopping: energy transfer rate

We now consider the energy transfer from a PKA energy $E$, mass $M_1$ to the electrons in the solid. The transfer is calculated differently depending on the ion energy.

For high energy ions, (in which the ion velocity $v_1 > 3 v_{EL}$, velocity of electrons), as the atom travels through the solid, some of its electrons are stripped off, causing the atom to become a charged particle of effective charge $Z_{\text{eff}}$. Because the effective charge changes with atom energy, it constantly changes as the atom loses energy while traveling through
the solid. If $Z_{\text{eff}}$ is known, then the Bethe formula gives an approximate expression for the electronic energy loss:

$$
\frac{dE}{dx}_{\text{EL}} = \frac{2\pi n_e Z_{\text{eff}}^2 e^4 (M_i/m_e)}{E} \ln \left[ \frac{4E}{(M_i/m_e)\bar{I}} \right]
$$

(12.15)

where $n_e$ is the electron density, $e$ is the electron charge, and $\bar{I}$ the average ionization energy. The value of the effective charge was computed by Bohr as

$$
Z_{\text{eff}} = \frac{Z_1}{e^2} \left( \frac{2E}{M_1} \right)^{1/2}
$$

(12.16)

where $\hbar$ is Planck’s constant divided by $2\pi$, and $Z_1$ is the atomic number of the energetic particle.

For the case of low energy ions ($v_1 < v_{EL}$), the energy transfer to an electron in an atom-electron collision is

$$
T_{EL} = \frac{1}{2} m_o (v_{ELf}^2 - v_{EL}^2)
$$

(12.17)

where $v_{ELf}$ and $v_{EL}$ are the final and initial electron velocities, and $m_o$ is the rest mass of the electron. But, from conservation of momentum,

$$
v_1 + v_{EL} = v_{ELf} - v_1 \quad \text{and} \quad \therefore v_{ELf} = v_{EL} \left( \frac{2v_1}{v_{EL}} + 1 \right)
$$

(12.18)

where $v_1$ is the PKA velocity. Thus,

$$
T_{EL} \approx 2m_o v_1 v_{EL} = 2m_o \left( \frac{2E}{M_1} \right) \left[ \frac{2(3\varepsilon_F / 5)}{m_o} \right] = A\sqrt{E}
$$

(12.19)

The energy transfer rate is given by

$$
\frac{dE}{dx}_{\text{EL}} = \frac{\text{collisions}}{PKA.s} \times \frac{\text{energy lost}}{\text{collision}} \times \frac{\text{distance travelled}}{PKA.s} = (\sigma_e J_{EL}) \times (T_{EL}) \div (v_1)
$$

(12.20)

where $\sigma_e$ is the cross section for atom-electron scattering, $J_{EL}$ is the flux of electrons seen by the moving PKA and is equal to $J_{EL} = n_{EL} (v_{EL} + v_1) \approx n_{EL} v_{EL}$ for low energy PKAs, but since below the Fermi level all states are occupied, the “excitable” fraction of electrons is $n_{EL} = \frac{T_{EL}}{\varepsilon_F} N_{EL}$ where $N_{EL}$ is the total electron density in the material.
Since the average electron initial kinetic energy is $3/5 \varepsilon_F$, and
\[
\frac{dE}{dx}_{EL} = (\sigma_e J_{EL}) \times (T_{EL} / v_i) = \sigma_e \left( \frac{T_{EL} N_{EL} v_{EL}}{\varepsilon_F} \right) (2m_e v_i v_{EL}) / v_i = 2.4 \sigma_e N_{EL} T_{EL} \quad (12.21)
\]

But $T_{EL} = A\sqrt{E}$, and for a given material, the cross section for electron-ion collisions varies slowly with energy, and the other terms are constant, so

\[
\frac{dE}{dx}_{EL} = K \sqrt{E} \quad (12.22)
\]

Detailed calculations by Lindhard show that

\[
K = 0.3 N_a Z^{2/3} \left( \frac{\sqrt{eV}}{A} \right) \quad (12.23)
\]

where $N_a$ is the atomic density (Å⁻³) and $Z$ is the atomic number. Thus, in the electron stopping region the energy loss rate by the PKA is proportional to the square root of the PKA energy.

### 12.3.3. Nuclear stopping

When the energetic particle slows down enough that it becomes difficult for it to transfer energy to the electrons, it starts to lose energy by collisions with the nuclei in the solid. For elastic collisions, a PKA with energy $E$ will strike an atom in the solid, and transfer energy $T$, leaving it with energy $E-T$. The moving atom can transfer to the atom in the solid any energy between 0 and $\Lambda E$. The probability that a particle energy between $E$ and $E+dE$ will transfer to an atom in the solid an energy between $T$ and $T+dT$ is given by the differential energy cross section $\sigma(E,T)$.

The differential cross section $\sigma(E,T)$ and the total cross section $\sigma(E)$ are related by

\[
\sigma(E) = \int_0^\Lambda \sigma(E,T) dT \quad (12.24)
\]

The average energy loss $dE$ in $dx$ (called the stopping power) is given by integrating equation 12.24 over all possible values of the transferred energy $T$:

\[
dE = \int_0^\Lambda N \sigma(E,T) T dT dx \quad (12.25)
\]
where $T_n=\Lambda E$, and thus the nuclear stopping power is given by

$$\left.\frac{dE}{dx} \right|_N = \int_0^E N\sigma(E,T) dT$$

(12.26)

The detailed process of atomic scattering and the energy loss for a single collision can be derived more exactly than in box 12.2. Using conservation of energy and momentum we can arrive at a relationship between the scattering angle in the center of mass system and the impact parameter, in the following.

### 12.3.4. Ion-Atom Scattering; General Binary Collision Dynamics

We study here a collision between two particles with a specified interaction potential $V(r)$, and which collide with an impact parameter $p$ as shown in Figure 12.6. The objective of this derivation is to find the orbit of two particles in an elastic collision and to relate the interaction potential to the differential cross section $\sigma(E,\theta)$.

![Figure 12.6: Geometry for derivation of elastic collision between energetic ion and atoms, interacting by a potential $V(r)$.](image)

In the system considered, a particle mass $M_1$ is moving initially with kinetic energy $E$ towards an initially stationary particle mass $M_2$. The center of mass CM is located on the line joining the two masses at a position

$$r_1 = \frac{M_2}{M_1 + M_2} r_1 \sin \alpha$$

and $r = r_1 + r_2$

(12.27)

from the mass $M_1$. The velocity of particle 1 in the center of mass system is $u_{10}$, and that is decomposed into two perpendicular components $\hat{r}_1$ and $\hat{S}_1$, such that $\hat{u}_{10} = \hat{S}_1 + \hat{r}_1$. The line between the particles makes an angle $\alpha$ with the initial direction of the particles in
the CM system. Only the initial kinetic energy in the CM system is convertible to potential energy, and this is written

\[ E_{co} = \frac{1}{2} (M_1 + M_2) v_{CM}^2 \]  

(12.28)

and using equation 12.3

\[ E_{co} = \frac{M_1}{M_1 + M_2} E \]  

(12.29)

where \( E \) is the initial kinetic energy of particle 1 in the laboratory frame. We now use conservation of energy and angular momentum during the collision to derive a relationship between the scattering angle in the center of mass \( \theta \) and the impact parameter \( p \). The geometry of the collision is shown in Figure 12.7, showing the trajectory of the particles as they interact and are deflected by angle \( \theta \).

**Conservation of Energy**

As the two energetic particles approach each other they convert kinetic energy into potential energy, so that at the distance of closest approach the kinetic energy is minimal. The conservation of energy for the system is written

\[
E_{co} = V(r) + \frac{1}{2} M_1 u_{10}^2 + \frac{1}{2} M_2 u_{20}^2 = V(r) + \frac{1}{2} M_1 (r_1^2 + \dot{S}_1^2) + \frac{1}{2} M_2 (r_2^2 + \dot{S}_2^2)
\]  

(12.30)

Figure 12.7: Geometry during the collision. As the particles approach they are scattered by the repulsive potential \( V(r) \).

