Interaction of high energy radiation such as $\alpha$, $\beta$ and $\gamma$ rays as well as particles such as electrons, protons, neutrons etc with crystal lattices give rise to defects/imperfections such as vacancies, self interstitials, ionization and electron excitation etc.

The microscopic defects produced in materials due to irradiation are referred to as **radiation damage**.

The crystal defects thus produced modify the macroscopic properties of materials which are referred to as **radiation effects**.

**Radiation Damage**

Following are radiation defects induced by intense nuclear radiation, in particular high energy \{E \textasciitilde 0.1 \text{ MeV}\} neutrons:

- Vacancies
- Interstitials
- Impurity atoms - produced by transmutation
- Thermal spikes - regions with atoms in high energy states
- Displacement spikes - regions with displaced atoms, vacancies, self interstitials [Frenkel pairs] produced by *primary* and *secondary* knock-on atoms
- Depleted zones - regions with vacancy clusters [depleted of atoms]
- Voids - large regions devoid of atoms
- Cavities - voids stabilized by filled gases such as He produced from (n,$\alpha$) reactions with B, Ni, Fe etc. $\text{B}^{10} + n \rightarrow \text{Li}^7 + \text{He}^4$; $\text{Ni}(n,\gamma)\text{Ni}^{59} \& \text{Ni}^{59}(n,\alpha)\text{Ni}^{56}$
- Replacement collisions - scattered [self] interstitial atoms falling into vacant sites after collisions between moving interstitial and stationary atoms and dissipating their energies through lattice vibrations
Primary Knock-on Atoms (PKA)

A lattice atom that is knocked off or displaced from its lattice position by intense radiation, say high energy neutron, and comes to rest in an interstitial position far from the vacant site created is known as PKA.

This process leads to the production of Frenkel pairs.

A neutron with sufficient energy produces a number of these PKAs which in turn produce knock-ons leading to displacement cascades. The atoms displaced by PKAs are known as secondary knock-on atoms. Thus a high energy neutron may produce a number of PKAs which lead to many secondary knock-ons resulting in a large number of atomic displacements.

Our goal is to calculate displacements per atom [dpa] using simple models and thus-evaluated dpa may be related to the changes in the macroscopic properties of the materials such as mechanical, physical, thermal, electrical, etc. (i.e., radiation effects).

It is important to note that many many atomic displacements occur due to neutron-lattice interactions but only a small fraction survive since most of the defects anneal out in-situ during irradiation mainly due to the proximity of the defects to the appropriate sinks.
Radiation Damage Model

A simple model for calculating the atomic displacements is due to Kinchin and Pease.

Before discussing this model, let us consider a collision between a high energy neutron \([\text{mass, } m]\) and a lattice atom of mass \(M\).

\(E_n = \text{energy of the neutron}\)

The atom is scattered with energy \(T\) transferred from the neutron.

\[\Rightarrow \text{But there exists a threshold energy, } E_d \text{ [displacement threshold energy] such that the atom with transferred energy } T \text{ will be displaced and becomes PKA if and only if } T > E_d \text{ (note } E_d \text{ is very small } \approx 25 \text{ eV)}\]

The neutron will now have an energy \([E_n-T]\) if the energy consumed in the scattering process is assumed negligible.

The neutron with energy \([E_n-T]\) and the PKA with energy \(T\) produce other knock-on atoms ⇔ higher-order knock-ons

\[\text{Table. Displacement Threshold Energies } \{E_d\}\]

<table>
<thead>
<tr>
<th>Element</th>
<th>Cu</th>
<th>Al</th>
<th>Ag</th>
<th>Au</th>
<th>Pt</th>
<th>Ni</th>
<th>Fe</th>
<th>Mo</th>
</tr>
</thead>
<tbody>
<tr>
<td>(E_d), eV</td>
<td>22</td>
<td>16</td>
<td>28</td>
<td>36</td>
<td>37</td>
<td>24</td>
<td>24</td>
<td>37</td>
</tr>
</tbody>
</table>

For isotropic elastic scattering:

\[v_{2f}^2 = \frac{2 M_1^2}{(M_1 + M_2)^2} v_{1o}^2 (1 - \cos \theta)\]

\[\therefore E_2 = \frac{1}{2} M_2 v_{2f}^2 = \frac{2 M_1 M_2}{(M_1 + M_2)^2} E_{1o} (1 - \cos \theta)\]

\[\therefore E_2 = \frac{1}{2} \Lambda E_n (1 - \cos \theta), \quad \theta \text{ is the scattering angle, Eq.1a}\]

Or, \(T_{\text{max}} = \Lambda E_n \) (Eq.1b) & \(\bar{T} = \frac{1}{2} \Lambda E_n \) (Eq.2) where \(\Lambda = \frac{4A}{(1+A)^2} \) (Eq.3).
$\phi(E_n) =$ flux [per cm$^2$ per sec] of neutrons with energy $E_n$

The rate of atomic displacements, $R_d$, is proportional to the number of target atoms per cc (N) and the displacement cross-section [$\sigma_d(E_n)$] for neutrons with energy $E_n$,

$$R_d = N \sigma_d(E_n) \phi(E_n). \quad \text{Eq. 4}$$

$$\therefore \text{dpa} = R_d \frac{t}{N} = t \int_{E_d/\Lambda}^{\infty} \sigma_d(E_n) \phi(E_n) dE_n \approx t \int_{0}^{\infty} \sigma_d(E_n) \phi(E_n) dE_n. \quad (\text{Eq. 5})$$

for neutrons with energies varying from $0$ to $\infty$.

