Radiation-induced damage in materials

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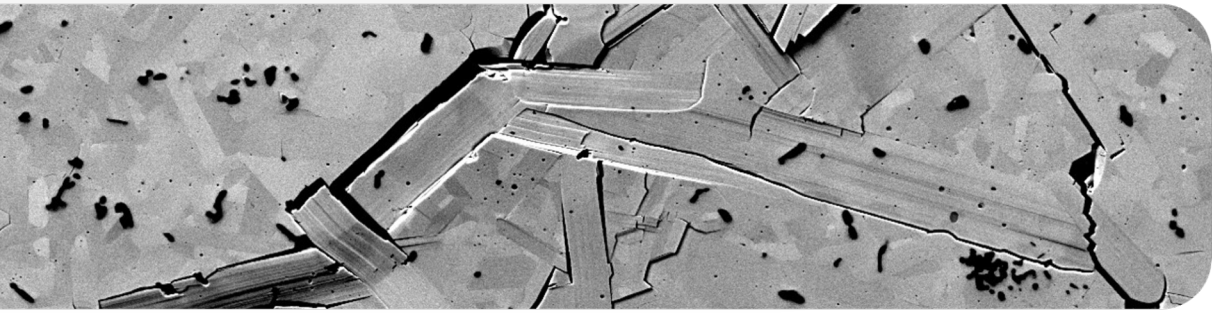

Introduction

Objectives and industrial context

❖ Why study radiation-induced degradation?

- In nuclear reactors, materials are constantly exposed to neutrons, γ-rays, ions, and electrons.
- This exposure causes atomic-scale damage that evolves and accumulates.
- Over time, this leads to macroscopic degradation:
  - ✓ swelling, embrittlement, amorphization, reduced ductility, cracking.

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↳ These effects are critical in reactor safety and lifetime management.

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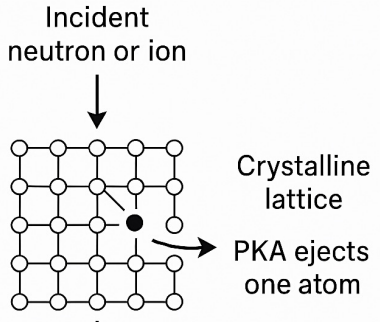
  - A high-energy particle displaces atoms from their lattice sites
    - ⇒ Formation of vacancies and interstitials.



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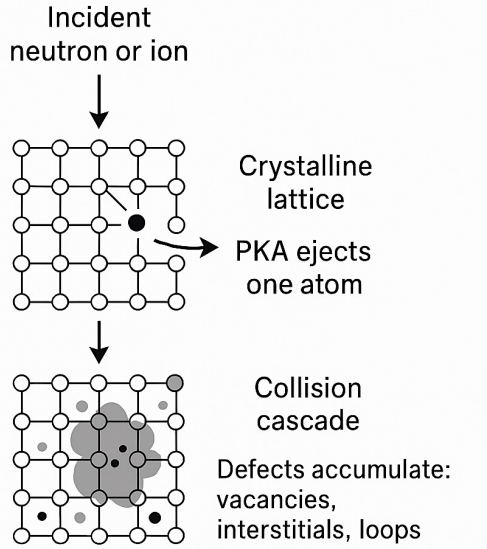

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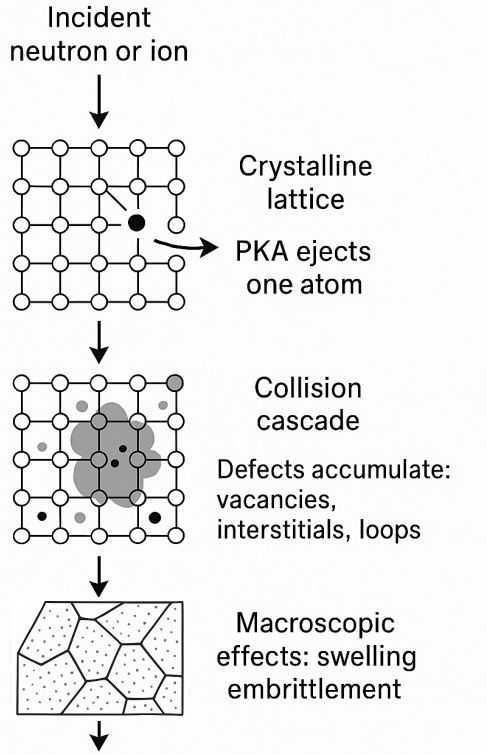

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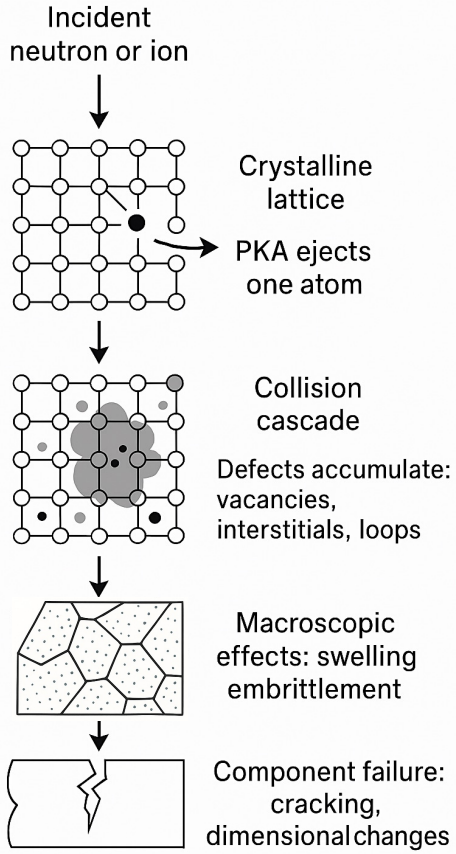

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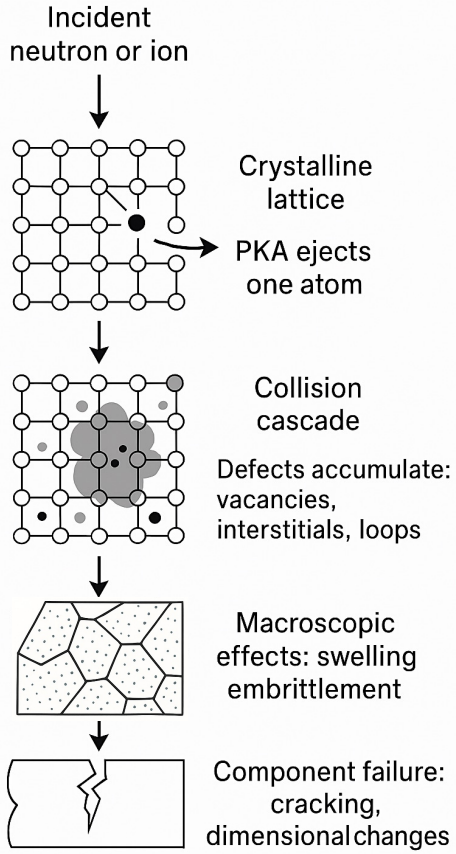

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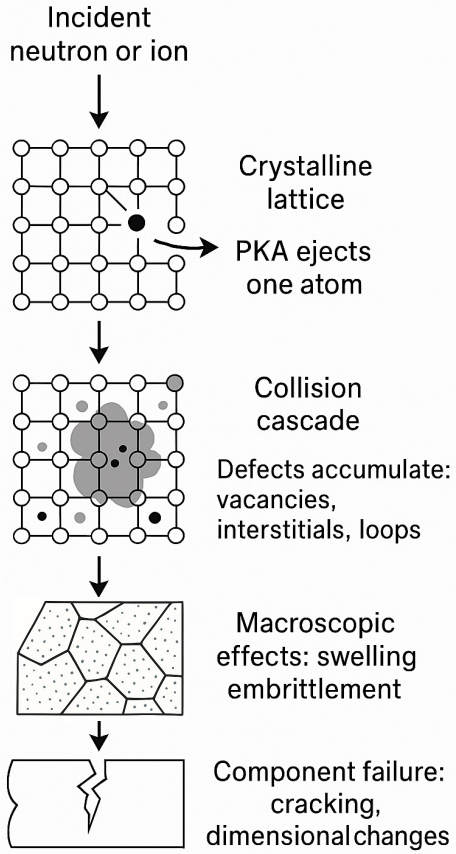
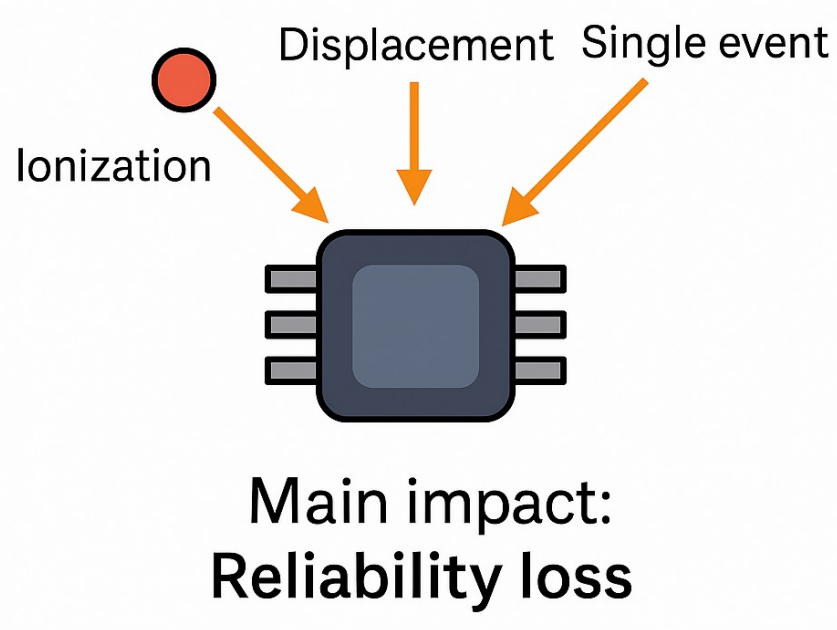
↳ Engineering solutions require linking scales: atomic → component.