The tangential speeds \( \dot{S} \) are equal to \( r \dot{\psi} \), and we can then write equation 12.30 as
\[ E_{co} = V(r) + \frac{1}{2} M_1 (r_1^2 + r_1^2 \psi^2) + \frac{1}{2} M_2 (r_2^2 + r_2^2 \psi^2) \]  
(12.31)

and using the definition of the center of mass

\[ E_{co} = V(r) + \frac{1}{2} \left( \frac{M_1 M_2}{M_1 + M_2} \right) (\dot{r}^2 + r^2 \dot{\psi}^2) \]  
(12.32)

but \[ \dot{r}^2 = \left( \frac{d\psi}{d\psi} \right)^2 + \left( \frac{dr}{d\psi} \right)^2 \dot{\psi}^2 \]  
(12.33)

so that

\[ E_{co} = V(r) + \frac{1}{2} \left( \frac{M_1 M_2}{M_1 + M_2} \right) \left( \left( \frac{dr}{d\psi} \right)^2 + r^2 \right) \dot{\psi}^2 \]  
(12.34)

**Conservation of Angular Momentum**

The angular momentum of a mass \( M \) about an axis is \( \vec{r} \times (\vec{M}\vec{u}) = rMu \sin \alpha = rM\dot{\mathbf{S}} \) where \( r \) is the distance between the particle and the axis, \( u \) is the velocity and \( \alpha \) is the angle between \( r \) and \( u \). Then, the total angular momentum in the CM system is equal to

\[ L = r_1 M_1 u_{10} \sin \alpha + r_2 M_2 v_{CM} \sin \alpha \]  
(12.35)

The tangential velocity \( \dot{\mathbf{S}} \) is equal to \( r\dot{\psi} \) and thus

\[ L = L_1 + L_2 = M_1 \dot{S}_1 r_1 + M_2 \dot{S}_2 r_2 = M_1 r_1^2 \dot{\psi} + M_2 r_2^2 \dot{\psi} \]  
(12.36)

Using the definition of CM velocity in equation 12.35 and equating to 12.36

\[ L = \frac{M_1 M_2}{M_1 + M_2} v_{10} (r_1 \sin \alpha + r_2 \sin \alpha) = \frac{M_1 M_2}{M_1 + M_2} v_{10} p = M_1 r_1^2 \dot{\psi} + M_2 r_2^2 \dot{\psi} \]  
(12.37)

from where using 12.27 in 12.37 we obtain an expression for \( \dot{\psi} \)

\[ \dot{\psi} = \frac{v_{10} p}{r^2} \]  
(12.38)

and thus we can eliminate the \( \dot{\psi} \) in equation 12.37

\[ E_{co} = V(r) + \frac{1}{2} \left( \frac{M_1 M_2}{M_1 + M_2} \right) \left[ \left( \frac{dr}{d\psi} \right)^2 + r^2 \right] \left( \frac{v_{10} p}{r^2} \right)^2 \]  
(12.39)

Then using 12.29 to eliminate \( v_{10} \) we obtain

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\[
\frac{d\psi}{dr} = \frac{p}{r^2} \left[ 1 - \frac{V(r)}{E_{co}} - \frac{p^2}{r^2} \right]^{-1/2} \tag{12.40}
\]

When the particles are at their closest distance \( r=r_o \) and \( \psi=\pi/2 \) and when \( r \) goes to infinity the angle \( \psi \) goes to \( \psi=\theta/2 \). We integrate equation 12.40 over half the orbit (from the distance of closest approach to infinity).

\[
\int_{\theta/2}^{\pi/2} d\psi = \frac{\pi}{2} - \frac{\theta}{2} \tag{12.41}
\]

and obtain the Classical Scattering Integral

\[
\theta = \pi - 2 \int_{r_o}^{\infty} \frac{pdr}{r^2 \left[ 1 - \frac{V(r)}{E_{co}} - \frac{p^2}{r^2} \right]^{1/2}} \tag{12.42}
\]

Equation 12.42 relates the impact parameter \( p \) to the scattering angle in the center of mass \( \theta \). At the distance of closest approach \( dr/d\psi=0 \) and

\[
1 - \frac{V(r_o)}{E_{co}} - \frac{p^2}{r_o^2} = 0 \tag{12.43}
\]

Equation 12.43 can be solved for the distance of closest approach as a function of impact parameter. In a head-on collision \( p=0 \) and equation 12.43 reduces to \( V(r_o)=E_{co} \), which using equation 12.27 yields the distance of closest approach in the head-on case.

**Relation of Impact parameter to Differential cross section**

![Figure 12.8: The geometry of the differential cross section.](image)

Equation 12.27 yields the distance of closest approach in the head-on case.
As shown in Figure 12.8, if the impact parameter is in the range \( p \) to \( p + dp \) the annular ring of area \( 2\pi dp \) is the area associated with the annular cone \( 2\pi \sigma(E, \theta) d(cos \theta) \) and thus

\[
\sigma(E, \theta) = \frac{1}{2} \frac{dp^2}{d(cos \theta)}
\]  

(12.44)

If the potential \( V(r) \) is known, then equation 12.42 can be integrated to give the final orbit of the particle after the scattering event, i.e., \( \theta \) as a function of \( p \). Then equation 12.44 allows the determination of the cross section. This process is only possible to perform analytically for a few simple potentials, and in most cases it is necessary to perform the integration numerically. One of these analytical cases is the Rutherford cross section, shown in Example 12.1.

**Example 12.1**

**Rutherford Cross Section**

The Rutherford cross-section arises from the substitution of the unscreened Coulomb potential

\[
V(r) = \frac{Z_1 Z_2 e^2}{r}
\]  

(12.45)

in equation 12.42 to give

\[
\theta = \frac{\pi}{2} - \int_0^1 \frac{du}{\left[1 - au - p^2 u^2\right]^{1/2}}
\]  

(12.46)

where \( u = \frac{r_o}{r} \), \( \alpha = \frac{C}{r_o E_{\text{co}}} \), \( C = Z_1 Z_2 e^2 \), \( P = \frac{p}{r_o} \)  

(12.47)

The analytical solution of equation 12.46 is

\[
\theta = \frac{\pi}{2} - \sin^{-1}\left(\frac{\alpha + 2P^2}{\sqrt{\alpha^2 + 4P^2}}\right) + \sin^{-1}\left(\frac{\alpha}{\sqrt{\alpha^2 + 4P^2}}\right)
\]  

(12.48)

The dimensionless form of equation 12.43 is

\[
P^2 = 1 - \alpha
\]  

(12.49)

Using 12.49 in 12.48 equation 12.48 reduces to

\[
\alpha = \frac{2 \sin(\theta/2)}{1 + \sin(\theta/2)}
\]  

(12.50)

Substituting equations 12.47, 12.50 into 12.49 we obtain
\[ p^2 = \frac{C^2}{4E_{\text{co}}} \left( \frac{1 + \cos \theta}{1 - \cos \theta} \right) \]  

(12.51)

The impact parameter \( p \) goes to zero as \( \theta \to \pi \) (head-on collision) and as \( \theta \to 0 \) \( p \to \infty \) (complete miss).

Now substituting equation 12.51 into equation 12.44, the Rutherford cross section results

\[ \sigma(E, \theta) = \frac{Z_1^2 Z_2^2 e^4}{16E^2} \left( \frac{M_1 + M_2}{M_2} \right)^2 \frac{1}{\sin^4(\theta/2)} \]  

(12.52)

This can be converted into an energy transfer cross section by noting that

\[ \sigma(E, T) = \left[ \frac{2\pi l(\cos \theta)}{dT} \right] \sigma(E, \theta) = \frac{4\pi}{\Lambda} \sigma(E, \theta) \]  

(12.52a)

and thus,

\[ \sigma(E, T) = \pi Z_1^2 Z_2^2 e^4 \left( \frac{M_1}{M_2} \right) \frac{1}{ET^2} \]  

(12.53)

The Rutherford cross-section decreases with increasing PKA energy. Note also that small scattering angles (which correspond to small values of the transferred energy \( T \)) are strongly favored also.

