Unit 3: Radiation Damage Mechanisms

ME 5203 – Nuclear Materials

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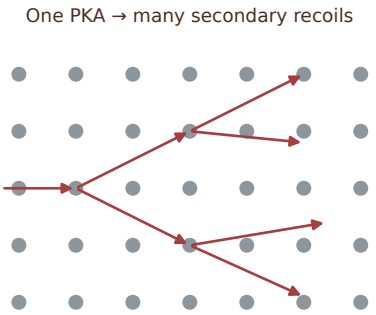
Fall 2026

One energetic particle can change many atomic sites

- A neutron transfers energy to a lattice atom.
- That recoil can transfer energy to more atoms.
- Some defects survive; others recombine.

Our task

Follow the energy, then count damage with a stated model.



Unit 3: from one collision to an irradiation dose

Step	Question
1. Collision	How much energy reaches the recoil atom?
2. Energy loss	How much remains for atomic motion?
3. Cascade	How many defects are predicted or retained?
4. Spectrum	How do we combine many recoil energies?
5. Dose	How do flux and exposure time give dpa?

Learning outcome

Calculate a model dose and explain what it does and does not measure.

Connect radiation damage to Unit 2

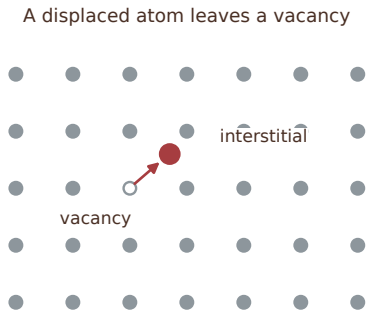
Starting structure

Atoms occupy lattice sites; an interstitial lies between normal sites.

Frenkel pair

A vacancy and a self-interstitial are created when an atom leaves its site.

The pair may disappear if the interstitial returns.



Three different stages of damage

Stage	What changes	Typical scale
Primary damage	Collisions and prompt relaxation	Sub-ps to tens of ps
Defect evolution	Migration, recombination, clustering	Material and temperature dependent
Property response	Strength, swelling, conductivity	Accumulated microstructure

Keep the stages separate

A primary-damage estimate is an input to later microstructure evolution.

Different radiation transfers energy differently

Radiation	Main routes relevant here
Neutrons	Nuclear scattering and reactions produce recoil atoms
Protons / ions	Nuclear collisions plus electronic excitation
Electrons	Electronic excitation; sufficiently energetic electrons can displace atoms
Photons	Electronic interactions; energetic secondary particles can cause damage

Scope

We focus on neutron-induced recoil cascades and displacement damage.

Separate scattering from nuclear reactions

Elastic scattering

Momentum and kinetic energy are conserved for the collision pair.

Inelastic scattering

The target nucleus is excited; some incident energy becomes internal excitation.

Other nuclear reactions

Capture and particle-emission channels can change species and generate energetic products.

Flux, fluence and cross section

Symbol	Meaning	Units
ϕ	Scalar flux: neutron density $\times$ speed (monoenergetic)	$\mathrm{cm}^{-2}\ \mathrm{s}^{-1}$
Φ	Time-integrated flux	cm^{-2}
σ	Interaction response per target	cm^{2}

$$\Phi = \phi t \quad \text{(constant flux)}; \qquad 1\ \mathrm{b} = 10^{-24}\ \mathrm{cm}^2$$

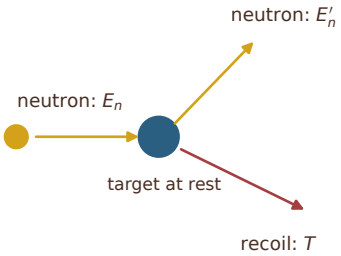
For a single-direction beam, flux equals particles crossing a perpendicular unit area per second. For a spectrum, sum over energies.

The primary knock-on atom: PKA

- The first target atom set in motion by the incident radiation is the PKA.
- E_n: incident neutron energy.
- T: kinetic energy of the PKA immediately after the collision.

Do not mix the two energies

The neutron usually transfers only part of E_n.

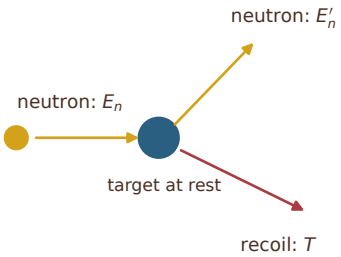


Elastic collision: start with conservation

$$E_n = E_n' + T$$

$$\mathbf{p}_n = \mathbf{p}_n' + \mathbf{p}_R$$

- Prime: outgoing neutron.
- $\mathbf{p}_R$: recoil momentum.
- Assume a stationary target and nonrelativistic kinematics.

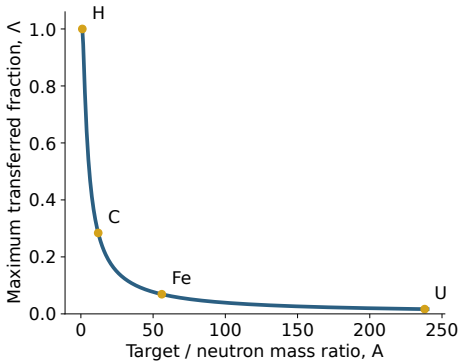


Mass ratio sets the maximum transfer

$$\Lambda = \frac{4mM}{(m+M)^2} = \frac{4A}{(1+A)^2}$$

$$T_{\max} = \Lambda E_n$$

- m: neutron mass; M: target mass.
- $A = M/m$; Λ is dimensionless.
- Equal masses permit complete transfer.



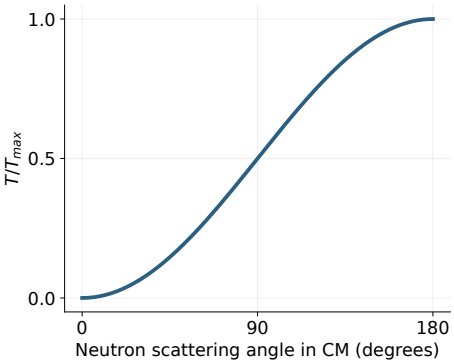
Angle sets where the recoil lies below the maximum

$$T = \frac{\Lambda E_n}{2}(1 - \cos\theta_{\mathrm{CM}})$$

- θ_{CM}: neutron scattering angle in the centre-of-mass frame.
- $0°$: no transfer; $180°$: maximum transfer.

Angle convention

Do not substitute the laboratory recoil angle into this equation.



Light and heavy targets: compare the fractions

Target mass ratio A	Λ	$T_{\max}$ **for 2 MeV**
H: 1	1.000	2000 keV
C: 12	0.284	568 keV
Fe: 56	0.0689	138 keV
Zr: 91	0.0430	86.0 keV
U: 238	0.0167	33.3 keV

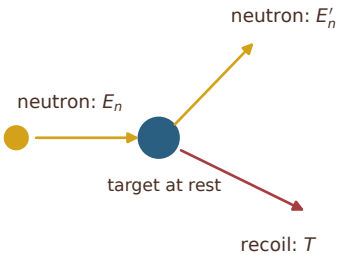
A small fraction can still matter

Even tens of keV greatly exceed the tens-of-eV threshold used in our examples.

Worked example: 2 MeV neutron on iron

Question

Use $A = 56$. Find the largest possible recoil energy.

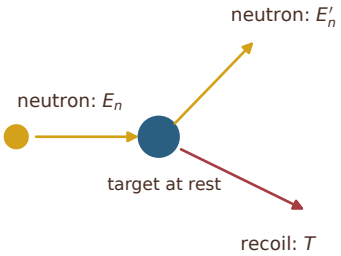


Worked example: 2 MeV neutron on iron

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$$\Lambda = \frac{4(56)}{57^2} = 0.06894$$



Worked example: 2 MeV neutron on iron

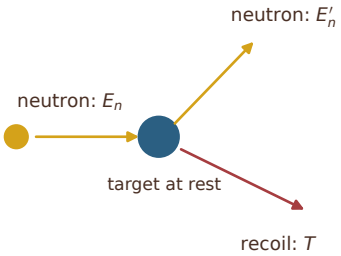
Question

Use $A = 56$. Find the largest possible recoil energy.

$$\Lambda = \frac{4(56)}{57^2} = 0.06894$$

Answer

$T_{\max} = 0.06894(2\text{ MeV}) = 0.1379\text{ MeV} \approx 138\text{ keV}$.



When is the mean recoil energy half the maximum?

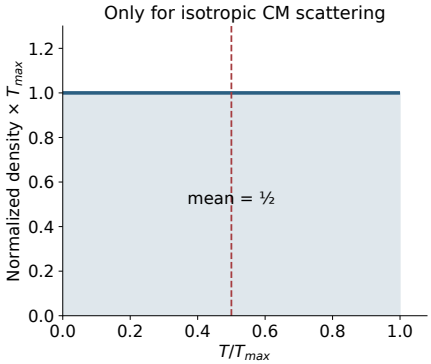
Special assumption

Elastic scattering is isotropic in the centre-of-mass frame.

- Then $\cos\theta_{\mathrm{CM}}$ is uniformly distributed.
- So T is uniform from 0 to $T_{\max}$.

$$\langle T \rangle = T_{\max}/2$$

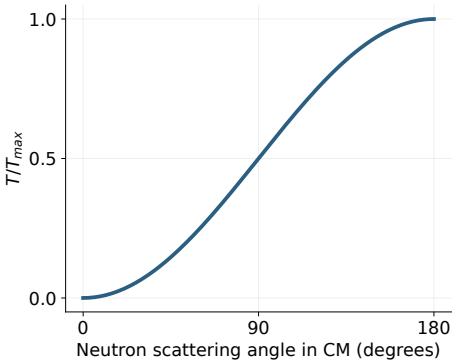
Real angular distributions can give a different mean.