Radiation effects on electronic components



- **Ionization**
  - Trapped charges in oxides
    ⇒ Leakage currents.
- **Displacement damage**
  - Defects in the silicon lattice
    ⇒Reduced carrier mobility, degraded performance.
- **Single Event Effects (SEE)**
  - Bit flips in memories, temporary malfunctions, or destructive latch-up.
- **Main impact**
  - Reduced reliability

↳Need for radiation-hardened designs in critical applications (aerospace, nuclear).

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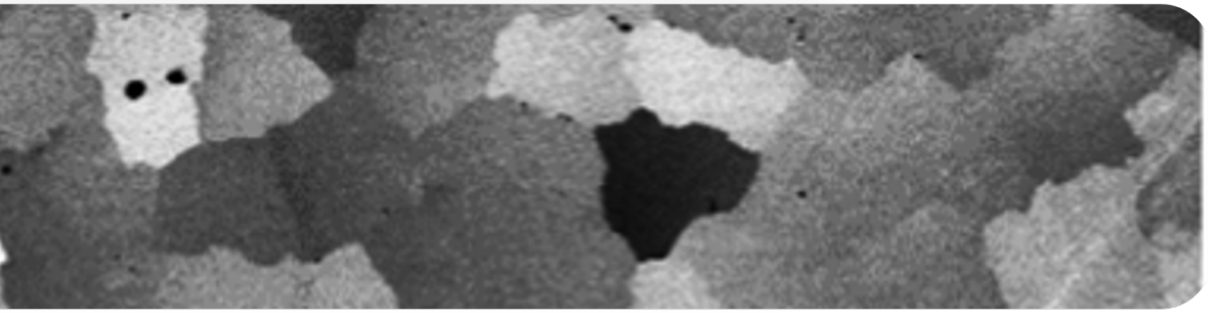
- **Embrittlement**
  - Loss of ductility caused by defect accumulation or segregation under irradiation. Makes materials more prone to fracture or cracking.

Overview of irradiating particles

Particle	Charge	Mass	Interaction mechanism	Typical effects in solids	Use in nuclear context
Neutron	0	$\sim 1\ u$	Elastic/inelastic nuclear collisions	Displacement cascades, transmutation	Primary cause of structural damage
Ion	± 1 to $\pm Z$	$> 1\ u$	Coulomb interaction (nuclei + electrons)	Dense cascades, high local damage	Material testing, ion implantation
Electron	-1	$\sim \frac{1}{1836}\ u$	Electromagnetic with electrons	Ionization, weak displacement ($> 1\ MeV$)	Radiation from decay or accelerators
Photon	0	0	Photoelectric, Compton, pair production	Ionization, excitation (especially in polymers)	γ irradiation, insulation aging

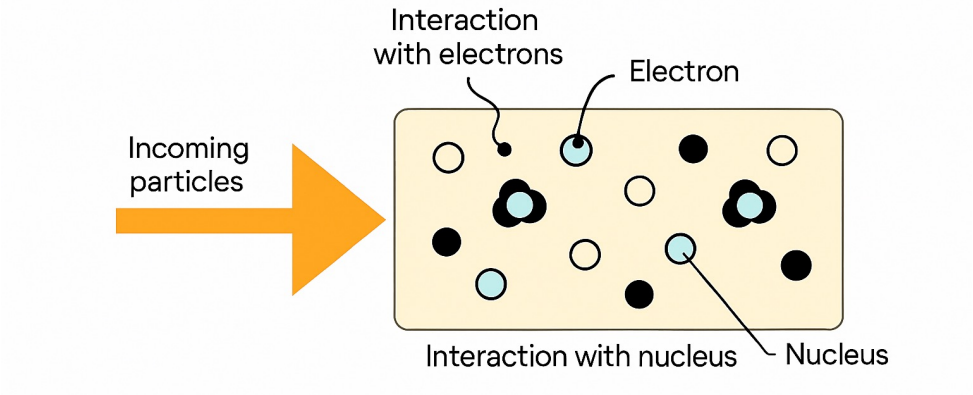
- **Neutrons:**
  - penetrate deeply, efficient at generating bulk displacement damage.
- **Ions:**
  - deposit energy locally ⇒ useful for simulating neutron damage.
- **Electrons:**
  - mostly cause ionization, rarely displacements unless highly energetic.
- **Photons:**
  - induce electronic excitations, chemical changes in sensitive materials.



General interactions between particles and matter

How is energy deposited in solids?

An incoming energetic particle enters the material and begins to lose energy.



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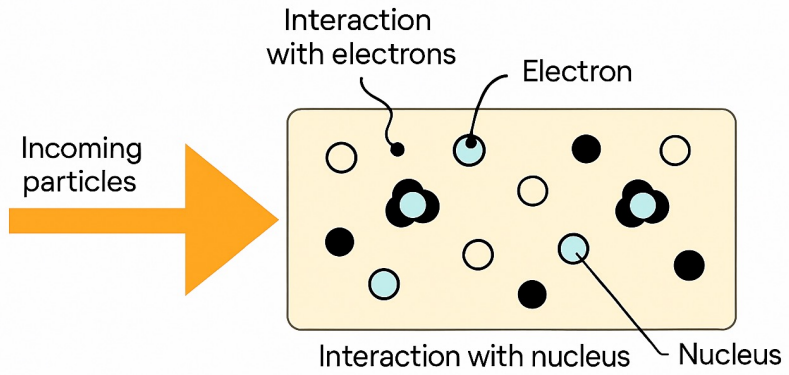

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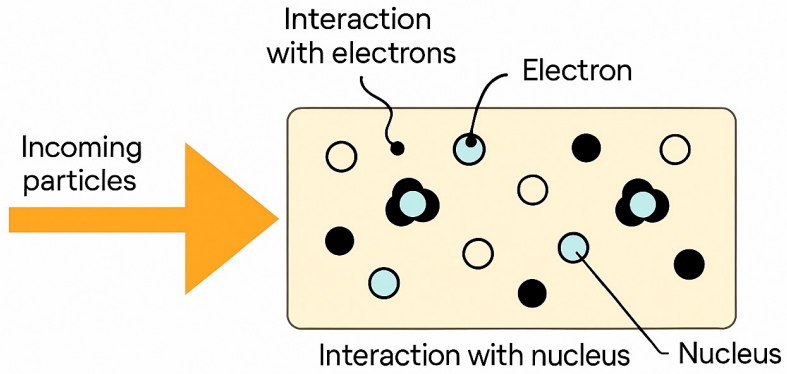

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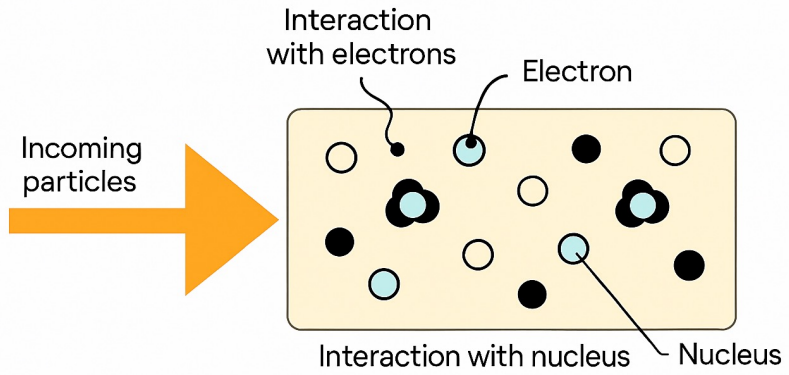
  - Can knock atoms out of place ⇒ defects, PKAs, cascades
  - Only nuclear interactions lead to permanent lattice damage

  ⇒ requires energy transferred > displacement threshold (E_d)