We have, so far, examined the stopping process from the point of view of the energetic particle, as it deposits energy in the solid. In metals, while the electronic energy loss in most cases does not lead to permanent accumulation of damage, the nuclear energy loss can lead to the displacement of atoms from their equilibrium lattice positions. This process is described in the next section.

### 12.4. The Displacement Process

#### 12.4.1. Threshold Displacement Energy

As a result of scattering of energetic particles, atoms in the solid can be displaced from their equilibrium lattice positions, creating a vacant lattice site and a self-interstitial atom (SIA). This vacancy-interstitial pair is called a Frenkel pair (FP).

Normally the struck atom is not the one that eventually ends as a SIA; instead, the struck atom starts a replacement collision sequence (RCS) along one of the close packed crystallographic directions. Figure 12.9 illustrates the displacement process schematically. If the initial energy of the struck atom is too low, the RCS propagates along the close packed direction and then returns each atom to its original location; if the energy is high enough, the RCS returns only partway to the original struck atom location. At the limit of the recovered and non-recovered parts a SIA atom is formed; thus a
replacement collision sequence causes each atom to displace its neighbor in a “domino” effect, with an interstitial atom at the end, thus creating a Frenkel pair. In the recovered part, only energy is transferred along the line of close packed atoms and no atom is permanently displaced; this is called a *focusson*. The minimum energy required to displace the atoms enough so that they do not return to its initial site is the displacement energy $E_d$. Depending on which crystallographic direction the displacement is originated, the original atom has to travel a longer or shorter distance. The limit of the minimum distance traveled to create a permanent FP is defined as the minimum distance to avoid athermal recombination (i.e. without need for an atomic jump to take place). The cross-shaped enclosure in Figure 12.9 shows schematically this recombination volume. Any vacancy inside this volume will spontaneously recombine with the interstitial at the center.

![Diagram](image)

*Figure 12.9 Schematic representation of the succession of atomic displacements involved in the creation of a permanent Frenkel pair [3]*

Clearly, because of this, the displacement energy depends on the crystalline orientation. This has been demonstrated, both experimentally and computationally. Figure 12.10 shows the variation of $E_d$ with crystalline orientation in pure Cu. The displacement energy is lowest along some of the low index crystallographic directions such as (110) and (100) but highest along (111).
Figure 12.10. The variation of displacement energy in with crystalline orientation in Cu as measured in-situ [3]

Because of the intrinsic uncertainties of displacement measurements and calculations, it is customary to use an average displacement energy. For metals the average displacement energy is on the order of 20-40 eV. Compilations of displacement energies for various materials can be found in [4], but it has been proposed that 40 eV be used whenever more precise knowledge does not exist [5]

For intermetallic compounds and ceramics, where sublattices and chemical ordering exist, the displacement energy can be much higher and also vary widely depending on the atomic species or sublattice considered [7]. In addition, point defects of one type can be unstable, decaying to the other type of defect (as discussed in Chapter 24). This is also true in solid solutions where displacements of the solvent and solute atoms occur at comparable rates, but if their formation energies differ widely, then one type of interstitial converts to the other type, which causes the interstitial population (and thus the interstitial flux to sinks) to be enriched in one or the other type of atom.

The simple picture of atomic displacement described above does not hold at much higher PKA energies. When the PKA energy is very high, so many atoms in a small region participate in the dissipation of energy that the very notion of crystalline lattice becomes difficult to define. As the PKA energy gets divided between many atoms, a displacement cascade is formed. The displacement cascade is a region where the dissipation of PKA energy causes many atoms to be displaced from their lattice positions. Figure 12.11 shows the results of a computer simulation of such a dissipation process at the end of a displacement cascade. Much clustering occurs in the cascade core, as well as recombination of interstitials and vacancies, thereby reducing the total damage. The region near the cascade also suffers a thermal spike, in which for a few ps the local temperature increases well beyond the melting point, as discussed below
12.4.2. Displacement Cascade and the Final Damage Structure

It is appropriate at this point to consider the actual defect distribution left in the debris of the cascade. In the calculations leading to the NRT formula in the following section we divide the PKA energy among all atoms in the cascade, counting as permanent atomic displacements all energy transfers above $E_d$. In reality, because of the close proximity in which these defects are created, they interact with each other, creating defect clusters and/or restoring the undamaged lattice. This causes the final number of interstitials and vacancies to be smaller than the total number of atoms displaced in the cascade. Since the subsequent microstructural evolution under irradiation depends on the actual number of defects and defect clusters created, it is useful to consider the physical processes occurring in the cascade.

Table 12.1 (adapted from Schilling [3]) Chronology of events during the slowing down of an energetic PKA, and its associated displacement cascade.

<table>
<thead>
<tr>
<th>Duration (ps)</th>
<th>Event</th>
<th>Result</th>
<th>Parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>$10^{-6}$</td>
<td>Transfer of energy from energetic particle</td>
<td>Primary knock on atom (PKA)</td>
<td>$\sigma(E_n, E)=$cross section for particle energy $E_n$ to transfer of energy $E$</td>
</tr>
<tr>
<td>$10^{-6}$ to 0.2</td>
<td>Slowing down of PKA, generation of a displacement cascade and thermal spike</td>
<td>Recoil atoms and Lattice Vacancies Formation of subcascades</td>
<td>$E_d=$displacement energy $\nu_{NRT}=$number of displaced atoms $T=$energy transferred to recoils</td>
</tr>
<tr>
<td>0.2-3.0</td>
<td>Thermal spike</td>
<td>Stable Interstitials</td>
<td>$\nu(T)=$number of stable point</td>
</tr>
</tbody>
</table>
The typical energy given to a PKA (on the order of keVs to 10s of keVs) is far in excess of thermal energies (on the order of hundredths of eVs), and thus energetic PKAs have a large excess of energy with respect to the surrounding atoms. Because the PKA interacts with the surrounding atoms via a screened Coulomb potential, this energy is quickly shared with other atoms, which in turn displace other atoms, until the energy per atom is smaller than the displacement energy. This process, whereby atoms in close proximity to the PKA receive large amounts of energy during a short time, is called the development of the displacement cascade.

As shown in table 12.1, the initial energetic particle-atom energy transfer occurs in a very short time, of the order of $10^{-15}$ s ($10^{-3}$ ps). During the several following picoseconds the PKA shares its energy with other nearby atoms through successive collisions. If one were to stop the process after a few tens of atoms were involved in the cascade, and calculate a “temperature” based on the average kinetic energy involved, this cascade core temperature would be far in excess of the melting temperature. Molecular dynamics simulations of displacement cascades show that during the first few picoseconds the region of the displacement cascade is similar to a molten drop [8].

This energetic thermal spike lasts only a few picoseconds, however, as the cascade is surrounded by a very large thermal reservoir which quickly absorbs the energy, in effect quenching the cascade. This very large difference between the PKA energies and thermal energies is at the root of many of the observed effects of irradiation. In fact, because these energies are so high, the material under irradiation explores crystal structures and defect configurations which are normally inaccessible under thermal driving forces, and which make non-equilibrium phases appear (see chapter 24).

During the “ballistic” or displacive part of the cascade development, a number of atoms $v(T)$ are displaced from their lattice sites, and which corresponds approximately to the value calculated from the Norgett-Robinson-Torrens model, section 12.5. The fate of these displaced atoms now determines the final damage state. Figure 12.12 illustrates the possible fate of these defects.
The interstitials and vacancies in the cascade can either react with similar defects or with opposite defects, or remain isolated. Because they have great mobility in the small time when the thermal spike is developing, during that time defects can cluster and recombine. As we will see in the next chapter, the defect structure created and their mobility at the irradiation temperature of interest are critical to the microstructure changes occurring under irradiation.

In order to quantitatively evaluate neutron irradiation damage on materials, we need to calculate the number of displacements per PKA as function of its energy $E$. This is done in the next section.