A kinematic maximum is not a typical event

Question

Every 2 MeV neutron colliding with Fe gives the atom 138 keV. True or false?



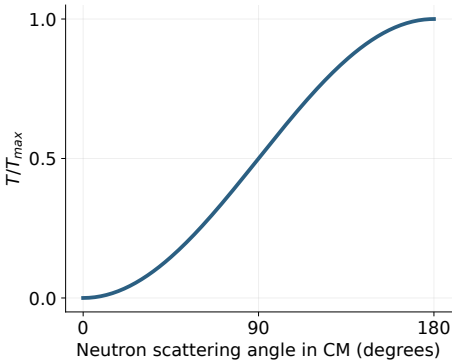
A kinematic maximum is not a typical event

Question

Every 2 MeV neutron colliding with Fe gives the atom 138 keV. True or false?

Answer

False. 138 keV is the upper bound. The recoil distribution depends on scattering angles.

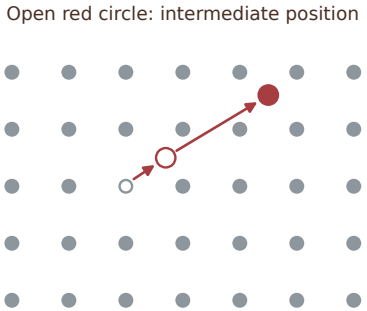


Threshold displacement energy is a dynamic threshold

E_d

Minimum recoil energy, for a stated direction and condition, that leaves a Frenkel pair after prompt relaxation.

- The atom must leave its site and avoid immediate return.
- A surviving primary pair can still anneal later.

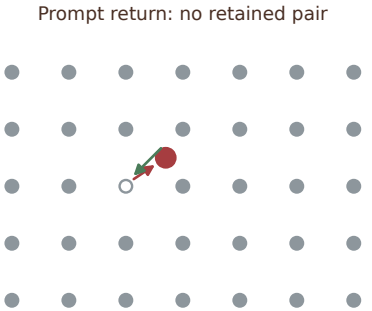


Below threshold: motion can end in recovery

- An atom can move away from its equilibrium position.
- The surrounding lattice also moves.
- If it returns during prompt relaxation, no retained Frenkel pair remains.

Motion alone is insufficient

Count the post-relaxation defect state.



Threshold energy is not defect formation energy

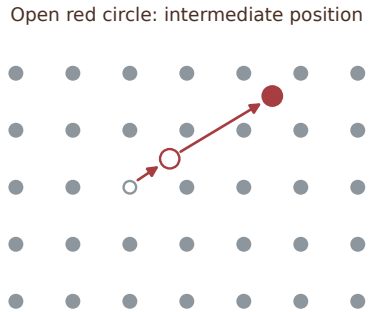
Formation energy

An energy difference between relaxed atomic configurations.

Displacement threshold

A kinetic threshold along a dynamic collision path.

Energy can spread into neighbouring atoms and vibrations before a stable separated configuration is reached.

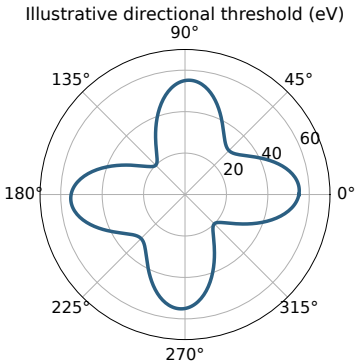


Threshold depends on recoil direction

- Different directions encounter different neighbouring atoms.
- Replacement sequences and return paths differ.
- A directional threshold $E_d(\hat{\mathbf{n}})$ is not a single universal number.

Illustrative anisotropy

The polar curve shows how the threshold can vary with direction.

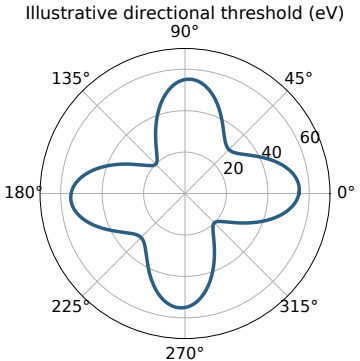


Choose and report an effective threshold

- A dose model often uses one effective threshold.
- Specify the material, model and adopted value.
- Do not mix a minimum directional value with an effective dose-model value.

Throughout our main calculations

We assume $E_d = 40$ eV for the Fe calculations.



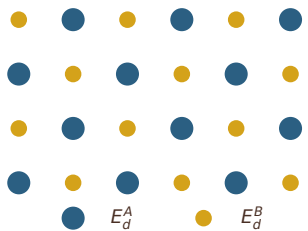
Compounds require species-aware accounting

- Different species can have different thresholds.
- Recoil production also depends on species.
- Species-resolved displacement counts preserve that information.

Why one number may fail

A single effective threshold cannot generally replace all recoil and energy-partition differences.

Two atomic species, two thresholds



A simplified compound threshold exercise

Question

Assume equal damage energy per atom of each species, with fractions $s_A = 1/3$, $s_B = 2/3$ and thresholds 40 and 20 eV. Find the equivalent high-energy threshold.

A simplified compound threshold exercise

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$$\frac{1}{E_d^{\text{eff}}} = \frac{1/3}{40} + \frac{2/3}{20}$$

A simplified compound threshold exercise

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$$\frac{1}{E_d^{\text{eff}}} = \frac{1/3}{40} + \frac{2/3}{20}$$

Answer

$E_d^{\text{eff}} = 24$ eV. This harmonic average applies only under the stated equal-partition simplification.

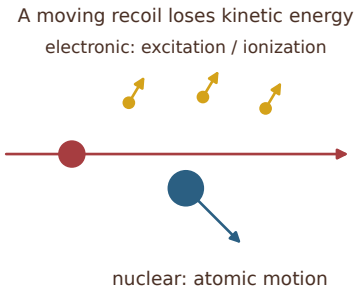
Stopping power measures energy loss along a path

$$S(E) = -\frac{dE}{dx}$$

- E: instantaneous moving-particle energy.
- x: distance along its path.
- $S > 0$ as the particle loses energy.

Units

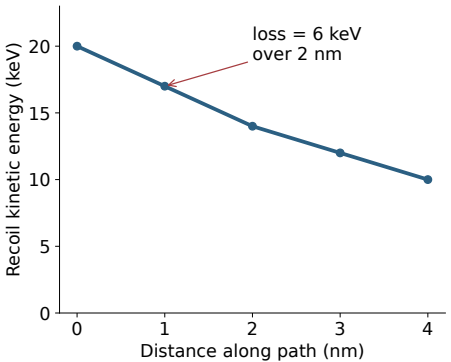
Energy per length, such as keV/nm.



Read stopping power from an energy-versus-distance plot

Question

The recoil drops from 20 to 14 keV over the first 2 nm. What is its average stopping power?

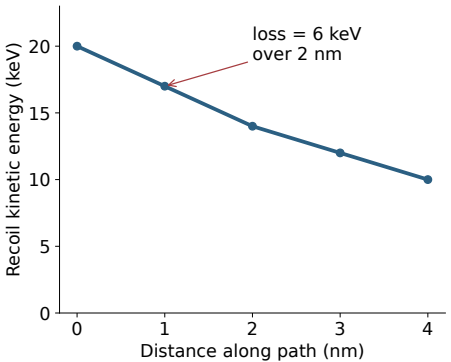


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Read stopping power from an energy-versus-distance plot

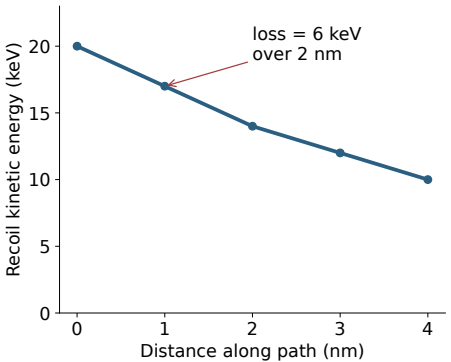
Question

The recoil drops from 20 to 14 keV over the first 2 nm. What is its average stopping power?

$$\overline{S} = \frac{20 - 14}{2} \text{ keV/nm}$$

Answer

$\overline{S} = 3$ keV/nm. This is an interval average, not the local derivative everywhere.



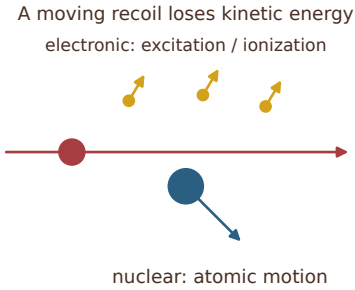
Nuclear stopping transfers energy to atoms

S_n

Energy transfer through collisions with target nuclei / atoms.

- Some transfers launch secondary recoils.
- Others are below the displacement threshold and become atomic vibrations.

Nuclear energy transfer is not identical to retained defect energy.



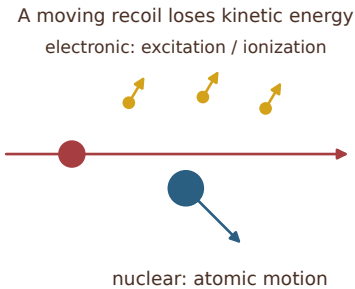
Electronic stopping transfers energy to electrons

S_e

> Energy transfer into electronic excitation and ionization.

- It reduces the energy available to the recoil cascade.
- Electron-lattice coupling can later heat the atoms.

In strongly excited materials, electronic energy deposition can itself cause structural change.