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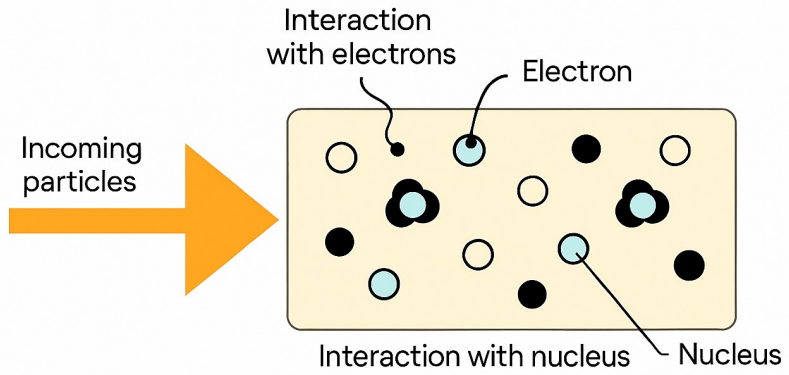
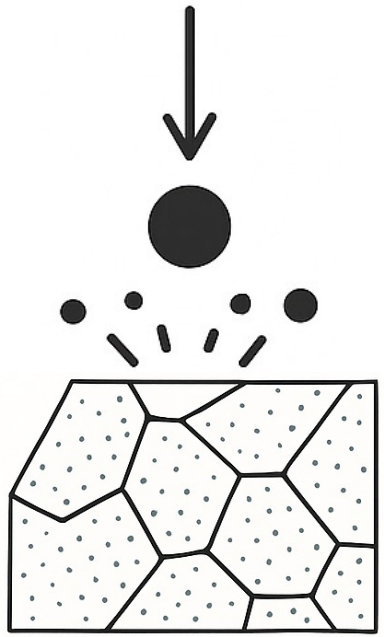
- The partition of energy between S_e and S_n depends on:
  - The mass and energy of the particle
  - The atomic structure of the target material



The main mechanisms of of particle-matter interaction

- **Elastic collision**
  - Atom ejection
  - Reflection
  - Desorption
  - Backscattered ions



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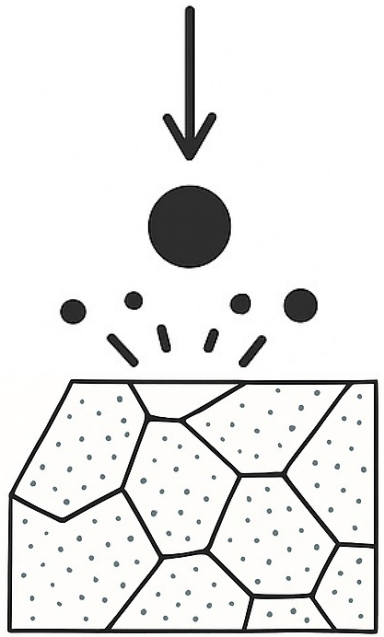

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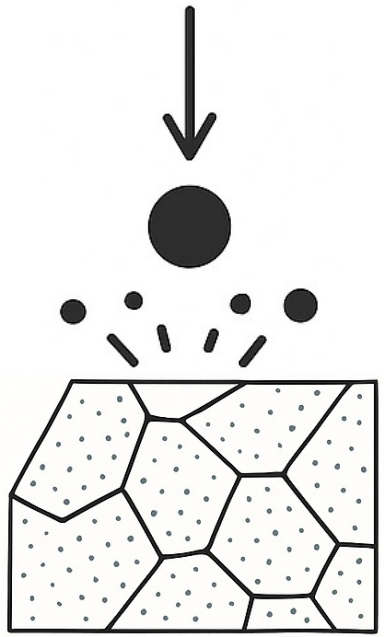

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- **In the target**
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  - Ionization
  - Atomic displacements
  - Implanted ions

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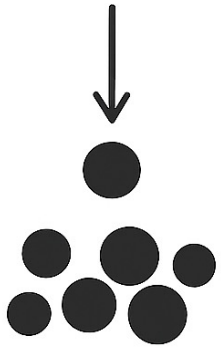

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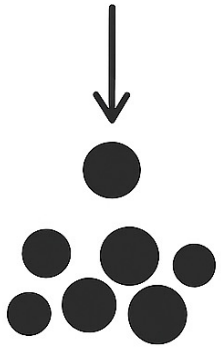

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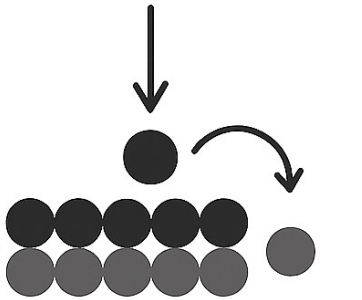

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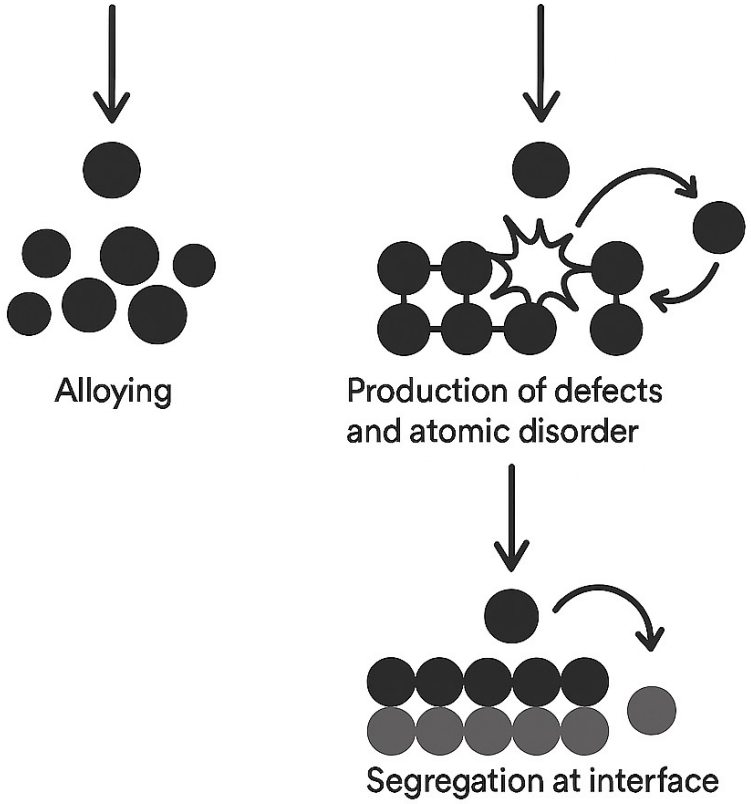

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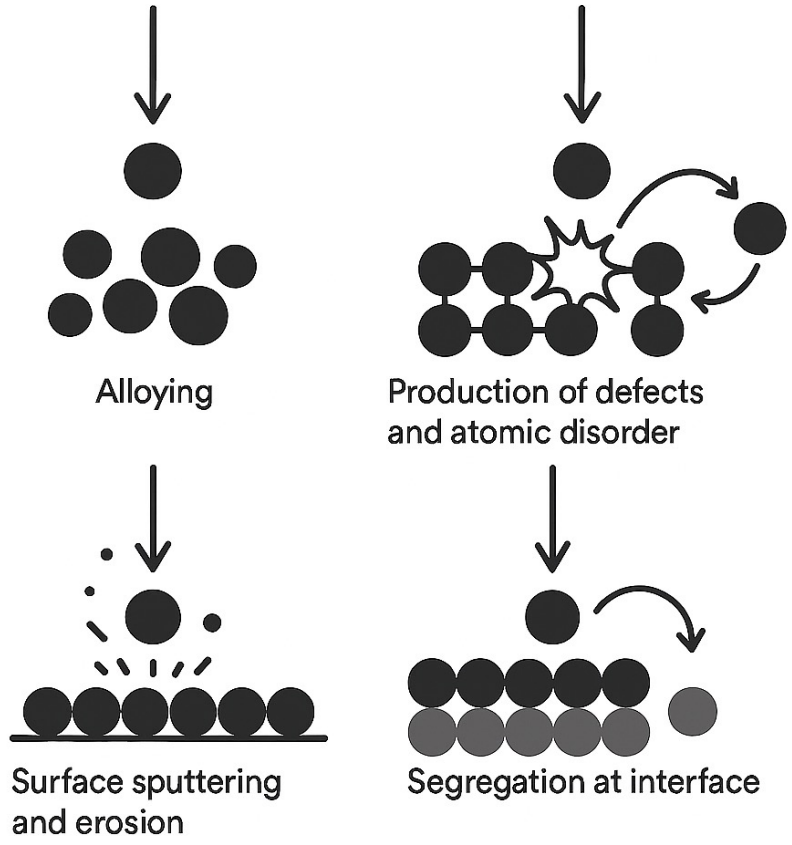
- **Surface sputtering and erosion: ($\sim 1 \rightarrow 100$ keV)**
  - Ejection of atoms from a surface when bombarded by high-energy particles, leading to material loss and surface modification.



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- **Assumptions for elastic collision calculations**
  - Binary collisions only (2 atoms involved)
  - Classical mechanics is valid
  - Electron excitation does not affect elastic collision
  - Target atom is initially at rest
  - Target atoms are randomly distributed
  - Elastic collision: No change in internal states of the particles.