### 12.5 Displacements per PKA

The PKA interacts with its neighbors causing many collisions and atomic displacements in a relatively small region. The final damaged state evolves as a result of intra-cascade clustering and recombination, and consists of a distribution of interstitial and vacancy clusters of different sizes. The spatial distribution of these defects is not homogeneous. Because the interstitials are energetic atoms, they are expelled from the center of the cascade through replacement collision sequences, and a vacancy-rich core forms along with an interstitial rich outer rim. This physical separation between interstitials and vacancies enhances defect clustering, relative to recombination. When the cascade cools down, a final damage state is created containing a certain number of point defects and point defect clusters. We arrive then at the stage where irradiation effects, i.e., the long-term interactions of the radiation damage with the microstructure, determine the microstructure evolution under irradiation, as described in Chapter 13.

The total number of displacements for a PKA energy $E$ can be estimated by the following derivation attributed to Kinchin and Pease [6], and also illustrated in Figure 12.13. If the initial PKA energy $E > 2E_d$, the PKA has the ability to cause further displacements in the solid. Assuming elastic collisions, after one collision, the number of displaced atoms is 2 and their average energy $T$ is $E/2$. After two collisions four atoms are involved and $T = E/4$, and after $n$ collisions, $2^n$ atoms are involved and $T = E/2^n$. The condition for the
displacement cascade to end is that $T \leq 2E_d$ (if the energy is more than $E_d$ and less than $2E_d$, the PKA can transfer enough energy to displace an atom, but it takes its place, thus creating no new defects) and thus

$$2E_d = \frac{E}{2^{n_f}} \tag{12.54}$$

where $n_f$ is the final number of collisions. But since after $n_f$ steps, $v=2^{n_f}$, then

$$v_{KP}(E) = \frac{E}{2E_d} \tag{12.55}$$

<table>
<thead>
<tr>
<th>Step</th>
<th>0</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>$n_f$</th>
<th>FINAL</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image.png" alt="Diagram" /></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Average Energy per atom</th>
<th>$E$</th>
<th>$E/2$</th>
<th>$E/4$</th>
<th>$\ldots \ldots$</th>
<th>$E/2^{n_f}$</th>
<th>$2E_d$</th>
</tr>
</thead>
<tbody>
<tr>
<td># of additional atoms</td>
<td>1</td>
<td>2</td>
<td>4</td>
<td>$\ldots \ldots$</td>
<td>$2^{n_f}$</td>
<td>$E/2E_d$</td>
</tr>
</tbody>
</table>

Figure 12.13: Illustration of the derivation of the Kinchin-Pease formula.

This is the Kinchin-Pease formula [9]. The arguments leading to equation 12.14 and adopted in the K-P model predict a sharp cutoff at an energy $E^*$, such that above $E^*$ all energy loss is electronic and below $E^*$ all energy loss is by elastic collisions with atoms. The displacements caused by such a PKA energy $E$ are thus given by:

$$v(E) = \frac{E^*}{2E_d} \text{ if } E > E^*$$

$$v(E) = \frac{E}{2E_d} \text{ if } 2E_d < E < E^*$$

$$v(E) = 1 \text{ if } E_d < E < 2E_d$$

$$v(E) = 0 \text{ if } E < E_d$$
Because it ascribes all of the atom energy to defect production, this model is approximately valid only in the nuclear stopping regime (i.e. for $E < E^*$) and even in this regime there is some electronic stopping. The Lindhard model addresses some of these concerns, by using a more realistic potential than hard-sphere (Thomas-Fermi) to predict the energy partition between electronic and nuclear stopping. Lindhard’s model provides a smooth transition from the electronic loss dominated regime to the nuclear stopping regime. Assuming that the nuclear stopping part of the deposited energy is converted into displacements, the number of displacements $\nu_L$ is

$$\nu_L(E) = \zeta(E,Z) \frac{E}{2E_d}$$

(12.56)

$$\zeta(E,Z) = \text{damage efficiency} = \frac{1}{1 + 0.88Z^{1/3}(3.4\varepsilon^2 + 0.4\varepsilon^3 + \varepsilon)}$$

(12.57)

where $\varepsilon = \frac{E}{2Z^2e^2/a}$; $a =$ screening radius = $\frac{\sqrt{2a_B}}{(Z_1^{28} + Z_2^{28})^{1/2}}$ with $a_B$ the Bohr radius. In the case of a self-PKA the screening radius is simply $a=a_B/Z^{1/3}$. The damage efficiency $\zeta(E,Z)$ originates from a numerical solution of the energy partition between electronic and nuclear stopping. This solution is plotted in Figure 12.15 and approximated by Eq (12.57)
Figure 12.15: Damage efficiency as a function of PKA energy for various elements. The dotted line shows the nuclear stopping limit [10].

The damage efficiency decreases slowly with PKA energy, and decreases more steeply for light elements than heavy elements. According to equation 12.14, the cutoff (dotted line in figure) would occur at different energy levels for different elements. We notice that for U the damage efficiency is higher than 0.7 at the cutoff, while, for Be, it is lower than 0.5.

In analyzing the figure above, and taking into account the fact that under neutron irradiation the energy of most recoils in metals of interest will be smaller than 50 keV, we arrive at the Norgett-Robinson-Torrens formula [7]

\[
\nu_{NRT}(E) \approx 0.8 \frac{E}{2E_d}
\]  
(12.58)

which is approximately valid over the full PKA range, especially for atoms with Z > 20. The two formulas above have various limitations. For example, they take no account of collisions between atoms of different masses; for calculations of displacements in polyatomic solids see [8], and as mentioned above, no account is taken of the variation of displacement energy with crystalline orientation. Nevertheless, equation 12.58 gives us an estimate of the total number of atoms displaced by a PKA and provides a useful basis for modeling and comparison.

### 12.6. Displacements caused by Neutron Irradiation

We are now ready to find the atomic displacement rate caused by a given particle flux incident on the materials of interest. This displacement rate is given in units of displacements per atom (dpa) per second, which is simply the volumetric displacement rate (displacements per second per unit volume) divided by the atom density. In reactor neutrons and gamma rays bombard the nuclear fuel and reactor components. To evaluate the displacement rate \( k \) in a neutron flux spectrum \( \phi(E_n) \), the displacement cross section \( \sigma_d(E_n) \) is needed. \( k \) in units of dpa/s is given by:
\[ k = \int_{E_d}^{\infty} \sigma_d(E_n)\phi(E_n) dE_n \] (12.59)

The lower limit of the integral represents the lowest neutron energy capable of transferring at least \(E_d\) to the atoms in the solid. The displacement cross section is

\[ \sigma_d(E_n) = \int_{E_d}^{\Lambda E_n} \sigma_s(E_n, E)\nu(E) dE \] (12.60)

For isotropic scattering (all PKA energies \(E\) equally probable), and if \(E_d << E_n\)

\[ \sigma_s(E_n, E) = \frac{\sigma_s(E_n)}{\Lambda E_n} \] (12.61)

and

\[ \sigma_d(E_n) = \frac{\sigma_s(E_n)}{\Lambda E_n} \int_{E_d}^{\Lambda E_n} \nu(E) dE \] (12.62)

Substituting equation 12.62 into equation 12.59 we obtain

\[ k = \int_{E_d}^{\infty} \phi(E_n) \left[ \frac{\sigma_s(E_n)}{\Lambda E_n} \int_{0}^{\Lambda E_n} \nu(E) dE \right] dE_n \] (12.63)

Using the NRT expression, equation 12.58 for \(\nu(E)\):

\[ k_{\text{NRT}} = \frac{\Lambda}{SE_d} \int_{E_d}^{\infty} \phi(E_n)\sigma_s(E_n)E_n dE_n \] (12.64)

To find the displacement rate from a given neutron flux, it is necessary to integrate equation 12.64.