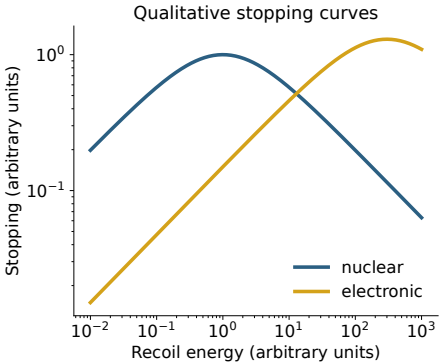
Nuclear and electronic stopping act together

$$S(E) = S_n(E) + S_e(E)$$

- Their relative importance changes with energy and species.
- A universal crossover energy does not exist.

Read the plot qualitatively

Both axes use arbitrary units; no material range can be calculated from this sketch.

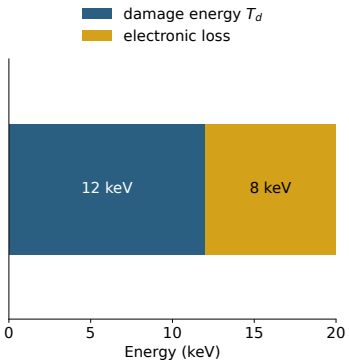


Lindhard partition: follow the cascade energy balance

$$T_d = f_n(T)\,T$$

- T: initial recoil energy.
- T_d: energy assigned to atomic motion after electronic losses.
- $f_n(T)$: nuclear energy-partition fraction, from 0 to 1.

It is a cascade partition, not simply the local ratio $S_n/(S_n + S_e)$ at the initial energy.



Worked example: split the recoil energy first

Question

For $T = 20$ keV, assume $f_n = 0.60$. Find the damage energy and electronic loss.

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$$T_d = 0.60(20 \text{ keV})$$

Worked example: split the recoil energy first

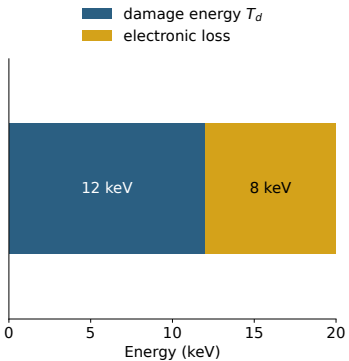
Question

For $T = 20$ keV, assume $f_n = 0.60$. Find the damage energy and electronic loss.

$$T_d = 0.60(20 \text{ keV})$$

Answer

$T_d = 12$ keV; electronic loss $= 8$ keV.



Two fractions answer different questions

Quantity	Question	Applied to
$f_n = T_d/T$	Where does the recoil energy go?	Energy
$\eta = \nu_{\mathrm{surv}}/\nu_{\mathrm{NRT}}$	How many primary defects survive relative to NRT?	Model count

Use them in order

$$T \longrightarrow T_d \longrightarrow \nu_{\mathrm{NRT}} \longrightarrow \nu_{\mathrm{surv}}.$$

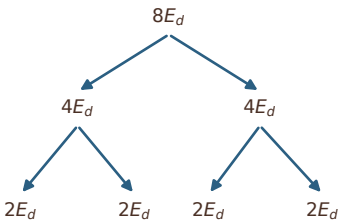
The two fractions describe different physics and need not have the same value.

Kinchin–Pease: a simple collision-count model

- Approximate the cascade as successive binary elastic collisions.
- Use equal-mass atoms and a sharp threshold.
- Neglect the real spatial structure and prompt recombination.

Purpose

Estimate the average displacement count as recoil energy is shared.



Equal energy sharing: schematic

KP: three low-energy regimes

Initial recoil energy T	KP model count
$T < E_d$	0
$E_d \le T < 2E_d$	1
$2E_d \le T < E_c$	$T/(2E_d)$

Meaning of the count

$\nu(T)$ is a model expectation; it need not be an integer for a given energy.

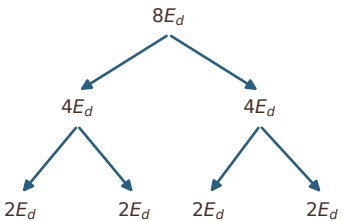
E_c is the idealized electronic cutoff in the original simplified model.

Why does the KP slope contain two?

- Secondary collisions divide the available recoil energy.
- Branches eventually fall below the displacement threshold.
- The equal-mass binary-collision model gives the mean count $T/(2E_d)$.

Interpretation

$2E_d$ is not the thermodynamic energy cost of one Frenkel pair.

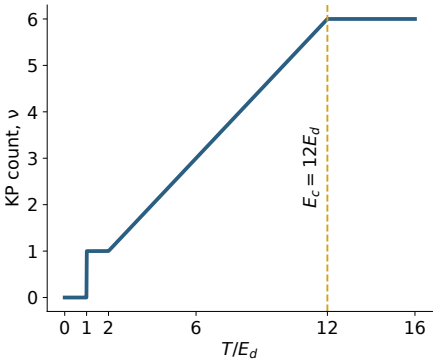


Equal energy sharing: schematic

KP: include the idealized electronic cutoff

$$\nu_{\mathrm{KP}}(T) = \begin{cases} 0 & T < E_d \\ 1 & E_d \le T < 2E_d \\ T/(2E_d) & 2E_d \le T < E_c \\ E_c/(2E_d) & T \ge E_c \end{cases}$$

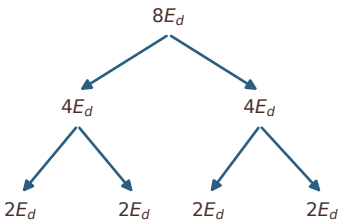
Above E_c, the simplified model sends the excess energy to electrons.



KP example: choose the branch before calculating

Question

Assume $T = 4$ keV, $E_d = 40$ eV and $E_c = 20$ keV. Find ν_{KP}.



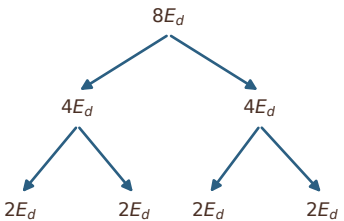
Equal energy sharing: schematic

KP example: choose the branch before calculating

Question

Assume $T = 4$ keV, $E_d = 40$ eV and $E_c = 20$ keV. Find ν_{KP}.

$2E_d = 80$ eV < 4000 eV $< E_c$: use the linear branch.



Equal energy sharing: schematic

KP example: choose the branch before calculating

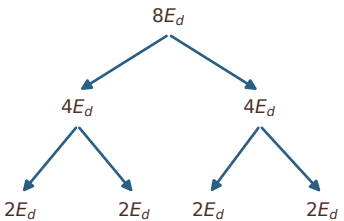
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$2E_d = 80$ eV < 4000 eV $< E_c$: use the linear branch.

Answer

$\nu_{\mathrm{KP}} = 4000/(2 \times 40) = 50$. The result is a model count.



Equal energy sharing: schematic

KP limitations point toward improved models

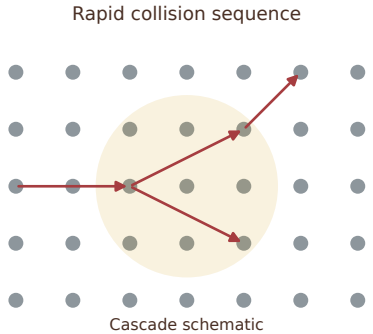
- Electronic losses vary continuously with energy.
- Atomic collisions are not ideal hard-sphere events.
- Dense cascades have many-body motion and recombination.
- The crystal controls directions and spatial clustering.

Next step

Use damage energy in NRT, then distinguish its count from surviving primary defects.

A cascade is more than a branching diagram

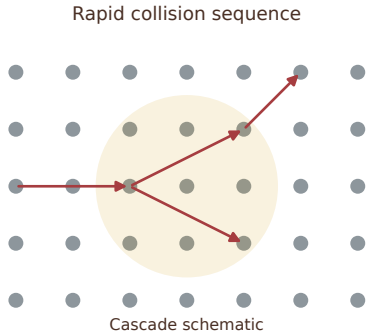
- One PKA generates secondary and later recoils.
- Trajectories overlap in a small excited region.
- Real atomic forces act simultaneously on many atoms.



Ballistic stage: rapid directed collisions

- Fast recoils transfer momentum to neighbouring atoms.
- The population far from lattice sites rises quickly.
- This stage is commonly sub-picosecond.

The exact duration depends on recoil energy and material.

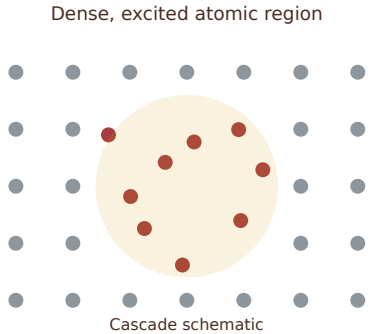


Thermal spike: a locally excited region

- Directed motion becomes collective, disordered motion.
- In some energetic cascades, a liquid-like core forms temporarily.
- Energy flows outward to the surrounding solid.

Use temperature carefully

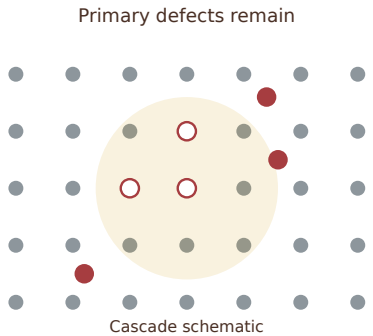
The earliest nonequilibrium motion need not have a well-defined local temperature.



Cooling and prompt recombination

- Atoms return toward lattice positions as the region cools.
- Nearby vacancies and interstitials can annihilate.
- The remaining primary defects may be isolated or clustered.

Relaxation commonly spans picoseconds to tens of picoseconds; there is no universal clock.