Elastic collisions: assumptions and framework

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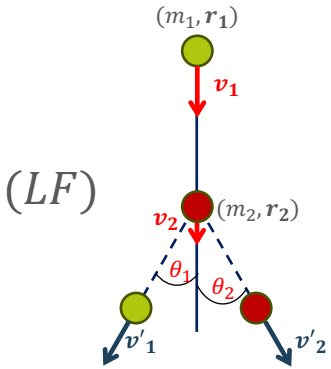
- Particles with masses m_1 and m_2 are located at M_1 and M_2 in the laboratory frame at the positions $\boldsymbol{r_1}$ et $\boldsymbol{r_2}$ respectively.



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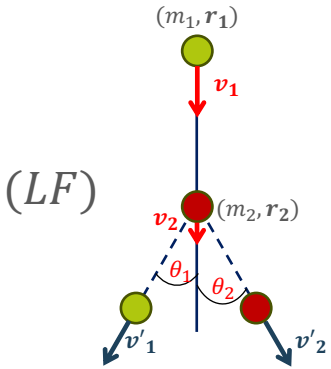

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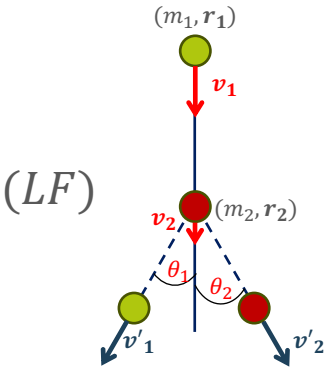
$$\mathcal{L} = E_k - E_p = \frac{1}{2}m_1\dot{\boldsymbol{r}}_{\boldsymbol{1}}{}^2 + \frac{1}{2}m_2\dot{\boldsymbol{r}}_{\boldsymbol{2}}{}^2 - U(r)$$



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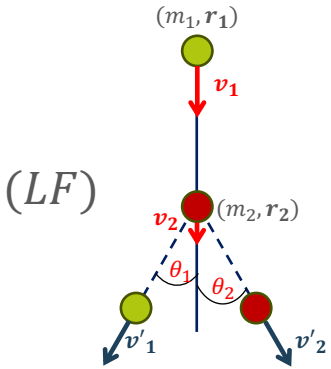

- In the center-of-mass frame (CMF):

$$(m_1 + m_2)\boldsymbol{OG} = m_1\boldsymbol{OM_1} + m_2\boldsymbol{OM_2}$$
$$m_1\boldsymbol{GM_1} + m_2\boldsymbol{GM_2} = \boldsymbol{0}$$

  - We set:

$$\boldsymbol{GM_1} = \boldsymbol{r_{G1}} = \frac{m_2}{m_1 + m_2}\boldsymbol{r}; \boldsymbol{GM_2} = \boldsymbol{r_{G2}} = \frac{m_1}{m_1 + m_2}\boldsymbol{r}$$
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$$\Rightarrow \mathcal{L} = \frac{1}{2}m\dot{\boldsymbol{r}}^2 + \frac{1}{2}m\dot{\boldsymbol{r}}^2 - U(r)$$

  - Where:

$$\frac{1}{m} = \frac{1}{m_1} + \frac{1}{m_2}$$

Elastic collisions: assumptions and framework

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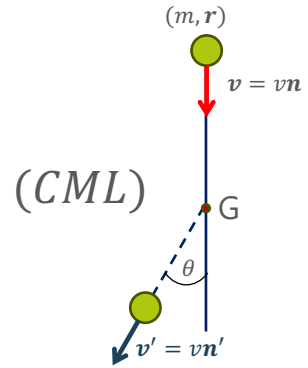

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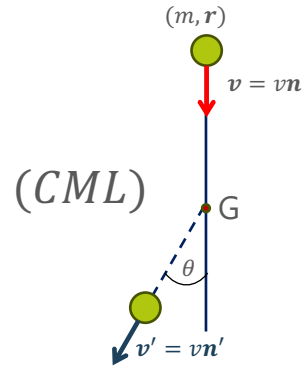

❖ The particle velocities in CMF after the collision:

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Elastic collisions: assumptions and framework

- To return to velocities and momenta in the laboratory frame, the velocity $\boldsymbol{V_G}$ of the center of mass must be added:

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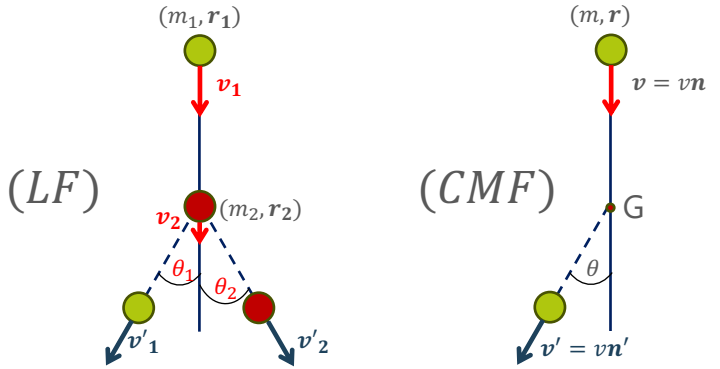

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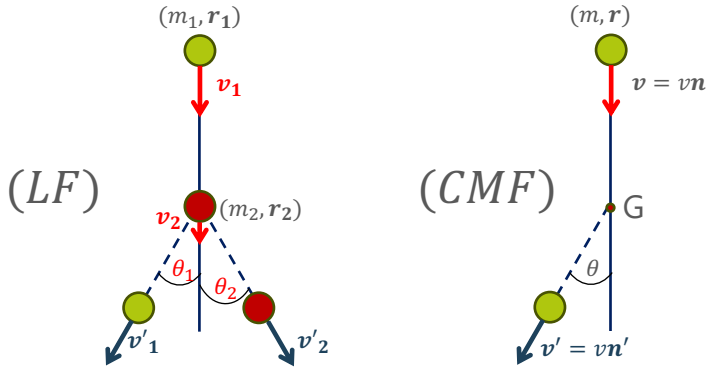

↳ The problem of elastic collision between two particles can be reduced, in the center-of-mass frame (CMF), to the study of the scattering of a fictitious particle (characterized by m, $\boldsymbol{r}$, and $\boldsymbol{v} = \dot{\boldsymbol{r}}$) in a potential field $U(r)$.

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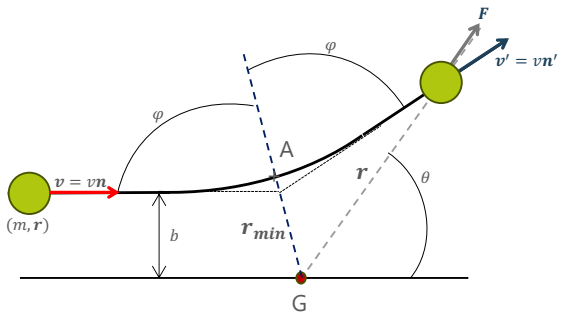

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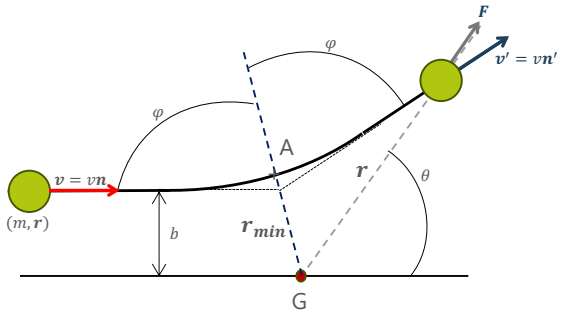

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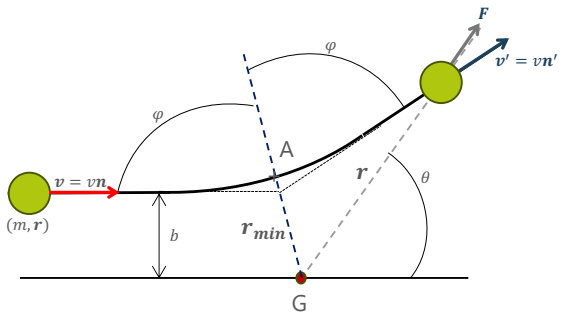

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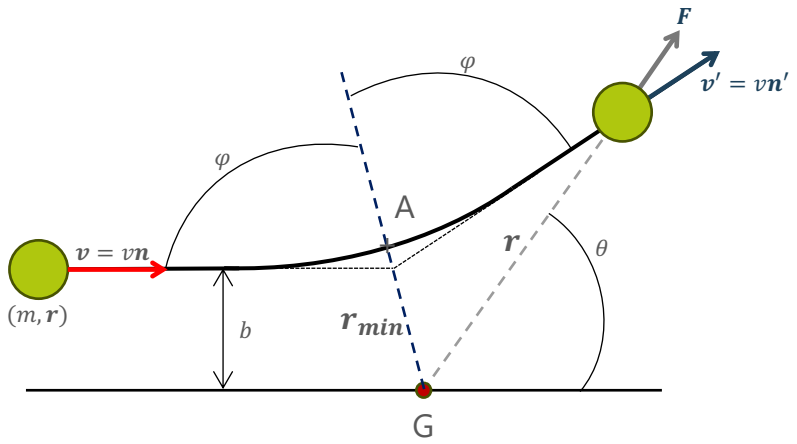