We use first the simple analytical approximation of a monochromatic neutron flux to obtain an order of magnitude of the number of atomic displacements created. The approximation is then to substitute the total neutron flux \(\phi_t\) at the average neutron energy for the overall flux, that is:

\[ \phi(E_n) \cong \delta(E_n - \bar{E}_n)\phi_t \] (12.65)
where \( \delta(E_n - \overline{E}_n) \) is the Kronicka delta, \( \phi_t \) is the total damage producing neutron flux given by

\[
\phi_t = \int_{\overline{E}_n}^{\infty} \phi(E_n) dE_n 
\] (12.66)

and \( \overline{E}_n \) is the average neutron energy given by

\[
\overline{E}_n = \frac{\int_{\overline{E}_n}^{\infty} \phi(E_n) E_n dE_n}{\phi_t} 
\] (12.67)

and so, for a monochromatic neutron beam of energy \( \overline{E}_n \),

\[
k_{NRT} \cong \frac{\phi_t \sigma_S(\overline{E}_n)}{5E_d} \Lambda \overline{E}_n
\] (12.68)

**Example 12.2:**

Calculate the number of displacements during one reactor cycle for a steel component subjected to a total flux of \( 5 \times 10^{13} \text{n/cm}^2\cdot\text{s} \) of monochromatic \( 1 \text{ MeV} \) neutrons, and assuming \( \sigma_S = 3 \text{ barns} \) and \( E_d = 25 \text{ eV} \). For iron-neutron collisions the energy transfer parameter is

\[
\Lambda_{nFe} = \frac{4(1.56)}{(1 + 56)^2} = 0.0689
\]

Using equation 12.68 we obtain

\[
k_{NRT} \cong 5 \times 10^{13} \left[ \text{n/cm}^2\cdot\text{s} \right] \frac{3 \times 10^{-24} \left[ \text{cm}^2 \right]}{5 \times 25 \left[ \text{eV} \right]} \times 0.069 \times 10^6 \left[ \text{eV} \right] = 8.3 \times 10^{-8} \text{dpa/s}
\]

If the reactor cycle lasts for 1.5 years (\( 4.73 \times 10^7 \text{s} \)) the total number of displacements per atom is \( 8.3 \times 10^{-8} \times 4.73 \times 10^7 = 3.93 \text{ dpa} \). Thus, during one reactor cycle, *each and every iron atom* in the solid is displaced on the average 4 times. Why does the solid not turn into powder after such enormous damage?

**end of example**

To obtain a more precise value of the displacement damage it is necessary to integrate equation 12.64 using more realistic expressions for the scattering cross section and neutron flux. We give one such example in the example 12.3 below

**Example 12.3:** Displacement rate in a fusion reactor first wall.
The D-T reaction in a fusion plasma produces monoenergetic 14 MeV neutrons. When these scatter from the atoms of the structure, a tail of low energy neutrons is produced, of the form

$$\phi(E_n) = \phi_{\text{max}} \exp[-1/3 \times (14 - E_n)]$$

as shown in Figure 12.16. For a first wall made of Zr for the scattering cross section is given in Figure 12.17 below.

![Neutron Flux in DT device](image1)

Figure 12.16: Neutron Flux for a plasma first wall in a DT fusion device

![Elastic Scattering Zr 91](image2)

Figure 12.17: Elastic scattering cross-section for Zr-91 [9]
Calculate the displacement rate by elastic scattering on the first wall of the device with such a neutron flux.

For the materials of interest, $\Lambda=0.043$ and thus $E_d/\Lambda=581$ eV.$=5.81 \times 10^{-4}$ MeV.

Substituting the flux above into equation 12.64, taking the upper integration limit as 14 MeV and considering that the scattering cross section is approximately constant (neglecting the portion below 2 MeV) and equal to $\bar{\sigma}=2$ barns we obtain

$$k_{NRT} = \frac{\Lambda}{5E_d} \left[ \phi_{\max} \exp[-(14 - E_n)/3] \right] \frac{E_n \sigma_s(E_n) dE_n}{\Lambda} = \frac{\Lambda \phi_{\max} \bar{\sigma} \exp[-14/3]}{5E_d} \int_{E_d}^{14} \exp[E_n/3] E_n dE_n$$

$$k_{NRT} = \frac{\Lambda \phi_{\max} \bar{\sigma} \exp[-14/3]}{5E_d} \left[ 3(E_n - 3) \exp(E_n/3) \right]_{5.81 \times 10^{-4}}^{14} = \frac{\Lambda \phi_{\max} \bar{\sigma} \exp[-14/3]}{5E_d} [33 \exp(14/3) + 9]$$

From where we obtain

$$k_{NRT} = 2.27 \times 10^{-7} \text{ dpa} / \text{s}$$

End of Example

However, most reactor physics calculations of the neutron flux spectrum involve discretization into individual energy groups, rather than analytical expressions. The displacement rate is given by the sum of the contributions of each energy group $j$.

$$k_{NRT} \cong \sum_{j=1}^{N} \frac{\Lambda \phi_{\max} \sigma_{sj} E_{nj} \Delta E_j}{5E_d} \quad (12.69)$$

The differential flux (or flux spectrum) $\phi$ has units of (n.cm$^{-2}$.s$^{-1}$.eV$^{-1}$). In addition to the flux spectrum, equation 12.69 requires scattering cross sections, like the one in Fig. 12.18 or evaluated for the equivalent energy group structure from databases such as ENDF-VI. The program SPECTER [10] takes a neutron flux such as given in Problem 12.10, and directly generates a displacement cross section compatible with the energy groups in which the flux is supplied.

**12.7 Other Displacement Mechanisms**

In addition to the approximations already mentioned associated with the inherent uncertainties involved in calculating a particle flux and in evaluating its effects, equation 12.64 only takes into account one of the processes of causing atomic displacements, i.e., elastic scattering of neutrons off the atoms in the solid. Other damage processes can also
cause atomic displacements, the main ones being (i) gamma induced displacements, (ii) thermal neutron reactions and (iii) inelastic scattering.

12.7.1. Gamma Displacement damage

Gamma rays do not deliver energy directly to atomic nuclei. Rather, electrons are energized by one of three interactions of the gamma ray with electrons of the solid: the photoelectric effect, Compton scattering, and pair production. These processes are each dominant at different energy ranges, but in all cases the net effect is to produce energetic electrons. These in turn cause displacement damage to the solid.

Compton scattering is by far the most important of these interactions. The Compton effect, as the interaction is called, describes an elastic collision between a gamma ray and a free electron initially at rest. Figure 12.18 diagrams the energy partitioning in the collision.

\[
\begin{align*}
\gamma' E & \quad E_\gamma \\
\theta & \\
E_e & \quad E'
\end{align*}
\]

Fig. 12.18: The Compton Effect

Conservation of energy gives:

\[ E_\gamma = E'_\gamma + E_e \quad (12.70) \]

Which, together with the momentum conservation equation, yields the Compton Formula\[11\]:

\[
E'_\gamma = \frac{E_\gamma \times m_e c^2}{m_e c^2 + E_\gamma (1 - \cos \theta)} \quad (12.71)
\]

where \( m_e c^2 = 0.51 \text{ MeV} \) is the rest energy of the electron.

The differential scattering cross section (per electron) is given by the Klein-Nishina Formula\[11\]:

\[
\sigma_s(E_\gamma, E'_\gamma) = \frac{0.15}{A^2 \times N_{Av}} \frac{m_e c^2}{E_\gamma \times E'_\gamma} \left[ 1 + \left( \frac{E'_\gamma}{E_\gamma} \right)^2 - \left( \frac{E'_\gamma}{E_\gamma} \right) \sin^2 \theta \right] \quad (12.72)
\]

where \( A \) is the mass number of the atoms of the solid and \( N_{Av} \) is Avogadro’s number. The \( \sin^2 \theta \) term can be expressed in terms of \( E'_\gamma \) by use of Eq (12.71). The range of \( E'_\gamma \) over which Eq (12.72) is obtained from Eq(12.71) by setting \( \theta = 0 \) (\( (E'_\gamma)_{\text{max}} = E_\gamma \)) and
\[ \theta = \pi \left( \left( E_\gamma' \right)_{\text{min}} = \frac{1}{2} \frac{m_e c^2}{E_\gamma} \right) \text{ if } E_\gamma \gg 0.255 \text{ MeV} \]

For calculating the damage due to the Compton electrons, we need the differential cross section in terms of the electron energy, not the energy of the scattered gamma ray. These two cross sections are related by:

\[
\sigma_s(E_\gamma, E_e) dE_e = \sigma_s(E_\gamma, E'_\gamma) dE'_\gamma
\]

or

\[
\sigma_s(E_\gamma, E_e) = \frac{dE'_\gamma}{dE_e} \left| \frac{dE'_\gamma}{dE_e} \right| = \sigma_s(E_\gamma, E_\gamma - E_e)
\]

(12.73)

The last equality results from taking the differential of Eq (12.43) and using the same equation to eliminate \( E'_\gamma \). Therefore, \( \sigma_s(E_\gamma, E_e) \) is obtained by replacing \( E'_\gamma \) by \( E_\gamma - E_e \) in Eq (12.45) and on the left hand side of Eq (12.44) and eliminating \( \theta \) between these two equations.