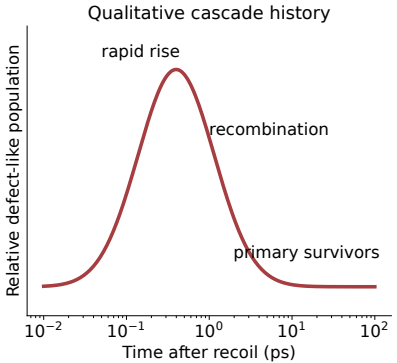


A large transient population can leave few defects

- The peak counts atoms far from lattice sites.
- The final primary count follows prompt relaxation.
- A later experimental count also includes migration and sinks.

Read the vertical axis

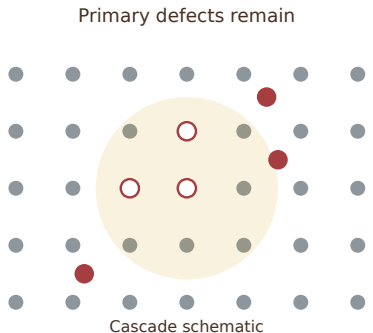
The curve shows a relative population on a schematic scale.



Vacancy-rich cores and outer interstitials

- Recoil motion can move atoms out of a central region.
- Vacancies can be concentrated near the core.
- Interstitials may occur farther out or in clusters.

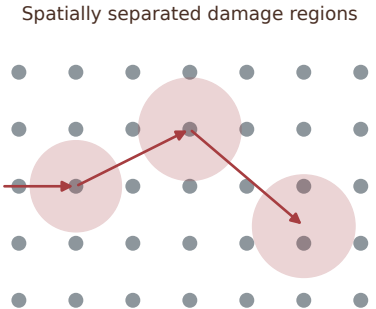
This is a useful physical picture; individual cascades are not perfect concentric shells.



Subcascades spread damage into separate regions

- An energetic recoil may travel between dense collision regions.
- It can initiate several spatially separated subcascades.
- Their overlap and recombination differ from a single compact region.

The onset depends on material and recoil energy.



Crystal rows can focus a collision sequence

- Momentum and energy can pass along an atomic row.
- Successive atoms may replace their neighbours.
- The final vacancy and interstitial can be separated by many sites.

A replacement event is not automatically a surviving Frenkel pair.

Energy passes along an atomic row



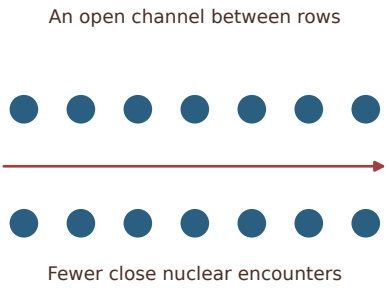
Successive replacements can move atoms without leaving a vacancy at every site

Channeling uses open crystal directions

- A particle moving between rows or planes can avoid close nuclear encounters.
- Its trajectory and penetration can change.
- Orientation therefore matters in ion experiments.

Distinction

Focusing transfers energy along rows; channeling guides motion between them.



Material dependence has several causes

Material feature	Possible cascade consequence
Atomic mass and collision potential	Energy transfer and scattering paths
Crystal structure and orientation	Focusing, channeling and defect configurations
Electronic energy loss	Energy remaining for atomic motion
Defect energetics and mobility	Recombination and cluster retention

Mass alone is insufficient to rank surviving damage in different materials.

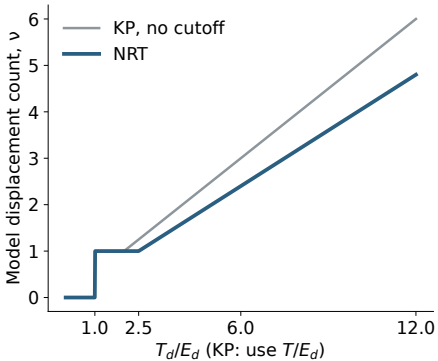
NRT replaces the simple KP energy budget

Norgett–Robinson–Torrens model

Use damage energy T_d and a factor 0.8 in the high-energy displacement estimate.

$$\nu_{\mathrm{NRT}} = \frac{0.8 T_d}{2E_d}$$

The 0.8 coefficient is part of the model calibration; it is not a universal 80% prompt-survival fraction.



Use the complete NRT piecewise function

$$\nu_{\mathrm{NRT}}(T_d) = \begin{cases} 0 & T_d < E_d \\ 1 & E_d \le T_d < 2E_d/0.8 \\ 0.8T_d/(2E_d) & T_d \ge 2E_d/0.8 \end{cases}$$

Branch boundary

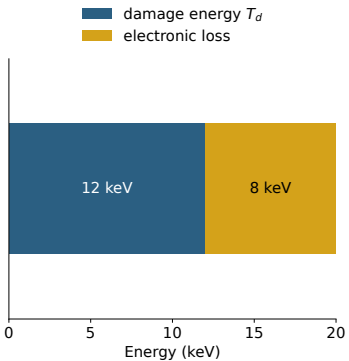
$2E_d/0.8 = 2.5E_d$. The linear branch reaches one at this point.

For $E_d = 40$ eV, the linear branch begins at $T_d = 100$ eV.

NRT example: carry the damage energy forward

Question

Use $T_d = 12$ keV and $E_d = 40$ eV. Find the NRT count.

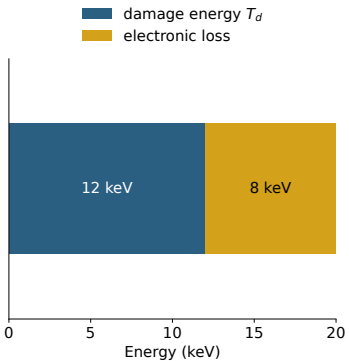


NRT example: carry the damage energy forward

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$$\nu_{\mathrm{NRT}} = \frac{0.8(12{,}000)}{2(40)}$$



NRT example: carry the damage energy forward

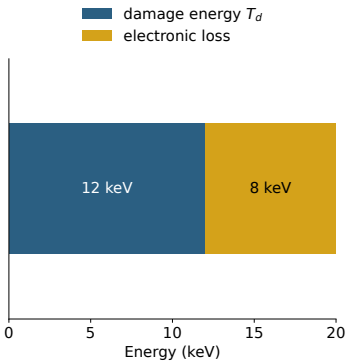
Question

Use $T_d = 12$ keV and $E_d = 40$ eV. Find the NRT count.

$$\nu_{\text{NRT}} = \frac{0.8(12{,}000)}{2(40)}$$

Answer

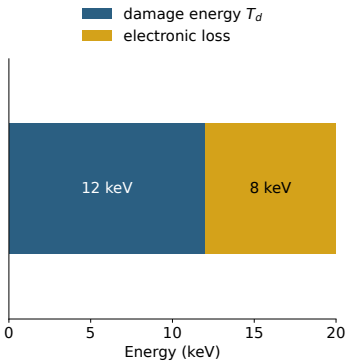
$\nu_{\text{NRT}} = 120$ model displacements per recoil.



Catch the energy-budget mistake

Question

A student uses the full 20 keV recoil and obtains 200 NRT displacements. What was omitted?



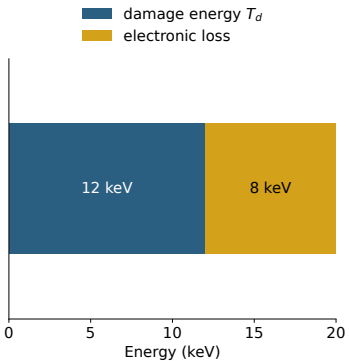
Catch the energy-budget mistake

Question

A student uses the full 20 keV recoil and obtains 200 NRT displacements. What was omitted?

Answer

The specified electronic loss. With $f_n = 0.60$, use 12 keV and obtain 120.



NRT near threshold

Question

For $E_d = 40$ eV, evaluate the count at $T_d = 30$, 60 and 200 eV.

NRT near threshold

Question

For $E_d = 40$ eV, evaluate the count at $T_d = 30$, 60 and 200 eV.

Check the two boundaries: 40 eV and 100 eV.

NRT near threshold

Question

For $E_d = 40$ eV, evaluate the count at $T_d = 30$, 60 and 200 eV.

Check the two boundaries: 40 eV and 100 eV.

Answer

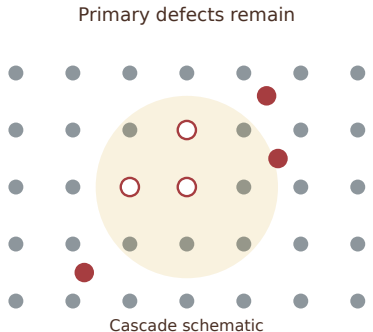
0, 1 and 2, respectively. Using the linear expression at 60 eV would incorrectly give 0.6.

What molecular dynamics adds

- Integrate atomic motion from a specified interatomic potential.
- Launch a PKA with chosen energy and direction.
- Include a stated treatment of electronic energy loss.
- Identify defects after a defined relaxation time.

A model still needs validation

Potential, cell size, boundaries, temperature and sampling affect predictions.

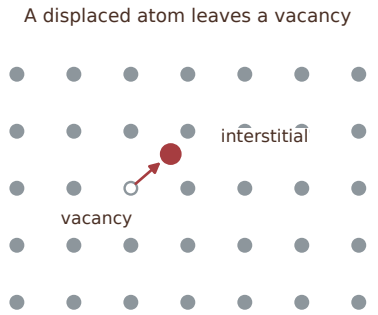


Define which defects a simulation counts

- Compare atoms with reference lattice sites.
- Empty sites indicate vacancies; excess occupancy indicates interstitial content.
- Group nearby defects only with a stated cluster criterion.

Report the observation time

Primary survivors after cooling differ from defects retained after long annealing.