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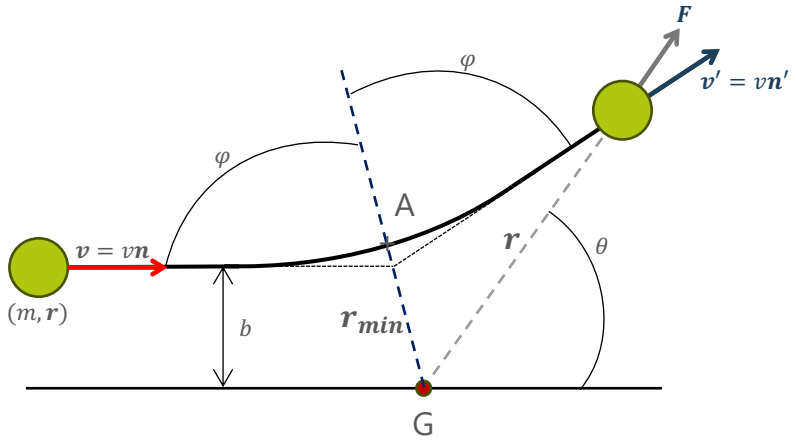

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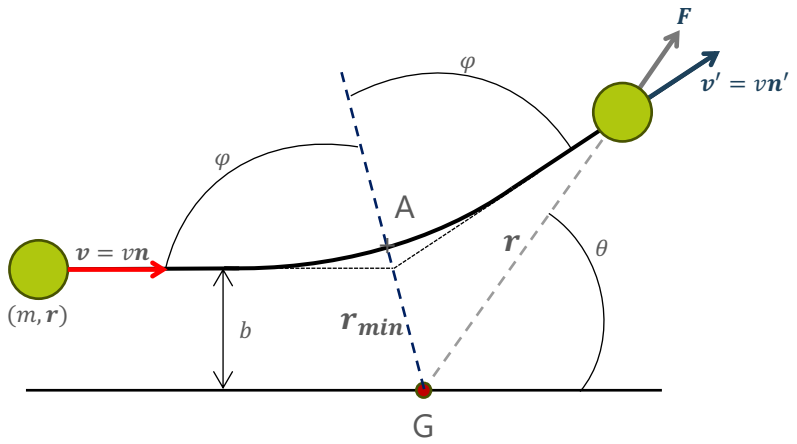

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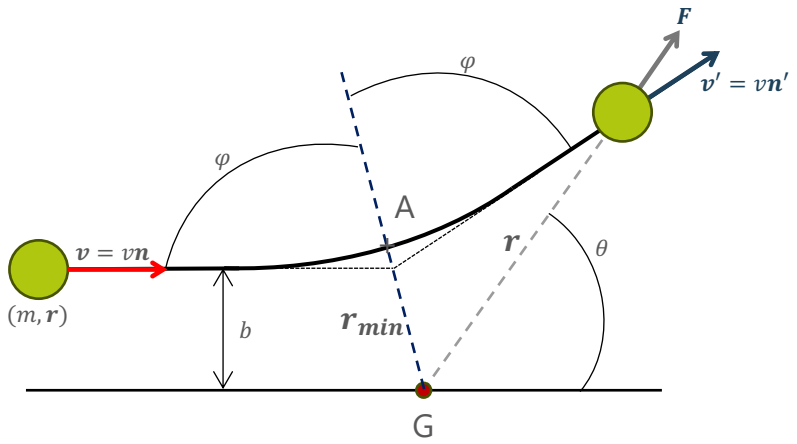
- Instead of using the quantities E_r and L, it is preferable to use the initial velocity far from the scattering center, where $U(r) = 0$, and then $L = mbv$

$$\theta = \pi - 2b\int_{r_{min}}^{\infty} \frac{\frac{1}{r^2}\mathrm{d}r}{\sqrt{1 - \frac{b^2}{r^2} - \frac{2U(r)}{mv^2}}}$$



Cross section

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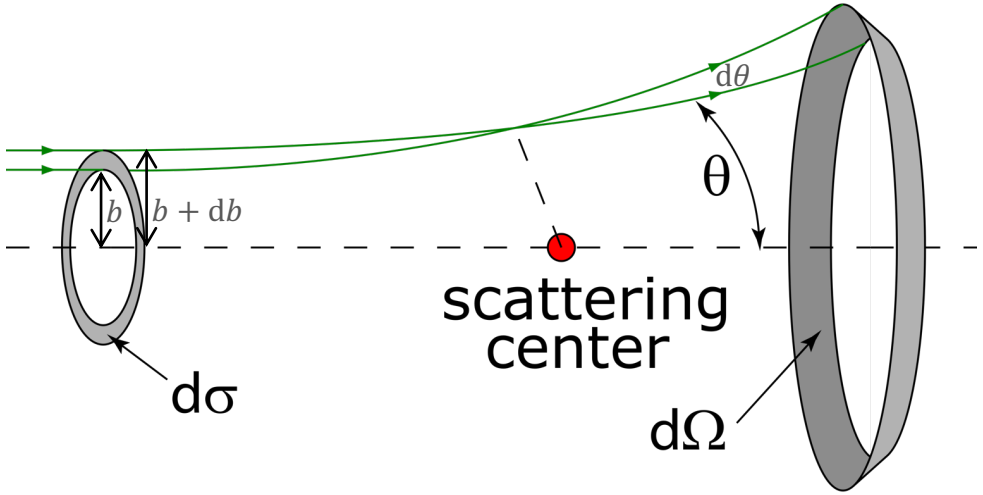

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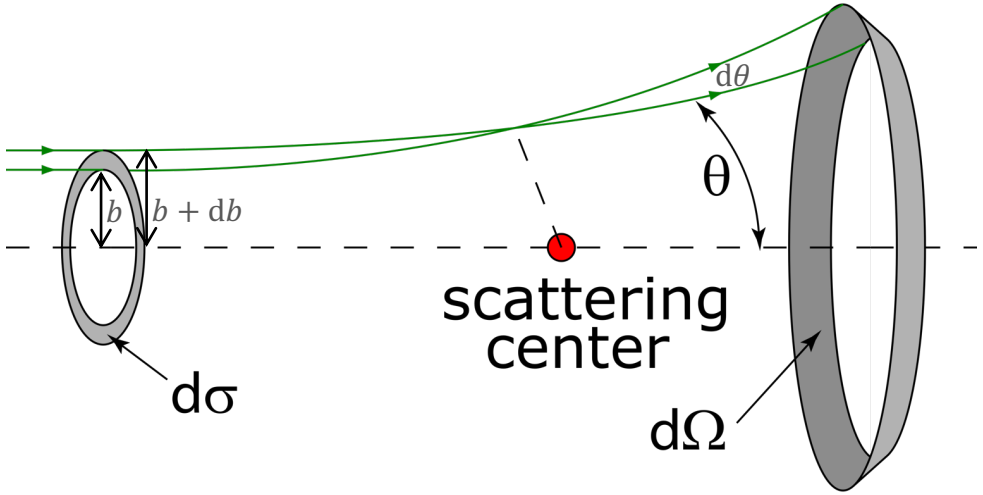
$$dN = 2\pi b n \mathrm{d}b$$



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- Let $\mathrm{d}N$ be the number of particles scattered per unit time into the angular range between θ and $\theta + \mathrm{d}\theta$:

$$dN = 2\pi b n \mathrm{d}b$$

- The scattering process is characterized by the ratio $\frac{\mathrm{d}N}{n}$, which has the dimension of an area:

$$\mathrm{d}\sigma = \frac{\mathrm{d}N}{n}$$

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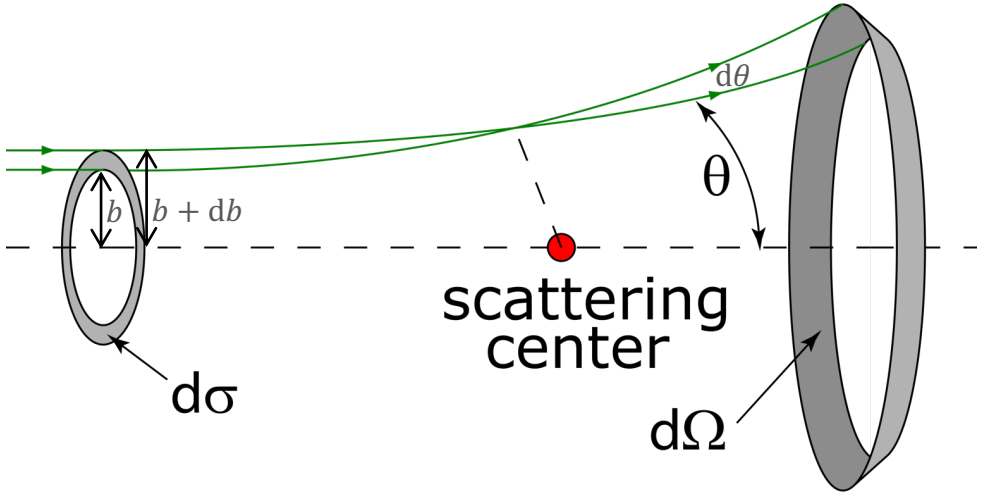