The displacement cross section for an photon of energy \( E_\gamma \) can now be calculated from the analog of the neutron case for the electron produced by Compton scattering (Eq (12.60)) and weighting the probability of a Compton electron with the Klein-Nishina formula (Eq (12.72)) converted to electron energy by Eq (12.73):

\[
\int \int \Lambda \gamma \gamma \sigma = \sigma
\]

(12.74)

where from Eq.(12.10) with \( M_1 = m_e \) and \( M_2 = A \), the mass number of the atoms in the solid, \( \Lambda = 2.2 \times 10^{-3} / A \). Sufficient energy transfer to cause a displacement in iron, for example, requires \( E_e \geq 0.65 \text{ MeV} \), assuming a displacement threshold \( E_d = 25 \text{ eV} \).

The total Compton scattering cross section for a gamma ray of energy \( E_\gamma \) is:

\[
\sigma_s(E_\gamma) = \int \sigma_s(E_\gamma, E_e) dE_e \]

(12.75)

Electron–atom scattering can be assumed to be isotropic in the center-of-mass system, so the differential energy transfer cross section is the electron analog of Eq (12.61) for neutrons:

\[
\sigma_s(E_e, E) = \frac{\sigma_s(E_e)}{\Lambda E_e}
\]

(12.76)

where \( \sigma_s(E_e) \) is the total scattering cross section for electrons and lattice atoms. To cause one or more displacements, the electron must interact with the bare nuclei of the atoms. The interaction for this process is purely Coulombic, so the cross section is given by the Rutherford formula.
Figure 12.19 shows the displacement cross sections calculated for Fe for all three sources of energetic electrons. It is clear that the dominant component is Compton scattering.

![Displacement cross sections](image)

Figure 12.19 Gamma displacement cross section as a function of gamma energy in iron [12]

Finally, the dpa rate due to a specified photon spectrum $\phi(E_\gamma)$ is, by analogy to Eq (12.32) for neutrons, given by:

$$k_\gamma = \int_{E_{\gamma\min}}^{\infty} \sigma_d(E_\gamma) \phi(E_\gamma) dE_\gamma$$  \hspace{1cm} (12.77)

where $E_{\gamma\min}$ is the photon energy that will just deliver energy $E_d/\Lambda$ to the struck electron, which in turn is just capable of imparting $E_d$ to a lattice atom. Eliminating $E_\gamma$ between Eqs (12.70) and (12.71), $E_{\gamma\min}$ is:

$$\frac{E_{\gamma\min}}{m_e c^2} = \frac{1}{2} B \left( \sqrt{1 + 2/B} + 1 \right)$$  \hspace{1cm} (12.78)

where

$$B = \frac{E_d/\Lambda}{m_e c^2}$$  \hspace{1cm} (12.79)

If $B$ were very large (which it is not), the result would be $E_{\gamma\min} = E_d/\Lambda$. For iron, $B = 1.28$, and Eq. (12.78) gives $E_{\gamma\min} = 0.85$ MeV.

Inside a reactor core, and in most cases for the pressure vessels too, the displacement rate caused by the gamma flux arising from both fission products and activation products decaying to their stable species is much smaller than the neutron elastic collision displacement rate (typically lower than 1%). In a few cases, however, especially when a large water gap exists between the core and the pressure vessel to thermalize the fast neutrons leaking from the core, $k_\gamma$ can be of the same order of magnitude as $k_n$. One well-known case relates to the accelerated embrittlement observed in the HFIR (High Flux Isotope Reactor) at Oak Ridge in the early 1990s [13]. The measured levels of embrittlement at the pressure vessel were found to be higher than expected for the levels of damage calculated by the NRT model (which considers only neutron damage). It was then realized that because of the large water gap, the gamma...
displacements were comparable to the neutron displacements. Taking Eq (12.77) into account removed the apparent discrepancy. Gammas are also important in situations where not only the total amount of damage but also the damage structure (in particular the freely migrating defect fraction) is important to evaluating the effects of irradiation. This will be discussed in more detail in the following section and in the next chapter.

12.7.2. Thermal Neutron Reactions

It is also possible to cause damage to reactor components by thermal neutron reactions. By this mechanism a thermal neutron absorbed by a nucleus undergoes radioactive decay, typically emitting an energetic gamma or alpha particle. By conservation of momentum, the decaying atom recoils in the opposite direction, often with an energy sufficient to cause further displacements. The emitted particle can also cause damage. The specific reaction depends on the atoms present, but several reactions are possible, including (n,α), (n,γ), (n,n’), (n,p), etc. One example, for gamma decay in Fe is shown below.

\[ ^{56}_{26}Fe + n \rightarrow ^{56}_{26}Fe + \gamma (7 \text{ MeV}) \]  

(12.80)

By conservation of momentum \( P_\gamma = \frac{E_\gamma}{c} = P_{Fe} \) and the energy of the recoil nucleus is \( E_{Fe} = \frac{P_{Fe}^2}{2M} \), which turns out to be about 460 eV, enough to cause 9 displacements according to equation 12.58 if \( E_d = 25 \text{ eV} \).

12.7.3 Inelastic Scattering

Inelastic scattering involves forming a compound nucleus by absorption of a fast neutron by the nucleus of an atom and subsequent emission of a neutron of lower energy. This reaction is called inelastic scattering or (n,n’). It only occurs above a certain threshold energy of the incident neutron, which for typical metals is above 1 MeV. Because the fission spectrum contains a considerable fraction of neutrons of energy above 1 MeV, the (n,n’) reaction is a significant damage mechanism.

The threshold neutron energy for inelastic scattering for an atom mass \( M \) is

\[ E_{nth} = \frac{M + 1}{M} E_{ex} \]  

(12.81)

where \( E_{ex} \) is the excitation energy, or the energy level above the ground state that is populated by the collision with the incident fast neutron. That the threshold energy is greater than the excitation energy is a consequence of momentum conservation. The analog of equation 12.9 for inelastic scattering is
\[
E = \frac{1}{2} \Lambda E_n \left[ 1 - \frac{1}{2} E_n^{th} \left( 1 - \frac{E_n^{th}}{E_n} \right)^{1/2} \cos \theta \right] \tag{12.82}
\]

The maximum energy transferred corresponds to \( \cos \theta = -1 \) and the minimum to \( \cos \theta = 1 \). Thus the analog of equation 12.11 is

\[
E_{\text{max,min}} = \frac{\Lambda E_n^{th}}{2} \left[ \alpha \left( 1 - \frac{1}{2\alpha} \pm \sqrt{1 - \frac{1}{\alpha}} \right) \right] \tag{12.83}
\]

where \( \alpha = \frac{E_n^{th}}{E_{ex}} \). Since inelastic scattering involves the formation of a compound nucleus, the emitted neutron is isotropic in the CM. The analog of equation 12.61 is

\[
\sigma_n^{in}(E_n, E) = \frac{\sigma_n^{in}(E_n)}{\Lambda E_n \left[ 1 - \frac{E_n^{th}}{E_n} \right]} \tag{12.84}
\]

and the displacement cross section for inelastic scattering is

\[
\sigma_d^{in}(E_n) = \frac{\sigma_n^{in}(E_n)}{\Lambda E_n \left[ 1 - \frac{E_n^{th}}{E_n} \right]} \int_{E_{\text{min}}}^{E_{\text{max}}} \nu(E) dE \tag{12.85}
\]

### 12.8. Other measures of damage

In the preceding sections we have seen that the number of displacements per atom from the NRT model is a useful measure of the damage caused by energetic particle irradiation. However, because (dpa)\text{NRT} measures only the \textit{total} number of atoms involved in the displacement cascade, it has only a correlational relationship to the actual damage structure and types of surviving defects. The actual damage characteristics have a great influence in the determining the types and production rates of specific radiation damage phenomena. Some of these more important but less accessible measures of damage are:

- The quantities of single (freely-migrating) defects surviving the cascade
- The percentages of clusters, the proximity of the defects after cascade cooldown,
- The number of replacements,
- The size of disordered or amorphous zones
The importance of these damage features depends on the type or macroscopic radiation effect that is of interest. For example, single, mobile defects are very important in irradiation creep and void swelling, but are less important than defect clusters in hardening a metal.