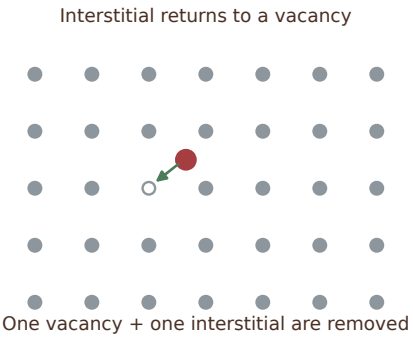


Prompt survival reduces the NRT estimate

$$\eta(T_d) = \frac{\nu_{\mathrm{surv}}(T_d)}{\nu_{\mathrm{NRT}}(T_d)}$$

- ν_{surv}: retained primary Frenkel-pair count after cascade cooling.
- η: model- and material-dependent survival factor.

A Frenkel pair contains one vacancy and one interstitial; avoid counting it twice.



A survival-factor calculation

Question

Assume $\nu_{\mathrm{NRT}} = 120$ and $\eta = 0.30$ for this recoil. How many primary Frenkel pairs are estimated?

A survival-factor calculation

Question

Assume $\nu_{\mathrm{NRT}} = 120$ and $\eta = 0.30$ for this recoil. How many primary Frenkel pairs are estimated?

$$\nu_{\mathrm{surv}} = 0.30(120)$$

A survival-factor calculation

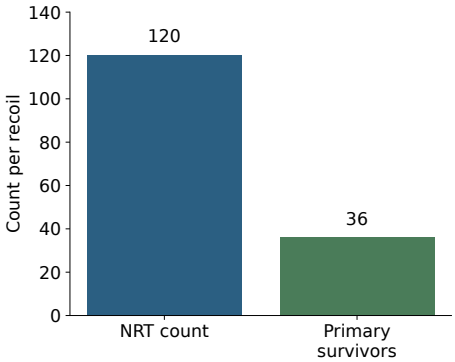
Question

Assume $\nu_{\mathrm{NRT}} = 120$ and $\eta = 0.30$ for this recoil. How many primary Frenkel pairs are estimated?

$$\nu_{\mathrm{surv}} = 0.30(120)$$

Answer

$\nu_{\mathrm{surv}} = 36$ pairs: 36 vacancies and 36 interstitials if the system conserves atoms and has no sinks.



ARC-dpa corrects for athermal recombination

$$\nu_{\mathrm{arc}}(T_d) = \eta(T_d)\nu_{\mathrm{NRT}}(T_d)$$

- ARC: athermal recombination corrected.
- The correction represents primary cascade survival.
- It does not include all later temperature-driven evolution.

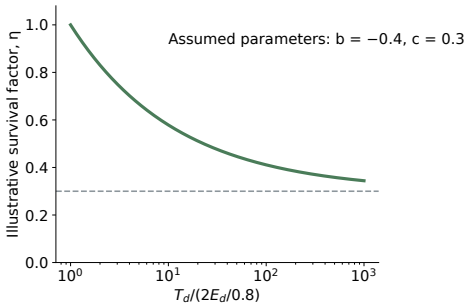
Use a material-specific parameterization and retain the threshold branches.

How the survival correction varies with energy

- The survival factor can fall as dense cascades develop.
- A high-energy plateau represents the subcascade regime.
- The illustrated curve uses assumed parameters.

Energy dependence

Use the correction appropriate to the recoil energy and material.



Displacements, survivors and mixing differ

- NRT supplies a conventional displacement estimate.
- ARC estimates primary surviving defects.
- Atomic mixing counts atoms transferred between sites, even if the lattice heals.

The moving-row example

Many atoms can change identity at lattice sites while only an end pair remains.

Energy passes along an atomic row



Successive replacements can move atoms without leaving a vacancy at every site

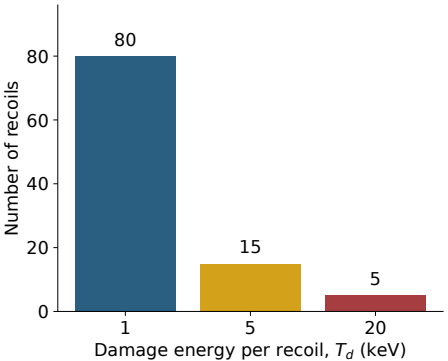
A recoil spectrum lists many different events

Spectrum

A distribution of recoil energies, usually also resolved by recoiling species.

- A single average recoil can hide the tail.
- A spectrum must state its normalization and units.

The next example spectrum contains exactly 100 recoil events.



Example: Recoil Spectrum

T_d per recoil	Number of recoils	Fraction
1 keV	80	0.80
5 keV	15	0.15
20 keV	5	0.05

Simplification

Here the bins are already damage energies, after electronic losses.

For a spectrum of initial PKA energy T, calculate $T_d(T)$ before weighting.

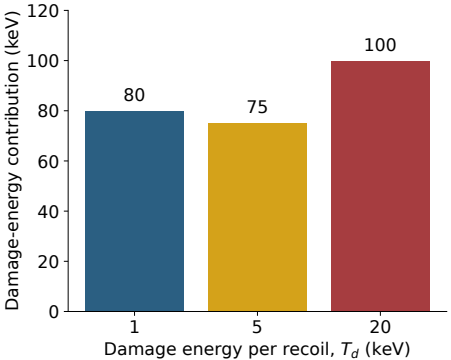
Count weighting and energy weighting tell different stories

$$\text{energy in bin } j = n_j T_{d,j}$$

- Low bin: $80 \times 1 = 80$ keV.
- Middle bin: $15 \times 5 = 75$ keV.
- High bin: $5 \times 20 = 100$ keV.

Total

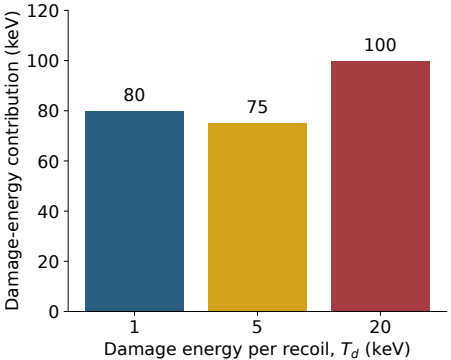
255 keV across the 100 recoil events.



Which bin matters most for damage energy?

Question

Only 5% of the recoils are in the 20 keV bin. What fraction of the total damage energy do they carry?

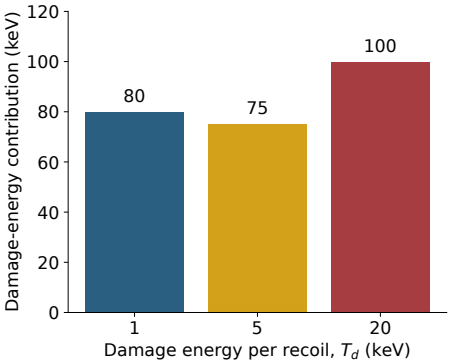


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Weight each recoil by its damage energy before normalizing.



Which bin matters most for damage energy?

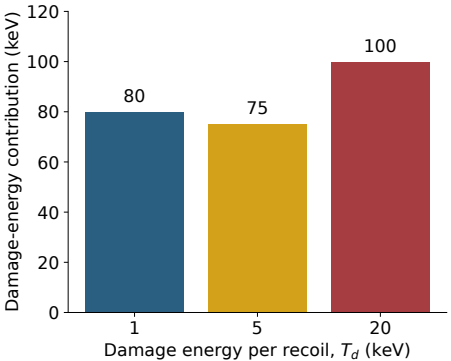
Question

Only 5% of the recoils are in the 20 keV bin. What fraction of the total damage energy do they carry?

Weight each recoil by its damage energy before normalizing.

Answer

$100/255 = 0.392$, or 39.2%. A small count fraction can carry substantial energy.

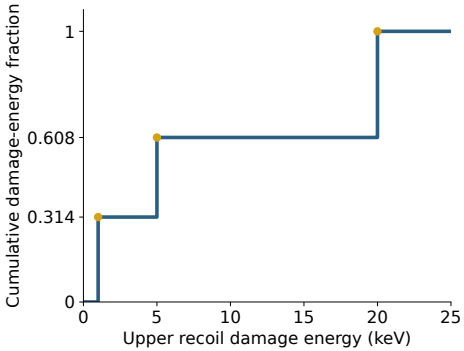


Build a cumulative damage-energy distribution

$$W(T_*) = \frac{\sum_{T_{d,j} \leq T_*} n_j T_{d,j}}{\sum_j n_j T_{d,j}}$$

- T_*: chosen upper damage-energy limit.
- Numerator: energy from bins at or below that limit.
- Denominator: energy from all bins.

The result is dimensionless and rises from 0 to 1.



Read cumulative values as fractions below a limit

Upper limit	Included energy	Cumulative fraction
1 keV	80 keV	$80/255 = 0.314$
5 keV	155 keV	$155/255 = 0.608$
20 keV	255 keV	1.000

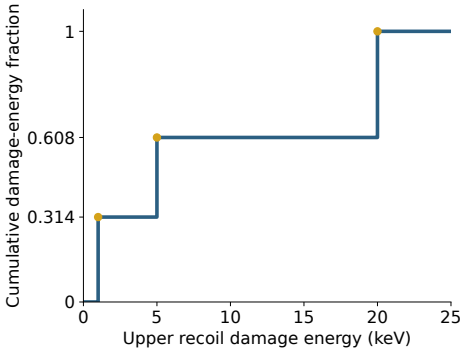
Between bin energies

The example curve is flat because no events were assigned to those gaps.

Read a fraction above a chosen energy

Question

How much damage energy in the example spectrum comes from recoils above 5 keV?