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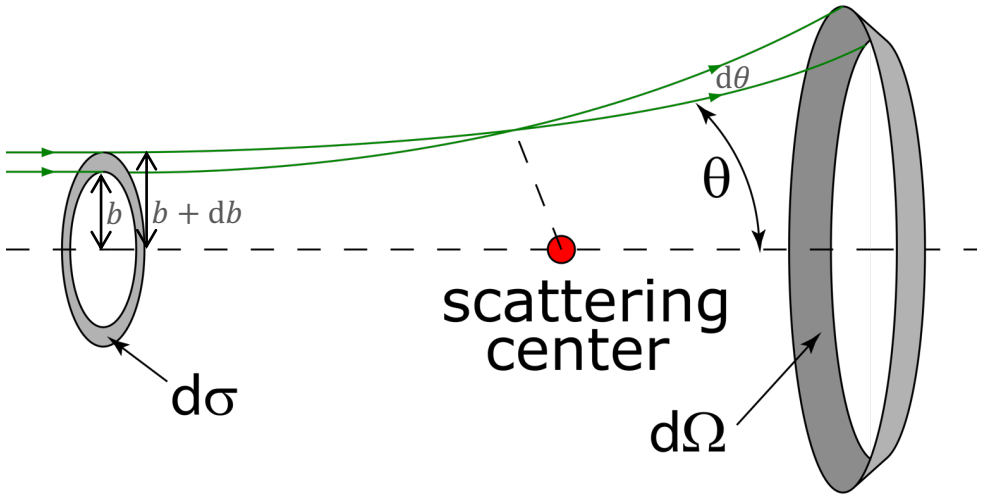
- There is a one-to-one correspondence between θ and b since only the particles with an impact parameter between b and $b + \mathrm{d}b$ are scattered into the angular range between θ and $\theta + \mathrm{d}\theta$.



The Rutherford cross section

- For the Colomb potential:

$$U(r) = \frac{q_1 q_2}{4\pi\varepsilon_0}\frac{1}{r} = \alpha\frac{1}{r}$$

$$\theta = \pi - 2b\int_{r_{min}}^{\infty} \frac{\frac{1}{r^2}\mathrm{d}r}{\sqrt{1 - \frac{b^2}{r^2} - \frac{2U(r)}{mv^2}}}$$

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↳ The Rutherford cross section provides a fundamental framework to quantify the probability of elastic scattering events between charged particles and target atoms. Understanding this cross section is essential for predicting the number and distribution of atomic displacements, which in turn control the nature and extent of irradiation-induced defects in materials.

The stopping powers and the total range

- The nuclear stopping power (S_n):
  - If E is the energy of the ions in the plane parallel to the surface at position x, they will lose an average energy $\langle \Delta E \rangle$ due to elastic collisions after passing through a layer of thickness Δx:
    $$\langle E \rangle = E_0 - \langle \Delta E \rangle$$
  - The probability $\mathrm{d}P$ that an ion undergoes an elastic nuclear collision within a layer of thickness Δx and a density of N, corresponding to a differential cross section $\mathrm{d}\sigma$, is:
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  - The average energy lost within Δx will be: (T is the energy transferred to m_2 in the LF)
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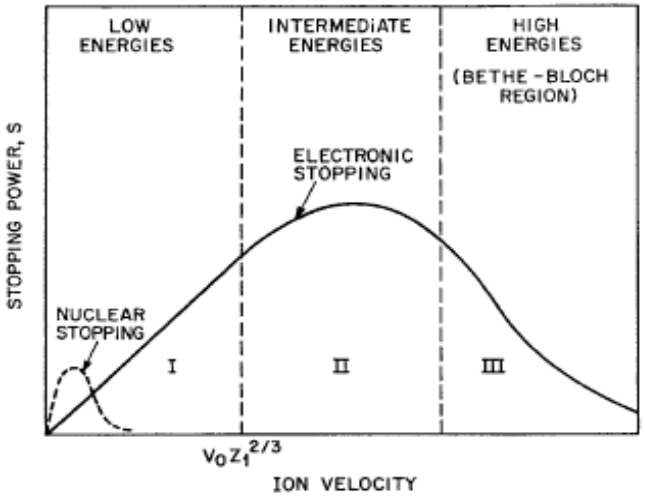
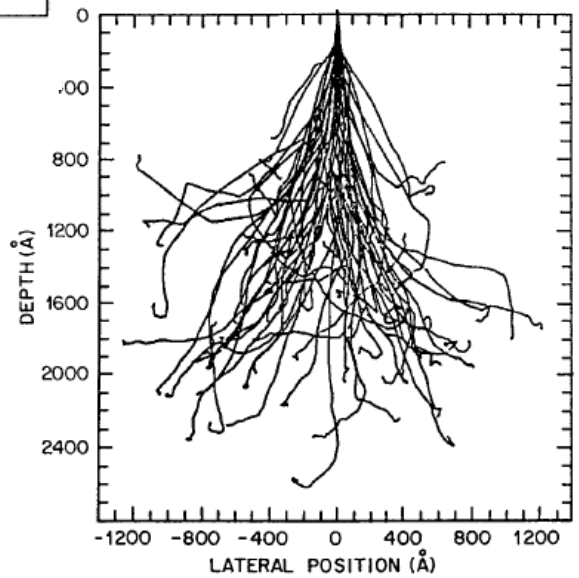


Trajectories of 128 B^+ ions at 50 keV in Si (Monte Carlo simulation)



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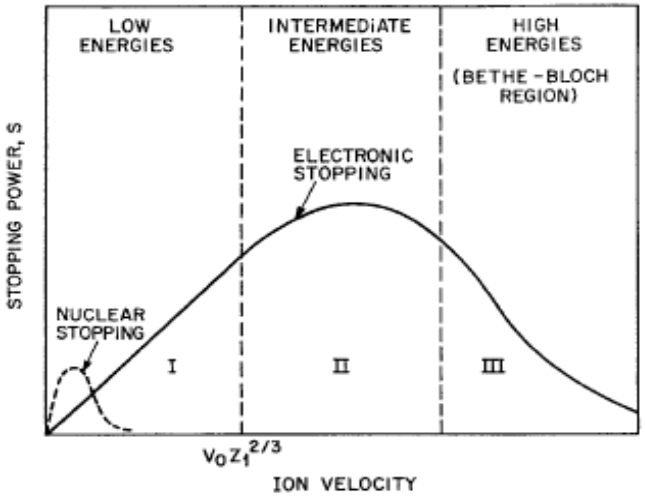

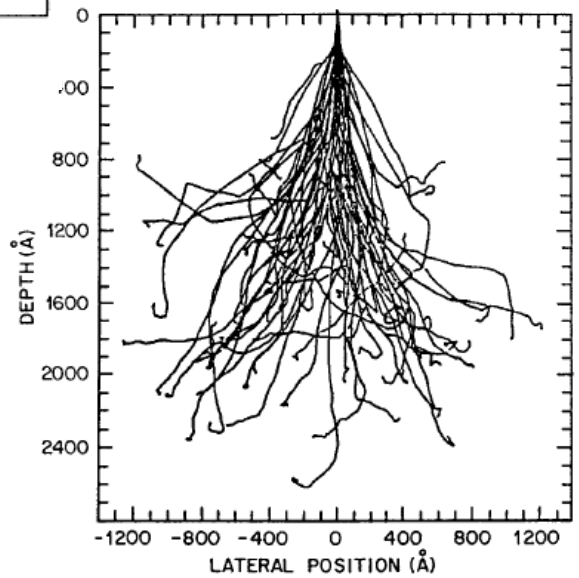

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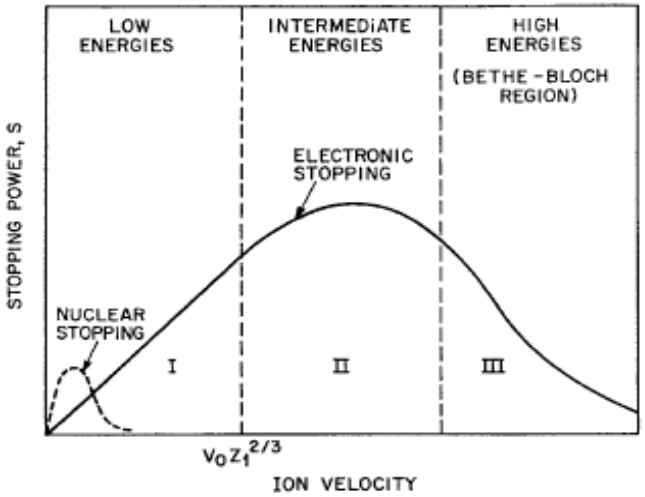
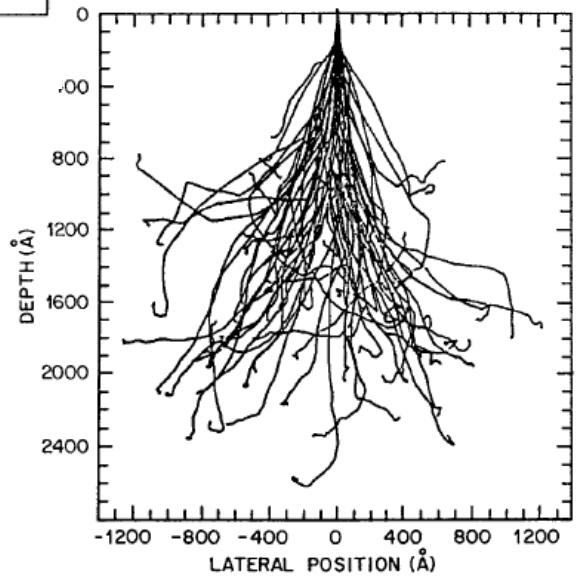
- Total range of the ions in the solid:
  $$R_T = \int_0^E \frac{\mathrm{d}E}{N(S_n + S_e)}$$

Since R_T is a broken (zigzag) path, it will be much greater than the projected range R_P along the direction perpendicular to the surface.