*Freely migrating defects:* a series of experiments has indicated that only a small fraction of defects survive the recombination and clustering processes that follow cascade formation [14]. Typical reported values are shown in table 12.2 (last row). Different types of irradiation produce different recoil spectra, which in turn change the cascade size, density, sub-cascade formation, all of which affect the final fraction of freely migrating defects. The fraction of the dpa_{NRT} that survive as mobile single vacancies and interstitials has to be taken into account in rate theory models that depend on long-range defect migration and absorption by sinks (Chapter 13).

### 12.9. Charged particle irradiation

For the sake of completeness, charged-particle irradiation (electrons and ions) generated by accelerators is discussed in this section. The motivations for using charged particle irradiation in experimental radiation damage studies are, first, displacement rates are orders of magnitude higher than those achievable under neutron irradiation, so equivalent doses (in dpa) are attained in hours instead of years; second the effects of experimental variables such as temperature and dose rate can be explored with greater ease; and third, ion or electron irradiated samples are less radioactive than samples irradiated with neutrons, making them easier to handle. The disadvantage of accelerator-produced particle irradiation is that the depth of damage is localized to at the most within a few tens of microns of the surface.

In general, the results obtained in such experiments do not have a one-to-one correspondence with results of neutron irradiation. Nor should close correspondence be expected, as the irradiations are quite different. Table 12.2 shows the differences between the different types of irradiation for typical values of irradiation parameters in reactors, accelerators and electron microscopes.

| Table 12.2 Comparison of neutron, ion and electron irradiation in metals: |
|---------------------------------|-----------------|-----------------|-----------------|
| **Typical Flux** (particle.cm\(^{-2}.s\(^{-1}\)) | **Fast Neutron** | **Ion (Heavy/Light)** | **Electron** |
| 5 \(\times\) 10\(^{13}\) | 10\(^{11}\)-10\(^{12}\) | 5 \(\times\) 10\(^{19}\) |
| **Displacement Rate** (dpa/s) | 10\(^{-7}\) | 10\(^{-4}\)-10\(^{-5}\) | 10\(^{-2}\)-10\(^{-3}\) |
| **Irradiation time to 1 dpa** | ~ 4 months | 4 to 40 h | 2-20 minutes |
| **Temperature** (Reactor temperature (coolant ~ 300 °C)) | adjustable | adjustable |
| **Macroscopic Spatial distribution of damage** | Small; follows neutron flux | Sharp nuclear stopping peak at the | Homogeneous in thin foil, but sharp |
### 12.9.1 Electron Irradiation

Energetic electrons include Compton electrons, beta particles from nuclear disintegrations and electrons produced by an accelerator. These electrons create atomic displacements by direct scattering off the atomic nuclei. Electron irradiation differs from neutron and ion irradiation in two ways: (i) even for energies in the MeV range the energy of the PKA created by an electron atom collision is not much greater than the displacement energy, and thus displacement cascades are rare and (ii) the electron velocities are high enough to require relativistic treatment of collision dynamics. Instead of the classical result, the maximum energy transferred to a struck nucleus is given by

$$E_{\text{max}} = \frac{1}{2} \Lambda \left( \frac{E_e}{m_e c^2} + 2 \right) E_e$$  \hspace{1cm} (12.86)

instead of the classical result $E_{\text{max}} = \lambda E_e$ used in the upper limit of the integral in Eq (12.74). The minimum electron energy to cause displacements is arrived at by setting $E_{\text{max}} = E_d$ in Eq (12.86) and rearranging

$$E_{\text{emin}} = m_e c^2 \left[ -1 + \sqrt{1 + \frac{2E_d / \Lambda}{m_e c^2}} \right]$$  \hspace{1cm} (12.87)

If the second term in the square root is small compared to unity, a Taylor series expansion gives the classical result $E_{\text{emin}} = E_d / \Lambda$.

### 12.9.2. Ion Irradiation

The principal difference between irradiation with ions and neutrons is that the former interacts with atoms with a cross section on the order of $10^{-16}$ cm$^2$, whereas typical neutron –nucleus cross sections are on the order of $10^{-24}$ cm$^3$. The result is an energy loss per unit target thickness much higher than that for neutron irradiation. This difference causes both a higher displacement rate due to ion interactions and a spatial gradient of damage as the displacement cross section increases with decreasing ion energy. Since irradiation effects are dependent on the balance between irradiation damage and thermal...
annealing, increasing the displacement rate affects phenomena such as, for example, the peak void swelling temperature. In Chapter 22, we show that this temperature is higher with ion irradiation than that observed under neutron irradiation.

Ion irradiation illustrates all the interactions of radiation with solids that were presented earlier in this chapter. In particular, the regions of electron stopping and nuclear stopping are illustrated in Fig. 12.20, which is a TEM micrograph of a cross-section of MgAl₂O₄ (spinel) irradiated with 2 MeV Al⁺ ions at 650°C to a level of 14.1 dpa. The contrast observed is the formation of dislocation loops which are more numerous in the nuclear stopping region, as seen from a TRIM simulation.
Figure 12.29 (a) TEM bright field image showing the variation of displacements damage with depth during 2 MeV Al+ ion irradiation of MgAl2O4 (spinel) [15]. (b) Plot of implanted ion distribution and (c) Displacements damage as a function of distance. Both simulations simulation performed using SRIM[2].

The energetic particles penetrate the solid from the left. At the beginning they interact mostly with electrons, causing very few displacements. After a distance of about 0.5-1 micron, corresponding to a decrease of ion (PKA) energy down to the energy limit between nuclear and electronic regimes, the ion starts interacting with nuclei. This is seen in the center of Figure 12.29 where the displacement rate then increases abruptly, thereby generating a higher defect concentration in that region. At the end of the displacement region, the ion comes to rest as a neutral atom.

box 12.3 TRIM code

**TRIM and SRIM: Monte Carlo codes to simulate ion transport and damage production in materials**

The TRIM and SRIM codes calculate the interactions of energetic ions with the atoms in the solid. The program relies on the development of a universal interatomic potential which depends on ion energy, and the masses and atomic numbers of the atoms in question. The potential is of the form

\[
V(r) = \frac{Z_1 Z_2 e^2}{r} \Phi \left( \frac{r}{a} \right)
\]

(12.88)

where \(Z_1\) and \(Z_2\) are the atomic numbers of the energetic ion and the target atoms, \(e\) is the electric charge, \(r\) the interatomic distance and \(a\) is an empirical screening length which depends on the atomic numbers of the two atoms by the semi-empirical formula:

\[
a = \frac{0.8854 a_{\text{Bohr}}}{Z_1^{0.23} + Z_2^{0.23}}
\]

(12.89)

where \(a_{\text{Bohr}}\) is the Bohr radius (the radius of the hydrogen atom, 0.53 Å). \(\Phi\) is the “universal” screening function determined by exact fitting of the calculated interatomic potentials of 521 randomly selected element combinations given by:

\[
\Phi \left( \frac{r}{a} \right) = \sum_{i=1}^{4} A_i \exp \left[ -B_i \left( \frac{r}{a} \right) \right]
\]

(12.90)
The remarkable feature of Equation 12.90 is that it depends only on the atomic numbers \( Z_1 \) and \( Z_2 \). It is very accurate for high energy collisions but does not accurately give the number of displacements for collisions less than a few tens of electron volts.