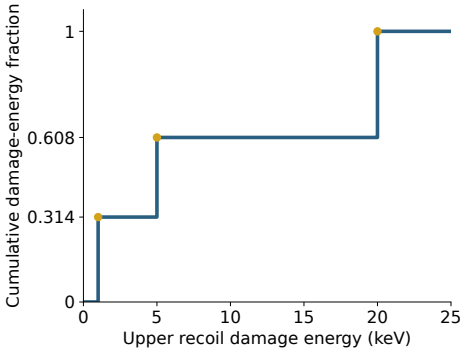


Read a fraction above a chosen energy

Question

How much damage energy in the example spectrum comes from recoils above 5 keV?

The cumulative value at 5 keV includes the 1 and 5 keV bins.



Read a fraction above a chosen energy

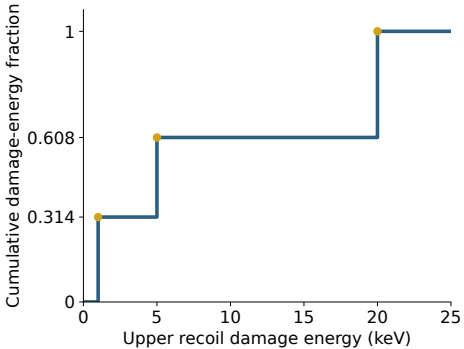
Question

How much damage energy in the example spectrum comes from recoils above 5 keV?

The cumulative value at 5 keV includes the 1 and 5 keV bins.

Answer

$1 - W(5) = 1 - 0.608 = 0.392$, or 39.2%.

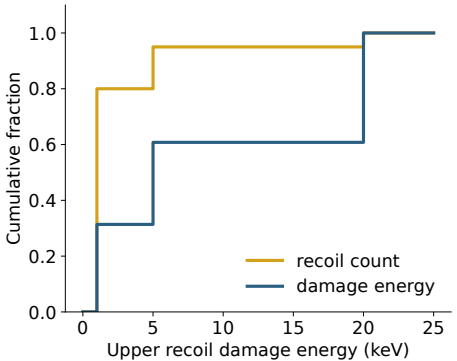


The same spectrum has two different cumulative curves

- Count cumulative: fraction of events at or below a limit.
- Damage-energy cumulative: fraction of energy at or below a limit.
- Both end at 1 because each uses its own total.

Axis label matters

Always ask what quantity was summed in the numerator.

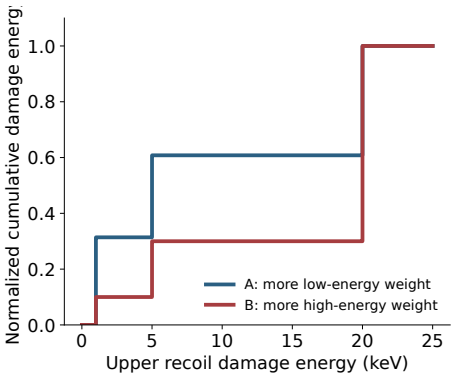


Compare normalized curves without losing their meaning

- Curve A reaches a given fraction at lower energy.
- Curve B has more of its energy in higher-energy recoils.
- Both end at 1 by normalization.

What you cannot infer

Equal final height does not imply equal total damage energy, event rate or dpa.

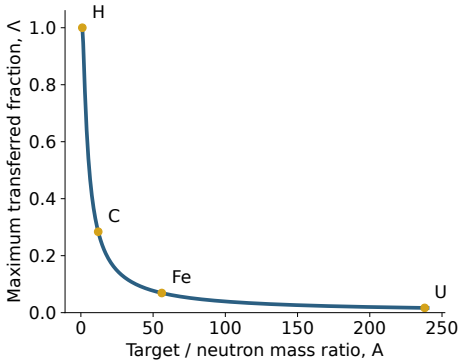


A spectrum endpoint is a kinematic limit, not a yield

$$T_{\max} = \frac{4mM}{(m+M)^2} E$$

- Compare the same target and the same incident energy.
- Protons and neutrons have nearly equal masses, hence nearly equal elastic endpoints.
- Their cross sections and recoil distributions can still differ.

For other projectile masses, recalculate the endpoint. A log axis can hide small differences.



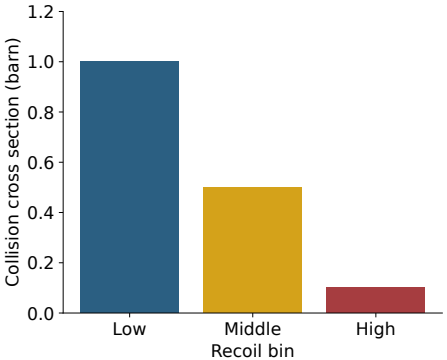
From recoil spectrum to displacement cross section

Two ingredients

How likely is each recoil bin, and how much model damage does each event cause?

$$\sigma_D \approx \sum_j \sigma_j \nu_j$$

- σ_j: collision cross section integrated over recoil bin j.
- ν_j: mean model displacement count for that bin.



A three-bin cross-section example

Bin	σ_j **(barn)**	ν_j	$\sigma_j \nu_j$ **(barn)**
Low	1.0	1	1
Middle	0.5	10	5
High	0.1	100	10

$$\sigma_{\text{coll}} = 1.6 \text{ b}, \qquad \sigma_D = 16 \text{ b}$$

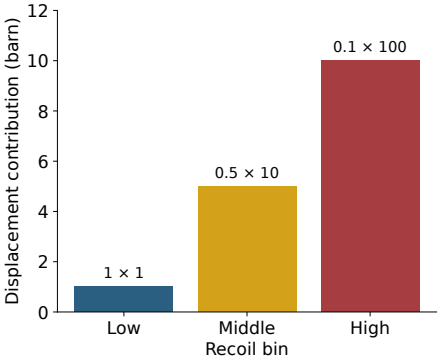
The bin means are assumed inputs at one incident energy.

Rare high-energy events can dominate the sum

- The high bin has the smallest collision cross section.
- Its events have the largest displacement count.
- The product determines its contribution to damage.

Read the vertical axis

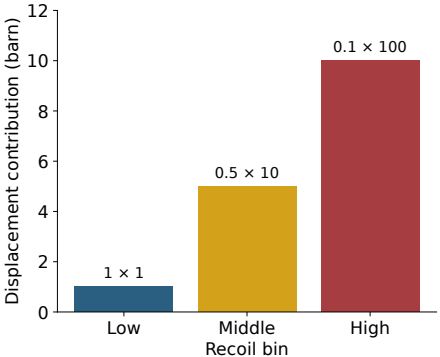
These bars show $\sigma_j \nu_j$, not collision probability alone.



Can displacement cross section exceed collision cross section?

Question

The example gives $\sigma_D = 16$ b but $\sigma_{\text{coll}} = 1.6$ b. Is this an error?



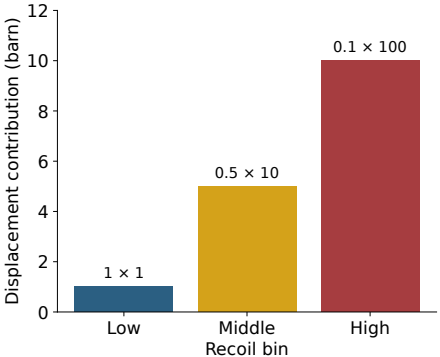
Can displacement cross section exceed collision cross section?

Question

The example gives $\sigma_D = 16$ b but $\sigma_{\text{coll}} = 1.6$ b. Is this an error?

Answer

No. Each collision can produce multiple model displacements. The collision-weighted mean count is $16/1.6 = 10$.



Why the differential cross section appears

$d\sigma/dT$

> Collision cross section per unit recoil energy, at a specified incident energy.

$$\sigma_j \approx \left(\frac{d\sigma}{dT}\right)_j \Delta T_j$$

- Units: barn/eV $\times$ eV $=$ barn.
- Unequal bin widths must be included.

An integral is the limit of a sum over narrower recoil bins.

Do not omit the energy-bin width

Question

A bin has $d\sigma/dT = 0.02$ b/keV, width 5 keV and mean count $\nu = 50$. What is its contribution?

Do not omit the energy-bin width

Question

A bin has $d\sigma/dT = 0.02$ b/keV, width 5 keV and mean count $\nu = 50$. What is its contribution?

$$0.02 \text{ b/keV} \times 5 \text{ keV} \times 50$$

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$$0.02 \text{ b/keV} \times 5 \text{ keV} \times 50$$

Answer

$\sigma_j = 0.10$ b and $\sigma_j \nu = 5$ b.

Use the same damage model throughout the sum

NRT displacement cross section

Weight each recoil bin with $\nu_{\mathrm{NRT}}[T_d(T)]$.

ARC displacement cross section

Weight it with $\nu_{\mathrm{arc}}[T_d(T)]$.

Because the correction depends on energy, a single survival factor may not represent the whole spectrum.

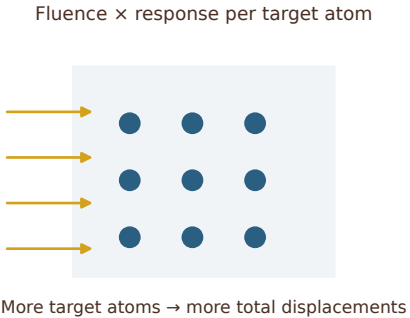
Derive dpa by counting a sample response

$$N_{\text{disp}} = N_{\text{target}}\,\Phi\,\sigma_D$$

$$\text{dpa} = \frac{N_{\text{disp}}}{N_{\text{target}}} = \Phi\sigma_D$$

- N_{target}: atoms represented by the calculation.
- Φ: local fluence; σ_D: matching model response.

Assume a uniform exposure and composition.