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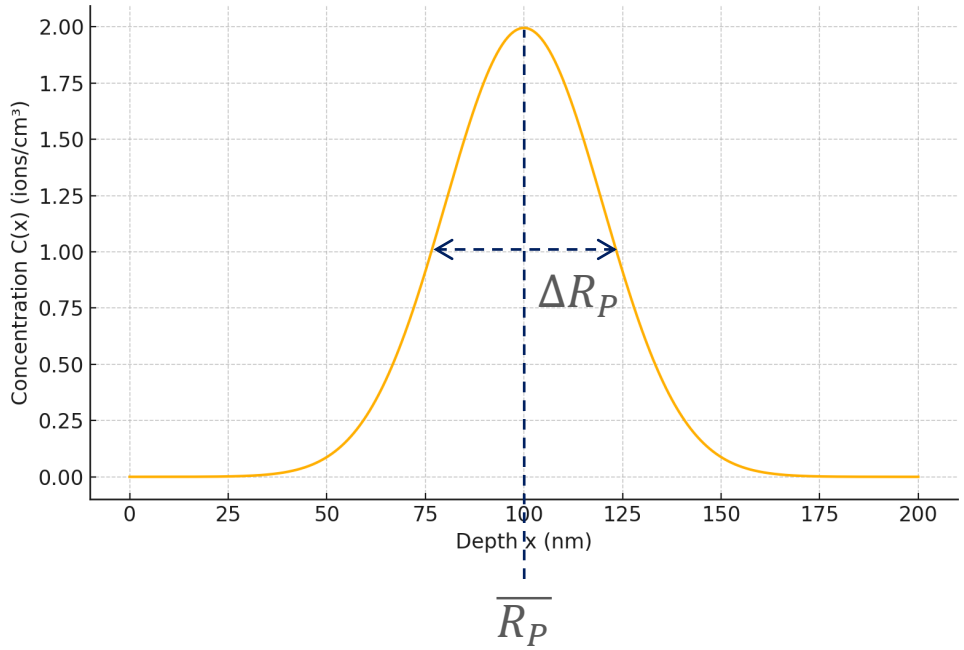
Distribution of implanted ions

- The concentration profile $C(x)$ for a fluence ϕ (ions/cm^2) of ions implanted into a target with atomic density N (atoms/cm^3) is reasonably well approximated at low fluence levels ($< 10^{16}$ cm^{-2}) by a Gaussian distribution:

$$C(x) = \frac{\phi}{\sqrt{2\pi N \Delta(R_P)}} \exp\left[-\frac{(x-\overline{R_P})^2}{2(\Delta R_P)^2}\right]$$



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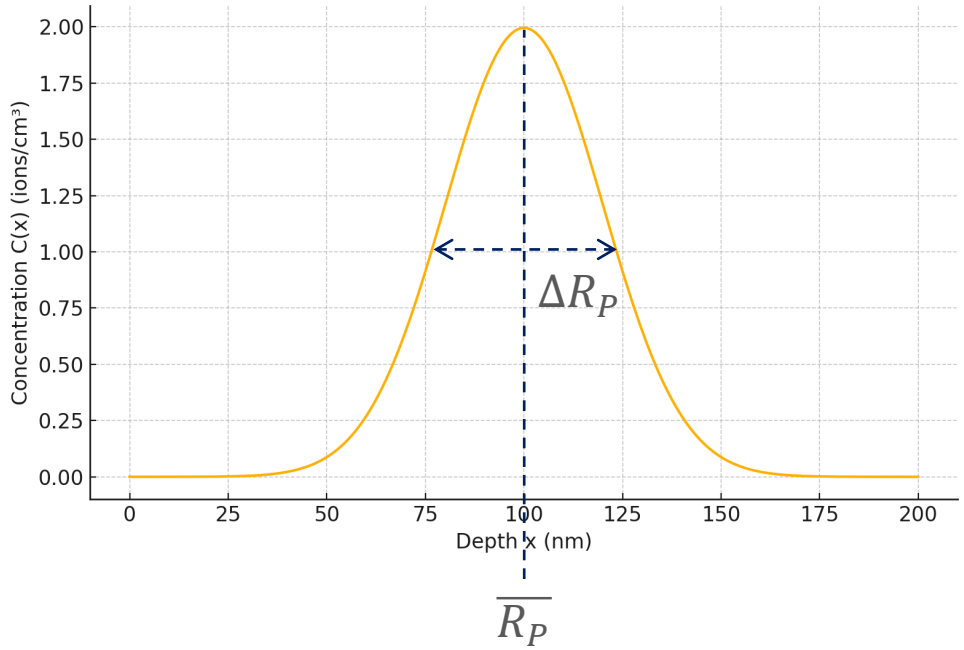
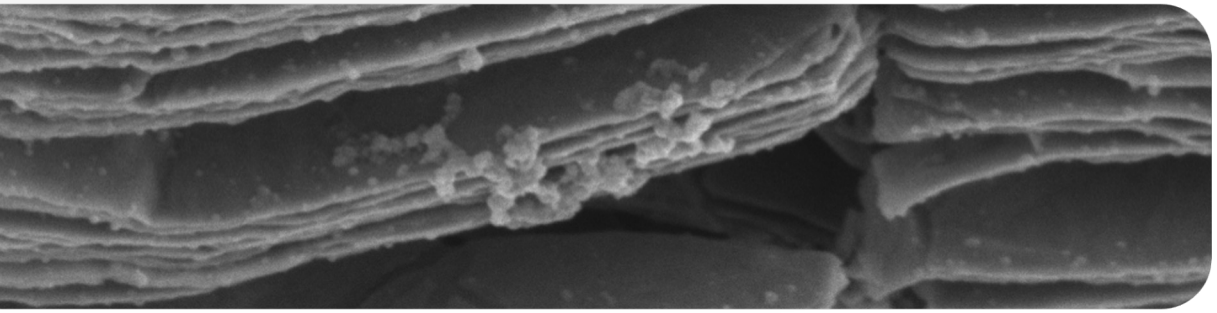
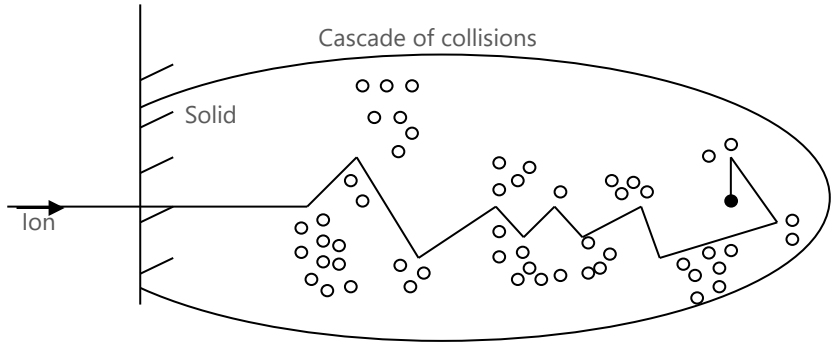




Damage induced by irradiation

Characteristics of the displacement cascade

- A displacement cascade is a sequence of atomic displacements initiated when a high-energy incident particle (such as an ion or neutron) transfers sufficient kinetic energy to a target atom in a solid, displacing it from its lattice site. This primary knock-on atom (PKA) can in turn collide with other atoms, creating a chain reaction of further displacements. The result is a localized region of atomic disorder, typically consisting of interstitials, vacancies, and defect clusters.