This empirical interatomic potential was validated by extensive comparison to experiment. It has been implemented into a code that gives the partitioning of energy loss between electrons and nuclei. The procedure is to substitute equation 12.88 into equation 12.42 to find a relation between impact parameter and angle \( \theta \). At the beginning of each calculation step the code calculates a “free flight” distance in the material equal to the target interatomic spacing at low energies and by a complicated function of the ion energy and scattering density at high ion energies. At the end of the free flight distance, the ion undergoes a nuclear collision with an atom at a randomly selected impact parameter. The analog of Equation 12.51 for the universal potential determines the energy transferred to the PKA and the scattering angle. If the ion energy after the collision, \( E' = E_i - E \), or the transferred energy \( E \) are lower than a specified displacement energy \( E_d \), the calculation is terminated. If not, the program recalculates the free flight distance for the two branches of the calculation (original ion and struck atom) and the process continues until the energies of all atoms involved fall below \( E_d \). The code keeps track of energy loss, number of displacements, ion range and various other parameters. The program does not consider nuclear reactions, the crystal structure of the material (materials is amorphous with a specified density) or the accumulation of damage (each ion sees virgin material). The program does explicitly account for polyatomic targets, atomic sputtering, and allows for up to 3 layers of material with up to 4 elements each. The program has been validated by comparison to experiments and is available for free download at www.ibm.org

**Problems**

1. Two atoms of the same kind interact with an energy transfer cross-section given by

\[
\sigma(E, T) = \frac{C}{\sqrt{ET}}
\]

where \( C \) is a constant. What is the probability of scattering with a center of mass angle greater than 90 degrees?

2. The \((n, \alpha)\) reaction in \( ^{59}\text{Ni} \) releases a prompt \( \alpha \)-particle of \( E_\gamma = \text{** MeV} \).

   a) Using momentum conservation, calculate the recoil energy of the \( ^{57}\text{Fe} \) product nucleus.

   b) Calculate the number of displaced atoms caused by the recoil according to the Kinchin-Pease and NRT models. Assume \( E_d = 25eV \)

   c) Using the K-P model, calculate the displacement rate (displacements/s.cm\(^3\)) due to this mechanism, in a thermal flux of \( 10^{13} \text{n/cm}^2\text{s} \), if the density of iron is 7.8 g/cm\(^3\) and the thermal absorption cross section for Fe is 2.5 barns.
d) Compare this displacement rate to the displacement rate caused by fast neutrons for a fast flux of $10^{13}$ n/ cm$^2$s, ($\bar{E} = 1$ MeV), also using KP. Assume elastic isotropic scattering and a scattering cross section of 3 b.

3. For a mononergic fast neutron flux of energy 0.5 MeV calculate the number of displacements per atom in iron after a fast neutron fluence of $10^{22}$ n.cm$^{-2}$. Compare this calculation with that due to the displacements for a flux of 10 MeV neutrons. The displacement cross section for the 10 MeV neutrons is 3000 b.

4. An iron primary knock-on atom (PKA) is created with an energy of 100 KeV. According to the Kinchin-Pease model of displacement calculation and the Lindhard electronic stopping formula, how far does the PKA travel before starting to interact with the nuclei in the solid?

5. The figure below shows a portion of a fission fragment track in UO$_2$. At one point the track changes direction indicating that the fragment has made a Rutherford collision with an atom at this point.
Assuming this is a $^{100}_{42}Mo$ fragment with a birth energy of 100 MeV, which has traveled 2 microns from where the fission took place to the place where it collides with the atom:

a) What is the effective charge of the fragment at birth?

b) Before the collision, the fragment loses energy by electronic excitation according to the Bethe formula. Calculate the energy at the point of the collision, assuming the mean excitation energy in the Bethe formula $\bar{T} = 8.8Z(eV)$.

c) If the scattering angle on the photograph is 5 degrees, calculate the energy transferred to the struck atom in the case of (1) an oxygen atom and (2) an uranium atom.

6. Calculate the average iron PKA energy in a fission neutron spectrum:

$$\phi(E_n) = A \times \exp(-E_n) \sinh(2E_n)^{1/2}$$

where $E_n$ is the neutron energy in MeV. How does this value compare with the approximation of calculating the average PKA energy due to collision with the neutron of average energy? Assume isotropic, elastic scattering and an energy independent scattering cross section.

7. It is desired to evaluate the number of displacements per atom suffered by a piece of Zircaloy cladding oxide subjected to a neutron flux in a BWR. For the purposes of this calculation, assume the material is 66 at% Zr, and 33% O and that both atoms have a displacement energy of 25 eV. Use the neutron flux provided below, divided into 47 energy groups. Consider that the total oxygen scattering cross section is constant and equal to 3 barns. Assume isotropic scattering (the probability of generating a PKA of energy $E$ is independent of $E$ for the energy range considered). For Zr scattering, use Figure 12.17. The methodology to be utilized is the following:

a). Each of these neutron energy groups will generate a distribution of energetic recoils of varying energy. Characterize each group by the total group flux at the average neutron energy in the group. Calculate the average recoil energy for each group.

b). Using the NRT formula, equation 12.68 find the displacement cross section for each energy group.
c). Multiply by the neutron flux per group to find the number of displacements per group and sum them over all energy groups to find the total number of displacements 
NRT for the material under consideration.

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</table>

8. It is desired to estimate the importance of considering polyatomic processes on displacement calculations in problem 12.7, and of considering KP and full damage cascade calculations. To do this use the TRIM code and compare it to the values calculated using the NRT model.

a) Choose two neutron groups and determine appropriate the maximum PKA energies $E_1$ and $E_2$. Divide the energy interval between 0 and $\Delta E_{ni}$ and derive a set of PKA energies to run TRIM.

b) Run TRIM (using full damage cascades) for the set of PKA energies for the two pure elements. Obtain from TRIM in each case i) the number of oxygen displacements and, ii) the number of Zr displacements created by the set of PKA energies $E$, for all intervals between 0 and $\Delta E_{ni}$.

c) Use the displacement values calculated to calculate a weighted displacement rate in the compound. Compare this value with the value obtained in problem 12.7 for the energy group in question.
d) Run TRIM for the compound material (2/3 O, 1/3 Zr). Compare the oxygen, zirconium, and total displacement rates obtained with those from part c). What are the differences?

9. It is an experimental observation that during electron irradiation of a material below a given electron energy no displacements are possible, as predicted by equation 12.48. Occasionally it is possible to observe damage even below $E_d$ as a result of secondary displacements through light element impurities. If bcc Fe has a displacement energy of 40 eV and contains C, calculate:
   a) The minimum electron energy to cause displacements in pure Fe.
   b) The minimum electron energy considering secondary displacements of the type electron $\Rightarrow$ C $\Rightarrow$ Fe. What is the maximum Fe recoil energy obtainable from 400 keV electrons through a secondary C displacement mechanism?
   c) What purity Fe would be necessary to ensure that secondary displacements are limited to 1/100 of the primary displacements at an electron energy of 900 keV? The displacement cross-section for 900 keV electrons is 30 b in Fe and 20 b in C.10. Given the following two-region neutron flux, incident on a Zr component, calculate the total displacement rate, from fast neutron collisions using the Norgett-Robinson-Torrens (NRT) model.

\[\Phi (n.cm^{-2})\]

\[10^{13} n.cm^{-2}\]

\[5 \times 10^{12} n.cm^{-2}\]

\[0.5 \text{ MeV} \quad 1.0 \text{ MeV}\]

$E_n$

The displacement energy for Zr is 33 eV. See Fig.12.17 for the scattering cross section of neutrons in Zr.

11. Redo the calculation in example 12.3, but taking into account the variation of the scattering cross section between 0 and 3 MeV, which you can approximate as a linear function.

12. Calculate the distance of closest approach for two particles that meet head-on, and whose interaction is governed by the unscreened Coulomb potential (equation 12.45)

13. A 40 eV atom of mass $M_1$ strikes a lattice atom of mass $M_2 = 2M_1$.
   a) What is the probability that the lattice atom is displaced?
   b) If the lattice atom is displaced, what happens to the other atom?
   Assume hard-sphere scattering and a displacement energy of 25 eV.
References