Constant flux gives dose rate and total dose

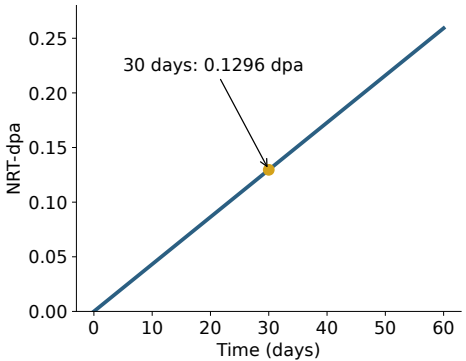
$$\dot{d} = \phi\sigma_D, \qquad d = \phi\sigma_D t$$

Symbols

d: dpa; $\dot{d}$: dpa/s; t: seconds.

$$(\mathrm{cm}^{-2}\mathrm{s}^{-1})(\mathrm{cm}^2) = \mathrm{s}^{-1}$$

dpa is dimensionless, but label it to identify the damage measure.



Worked dose example: collect the inputs

Assumed spectrum-averaged NRT response

$\overline{\sigma}_D = 500 \text{ b} = 5.00 \times 10^{-22} \text{ cm}^2$.

Exposure

$\phi = 10^{14} \text{ cm}^{-2}\text{s}^{-1}$ for 30 days.

$$t = 30(24)(3600) = 2.592 \times 10^6 \text{ s}$$

Worked dose example: rate first, then time

Question

Use the previous inputs. Find the dpa rate and 30-day dose.

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$$\dot{d} = (10^{14})(5.00 \times 10^{-22}) = 5.00 \times 10^{-8}\ \mathrm{s}^{-1}$$

Worked dose example: rate first, then time

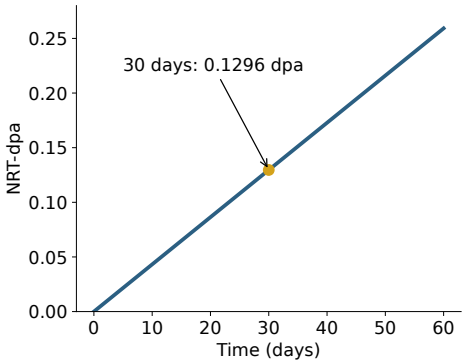
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$$\dot{d} = (10^{14})(5.00 \times 10^{-22}) = 5.00 \times 10^{-8}\ \mathrm{s}^{-1}$$

Answer

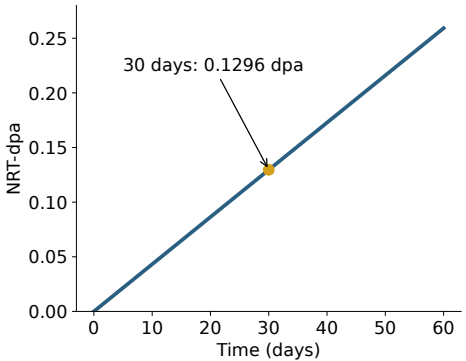
$d = (5.00 \times 10^{-8})(2.592 \times 10^{6}) = 0.1296$ NRT-dpa.



How long to reach one dpa?

Question

At $\dot{d} = 5.00 \times 10^{-8}$ dpa/s, find the time to 1 dpa.

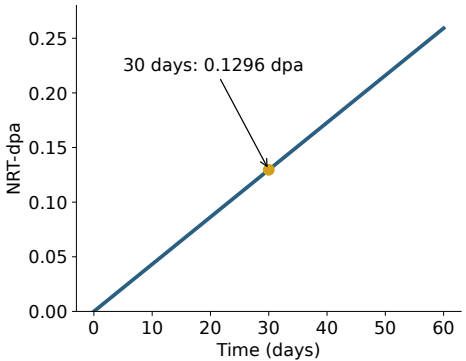


How long to reach one dpa?

Question

At $\dot{d} = 5.00 \times 10^{-8}$ dpa/s, find the time to 1 dpa.

$$t = d/\dot{d}$$



How long to reach one dpa?

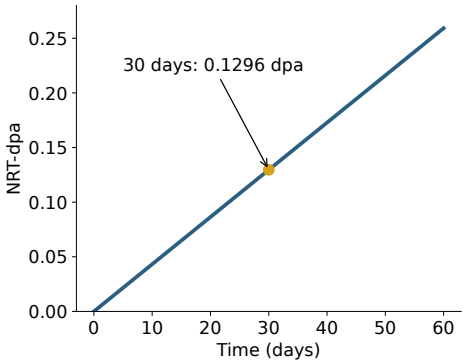
Question

At $\dot{d} = 5.00 \times 10^{-8}$ dpa/s, find the time to 1 dpa.

$$t = d/\dot{d}$$

Answer

$t = 2.00 \times 10^{7}$ s ≈ 231 days, assuming the rate stays constant.



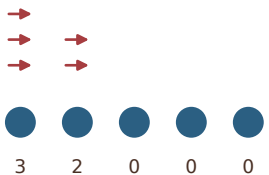
One dpa does not mean every atom moved once

- dpa is a model count normalized by target atoms.
- Some atoms can move repeatedly; others may not move.
- Most displaced atoms need not remain as defects.

Counting analogy

Five moves among five atoms do not require one move per atom.

Five counted moves / five atoms = 1



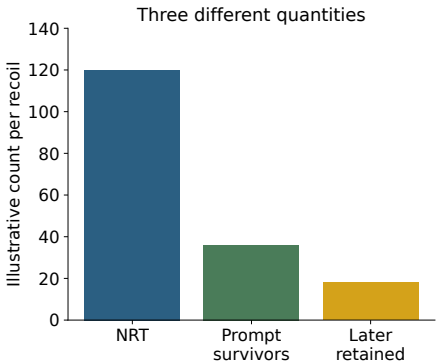
Schematic counts: 3 + 2 + 0 + 0 + 0

dpa is not the residual defect fraction

- A dose records an accumulated model production measure.
- Prompt recombination removes many defect pairs.
- Migration and sinks change the later population.

Example

120 NRT → 36 primary pairs → 18 later pairs illustrates three separate quantities.



Same fluence can produce different dpa

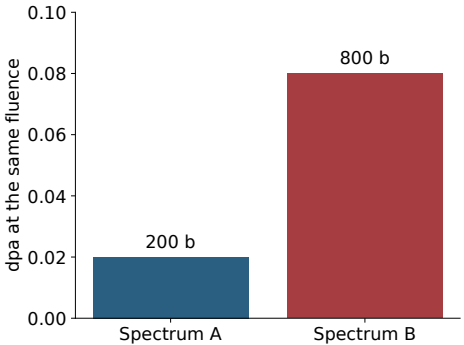
Assume

$\Phi = 10^{20}$ cm^{-2}.

$$d_A = \Phi(200\text{ b}) = 0.020$$

$$d_B = \Phi(800\text{ b}) = 0.080$$

The spectral response differs, so the dose differs even at equal particle fluence.



Add incident-energy groups before averaging

$$\dot{d} = \sum_i \phi_i \sigma_{D,i}$$

- i: incident-energy group, distinct from recoil bin j.
- ϕ_i: group-integrated flux.
- $\sigma_{D,i}$: response averaged consistently within that group.

Two levels of weighting

First combine recoil damage at each incident energy; then combine the incident-energy groups.

A two-group neutron-field calculation

Question

Let $\phi_1 = 8 \times 10^{13}$ and $\phi_2 = 2 \times 10^{13}$ $\mathrm{cm}^{-2}\mathrm{s}^{-1}$, with responses 100 and 900 b.

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A two-group neutron-field calculation

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$$\dot{d} = [(8 \times 10^{13})(100) + (2 \times 10^{13})(900)]10^{-24}$$

Answer

$\dot{d} = 2.6 \times 10^{-8}$ dpa/s; $\overline{\sigma}_D = 260$ b for total flux 10^{14}.

Same dpa still does not imply the same material state

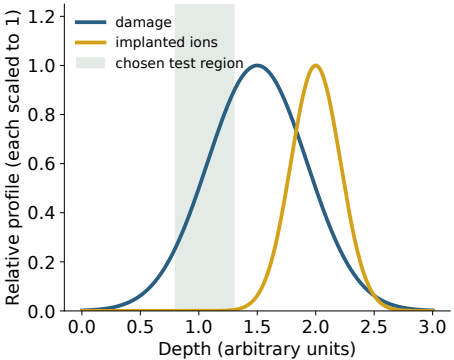
Also compare	Why it matters
Temperature	Defect mobility and recombination
Dose rate	Time between production events
Recoil spectrum	Cascade size and clustering
Gas production	He / H interactions with defects
Depth and microstructure	Surfaces, sinks and spatial gradients

dpa supports comparisons; it does not remove all differences between irradiation conditions.

Ion irradiation gives a depth-dependent experiment

- Damage changes with depth.
- Implanted ions can change composition.
- Near-surface sinks affect defect retention.
- Choose the sampled depth when reporting dose.

The illustrative profiles are each normalized to their own maximum.

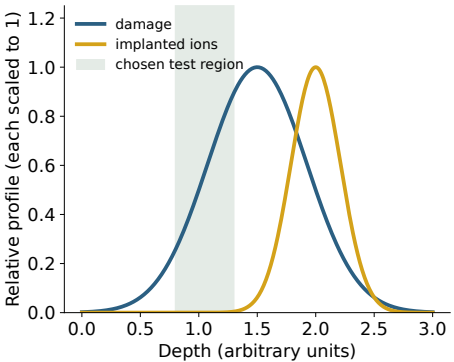


What must be matched in an ion–neutron comparison?

- Material composition and starting microstructure.
- Temperature, model dose and dose rate.
- Recoil energies and defect-cluster production.
- Gas production, injected species and analysis depth.

Practical use

Ion studies can isolate mechanisms; transferring results requires these comparisons.