[Note that neutrons with $E_n < E_d/\Lambda$ do not produce any displaced atoms since $T$ should be $\geq E_d$ {i.e. the maximum transferable energy given by $\Lambda E_n \geq E_d$ to produce a knock-on atom}]

The displacement cross-section is given by the sum of the number of atomic displacements {$v(E)$} produced by PKAs with energies $E$ from $E_d$ [this is the minimum needed] to $T_{\text{max}}$ {$= \Lambda E_n$}. The interaction probability is given by the differential energy transfer cross-section $\sigma_n(E_n,E)dE$ for producing a PKA with energy $(E,dE)$ due to interaction with a neutron of energy $E_n$.

$$\therefore \sigma_d(E_n) = \int_{E_d}^{\Lambda E_n} \sigma_n(E_n,E) v(E) dE. \quad (\text{Eq. 6})$$

Note: here, the minimum energy of the PKA to produce displacements is $E_d$, [$\Lambda=1$, since scattering between like atoms] and the maximum energy of PKA is $T_{\text{max}}$ {$= \Lambda E_n$}.

The Kinchin and Pease model is based on the following assumptions:

- 2-body elastic collisions
- hard sphere model
- atomic displacements occur only when $T \geq E_d$
- no energy is consumed in displacing a lattice atom
- atomic arrangement in the material is random [no crystallography]
- no annihilation

According to K-P model,

$$v(E) = \frac{E}{2E_d} \quad (\text{Eq. 7})$$
Or
\[ R_d = N \int_{E_d}^{\infty} dE_n \phi(E_n) \frac{\Lambda E_n}{E_d} \int_{E_d}^{\Lambda E_n} \sigma_n(E_n,E)\nu(E)dE \]

From the theory of the elastic scattering, we find that
\[ \sigma_n(E_n,E) = \frac{\sigma_{el}(E_n)}{\Lambda E_n} \quad \text{(Eq.9)} \]
where the elastic collision cross-section is weakly dependent on the neutron energy, \( E_n \). Thus,
\[ R_d = \frac{N\Lambda\sigma_{el}(\bar{E}_n)}{4E_d} \bar{E}_n \Phi \quad \text{(Eq.10)} \]

and
\[ \text{dpa} = \frac{R_d t}{N} = \sigma_{el} \frac{\Lambda \bar{E}_n}{4E_d} \Phi t \quad \text{(Eq.11)} \]

Here, \( \Phi \) is the total integrated neutron flux given by
\[ \Phi = \int_{0}^{\infty} \phi(E_n) dE_n \quad \text{(Eq.12)} \]

Note that the weighted average energy of neutrons is given by
\[ \bar{E}_n = \frac{\int_{0}^{\infty} E_n \phi(E_n) dE_n}{\int_{0}^{\infty} \phi(E_n) dE_n} \quad \text{(Eq.13)} \]

**Example**: Consider 0.5 MeV neutrons interacting with iron [\( A=56 \)] target. Find \( R_d \).

\[ \bar{E}_n = 0.5 \text{ MeV} \quad N = 0.85 \times 10^{23} \text{ atoms/cc} \quad \sigma_{el} = 3 \text{ b} \quad E_d = 24 \text{ eV} \quad \Phi = 10^{15} \text{ n/cm}^2\text{-s} \]

\[ \therefore \Lambda = \frac{4A}{(1+A)^2} = 0.069 \quad \text{and} \quad \frac{\Lambda \bar{E}_n}{4E_d} = 350 \text{ dpa per neutron collision} \]

and,
\[ R_d = 9 \times 10^{16} \text{ displacements/cc-s} = 10^{-6} \text{ dpa/s} \]
Example:
If a copper \((A=64)\) specimen is exposed to monoenergetic (2 MeV) neutrons of flux, \(\phi = 2 \times 10^{15} \text{ n/cm}^2\text{-s}\) for 6 days continuously, show that the number of atomic displacements per atom (dpa) is 2.856. \((E_d=22 \text{ eV, } \sigma_{el}=2b)\).

----- What will be the enhancement in self diffusion of copper at 500 C if only one vacancy survived for million displacements (due to in-situ annealing) ?

Cu is fcc \((z=12, a=2.2 \text{ Å})\) – \(Q_v=20 \text{ kCal/mole, } Q_m=18 \text{ kCal/mole, } v_D=10^{13} \text{ sec}^{-1}\).