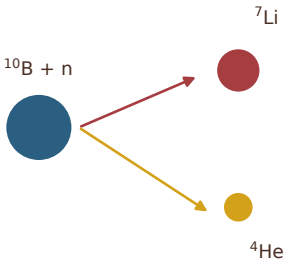


Transmutation changes chemistry as well as damage

$$^{10}\mathrm{B} + n \longrightarrow {}^{7}\mathrm{Li} + {}^{4}\mathrm{He}$$

- The products are different chemical species.
- Energetic charged products also deposit energy.
- Some branches include an excited nucleus and gamma emission.

Gas production cannot be inferred from dpa alone.



Nickel illustrates a two-step helium route

$$^{58}\mathrm{Ni}(n,\gamma)^{59}\mathrm{Ni}$$
$$^{59}\mathrm{Ni}(n,\alpha)^{56}\mathrm{Fe}$$

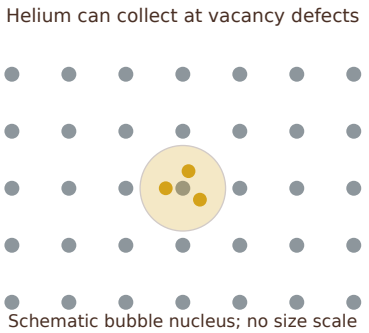
- The first reaction changes the isotope inventory.
- The second produces an alpha particle, which becomes helium.
- Rates depend on spectrum and irradiation history.

Helium adds another variable to the comparison

- Helium can bind to vacancy defects and collect in bubbles.
- Gas content changes the evolution of cavities.
- Report gas concentration as well as displacement dose.

$$1 \text{ appm} = 10^{-6} \text{ atomic fraction}$$

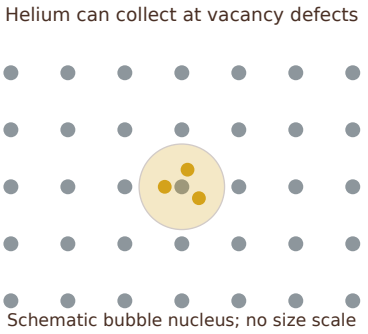
He/dpa is environment- and composition-dependent.



A gas-production bookkeeping example

Question

Assume a constant production ratio of 8 appm He/dpa. What is produced over 0.25 dpa?

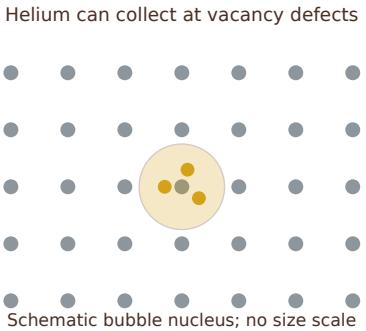


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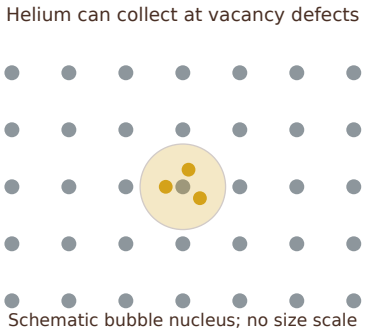
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$$8\ \frac{\text{appm}}{\text{dpa}} \times 0.25\ \text{dpa}$$

Answer

2 appm He, or atomic fraction 2×10^{-6}. Retention may differ if helium escapes.



Summary: From Recoil Energy to Dose

Stage	Input / result
Collision	Determine recoil energy distribution
Partition	$T = 20$ keV, $f_n = 0.60 \Rightarrow T_d = 12$ keV
Count	$E_d = 40$ eV $\Rightarrow \nu_{\mathrm{NRT}} = 120$
Survival	Assumed $\eta = 0.30 \Rightarrow 36$ primary pairs
Dose	Weight all recoil events, then multiply response by fluence

The one-recoil example supplies a count, not a sample dpa by itself.

Final check: identify three separate errors

Question

A report says: “20 keV gives 200 stable defects, so 1 dpa means every atom is now a defect.”

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Use T_d, identify the damage model, and specify when defects are counted.

Final check: identify three separate errors

Question

A report says: “20 keV gives 200 stable defects, so 1 dpa means every atom is now a defect.”

Use T_d, identify the damage model, and specify when defects are counted.

Answer

It omitted the stated energy partition; equated NRT with retained defects; and treated a normalized production count as a residual defect fraction.

Unit 3: Summary of Equations

Equation	Job
$T_{\max} = \Lambda E_n$	Bound the recoil energy
$T_d = f_n(T)T$	Remove electronic energy loss
$\nu_{\mathrm{NRT}} = 0.8T_d/(2E_d)$	Count in the high-energy branch
$\sigma_D \approx \sum_j \sigma_j \nu_j$	Combine recoil events
$\dot{d} = \sum_i \phi_i \sigma_{D,i}$	Combine incident-energy groups
$d = \dot{d}\,t$	Accumulate a constant dose rate

Check model, branch, units and normalization before substituting numbers.

Practice: one independent recoil-to-dose exercise

Given

At one incident energy, recoil bins have cross sections 0.2 and 0.05 b, initial energies 2 and 20 keV, and partition fractions 0.80 and 0.60. Use $E_d = 40$ eV and NRT.

Exposure

$\Phi = 10^{21}$ cm^{-2}. Find each T_d, each ν, σ_D and dpa.

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Answer

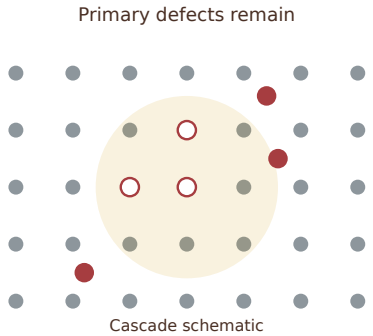
T_d: 1.6, 12 keV; ν: 16, 120; $\sigma_D = 9.2$ b; $d = 0.0092$ NRT-dpa.

From primary damage to Unit 4

- Primary cascades supply vacancies, interstitials and clusters.
- Diffusion moves these defects after the cascade cools.
- Sinks and reactions determine how the microstructure develops.

Carry forward

A defect production rate needs a kinetic evolution model before it predicts swelling or hardening.



Optional backup: the recoil-energy integral

$$\sigma_D(E_n) = \int_0^{T_{\max}(E_n)} \frac{d\sigma(E_n, T)}{dT}\, \nu[T_d(T)]\, dT$$

- E_n is fixed during this integral.
- T labels recoil energy; $d\sigma/dT$ has area/energy units.
- ν is the chosen NRT or ARC count; subthreshold recoils contribute zero.

This expression shows one elastic recoil channel. General calculations sum reaction channels and recoil species.

Optional backup: incident spectrum and changing flux

$$d = \int_0^{t_f} dt \int_0^{\infty} \phi(E,t)\sigma_D(E)\, dE$$

- $\phi(E,t)$: differential flux, $\mathrm{cm}^{-2}\mathrm{s}^{-1}\mathrm{eV}^{-1}$.
- t_f: final exposure time.
- $\sigma_D(E)$: area, calculated for the chosen material and damage model.

$$\overline{\sigma}_D = \frac{\int \phi(E)\sigma_D(E)\, dE}{\int \phi(E)\, dE}$$

For a fixed spectrum and constant total flux, $d = \phi_{\text{total}}\overline{\sigma}_D t$.

Optional backup: damage-weighted recoil cumulative

$$W(T_*) = \frac{\int_0^{T_*} T_d(T)\, r(T)\, dT}{\int_0^{T_{\max}} T_d(T)\, r(T)\, dT}$$

- $r(T)$: differential recoil rate for a stated exposure and species.
- T_* is now a limit on initial recoil energy, not damage energy.
- $W(T_{\max}) = 1$ if the denominator is nonzero.

For displacement weighting, replace $T_d(T)$ with the chosen count $\nu[T_d(T)]$. They are proportional only in a common linear regime.

Optional backup: KP linear branch from the model

$$\nu(T) = \frac{2}{T}\int_0^T \nu(u)\,du \qquad (T \geq 2E_d)$$

The equal-mass hard-sphere model averages the two outgoing energy branches.

$$T\nu(T) = 2\int_0^T \nu(u)\,du \quad \Rightarrow \quad T\nu'(T) = \nu(T)$$

Thus $\nu = CT$. Matching $\nu(2E_d) = 1$ gives $C = 1/(2E_d)$.

Domain

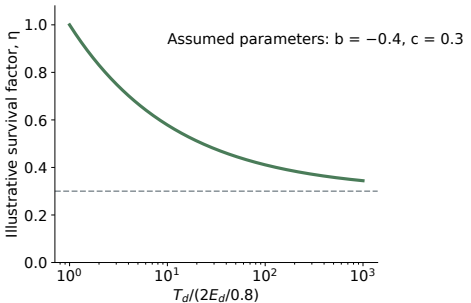
This derivation describes the idealized KP assumptions below its electronic cutoff.

Optional backup: ARC correction function

$$\eta(T_d) = (1 - c)\left(\frac{T_d}{2E_d/0.8}\right)^b + c$$

- Use this branch for $T_d \geq 2E_d/0.8$.
- $b < 0$: energy dependence; c: high-energy limiting factor.
- Material-specific parameters come from an appropriate fit.

At the branch boundary, $\eta = 1$. Keep the zero and one-displacement threshold branches below it.



Optional backup: useful conversions and checks

Conversion / check	Value
Energy	1 keV = 1000 eV; 1 MeV = 1000 keV
Time	1 day = 86,400 s
Area	1 barn = 10^{-24} cm^2
Rate	1 dpa per 365-day year $\approx 3.17 \times 10^{-8}$ dpa/s
Energy balance	$0 \leq T_d \leq T \leq T_{\max}$
Normalization	A nonzero cumulative weighted distribution ends at 1