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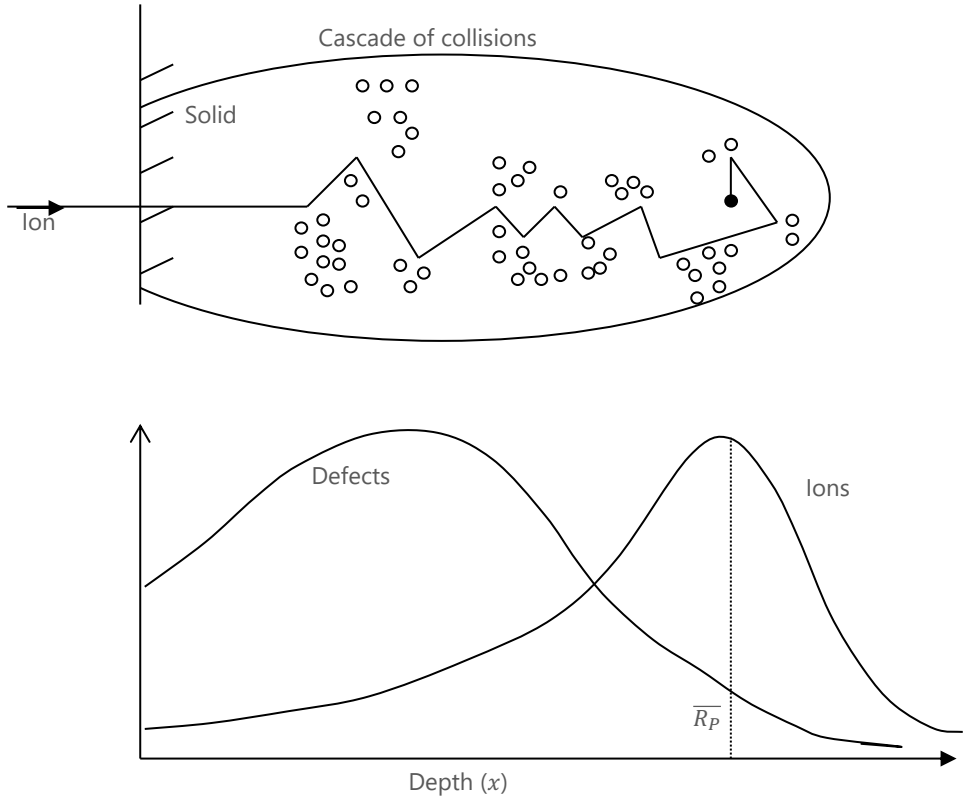

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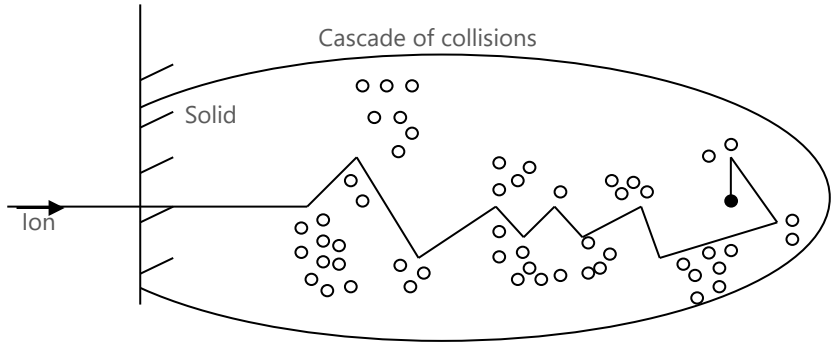

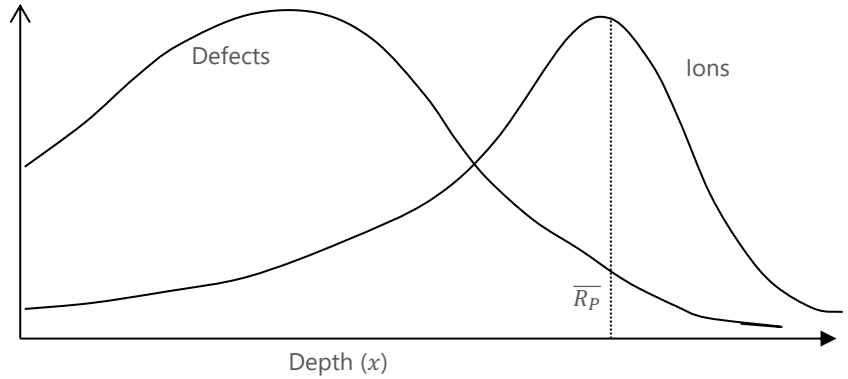

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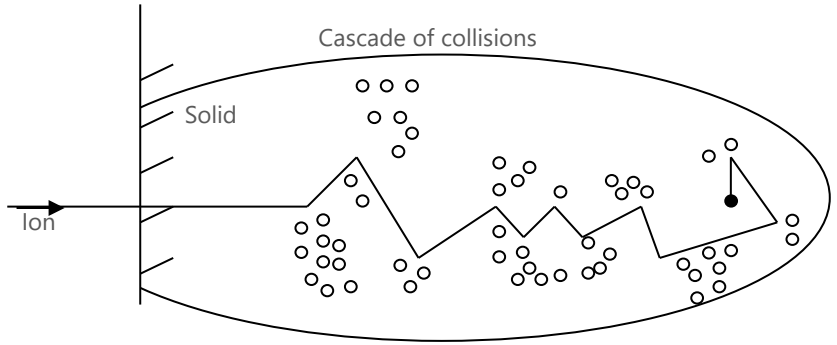

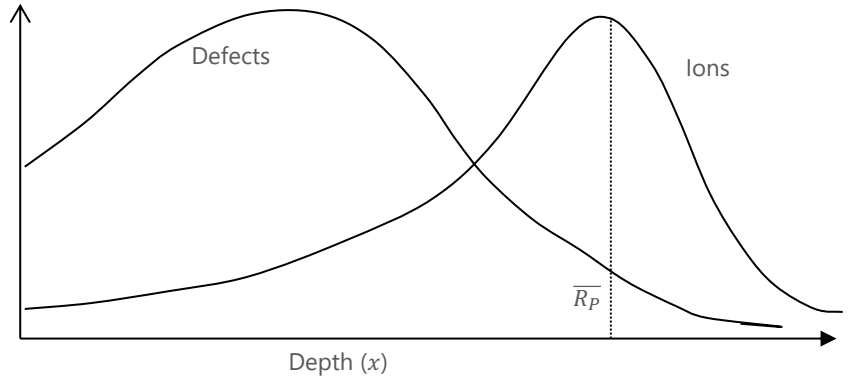

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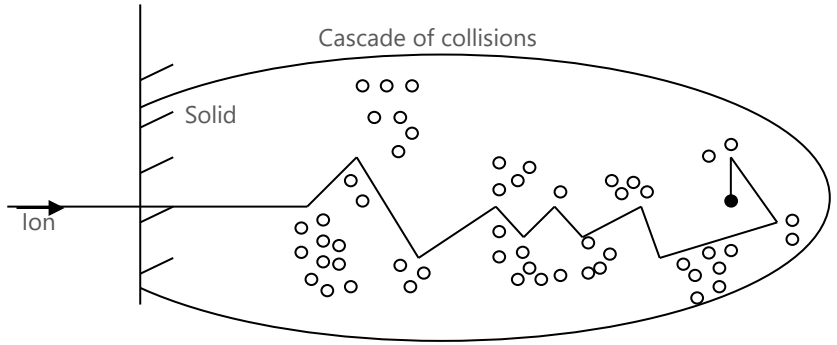
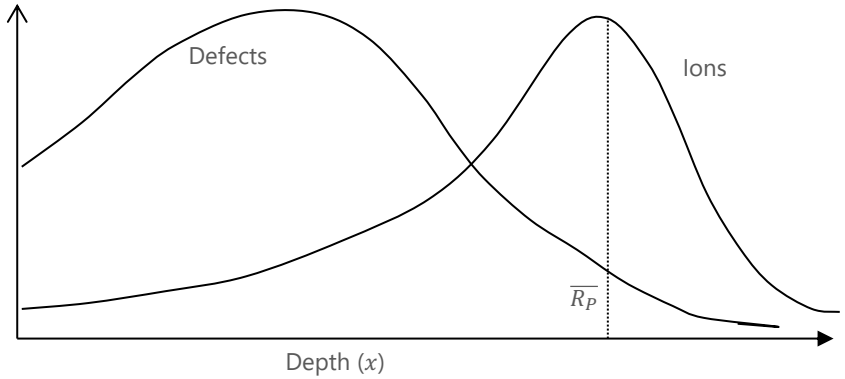
    $$dpa = \frac{0.8}{2E_d} S_n \frac{\Phi}{N}$$

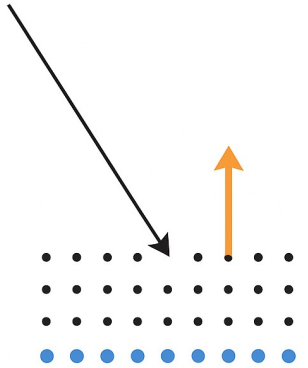
(E_d is the energy lost by each incident ion through elastic collisions)





Surface sputtering and erosion

- There are three sputtering mechanisms:
  - Single-impact regime: surface target atoms receive enough energy from individual ion impacts to be ejected.



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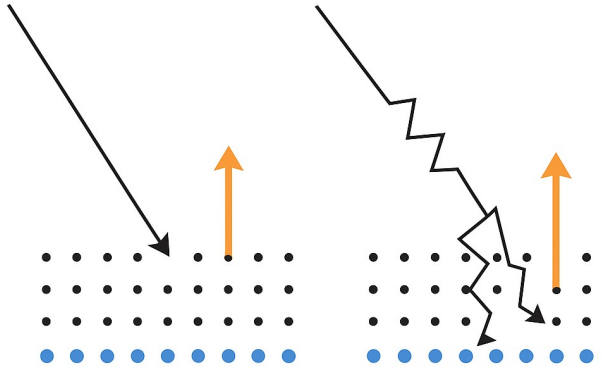

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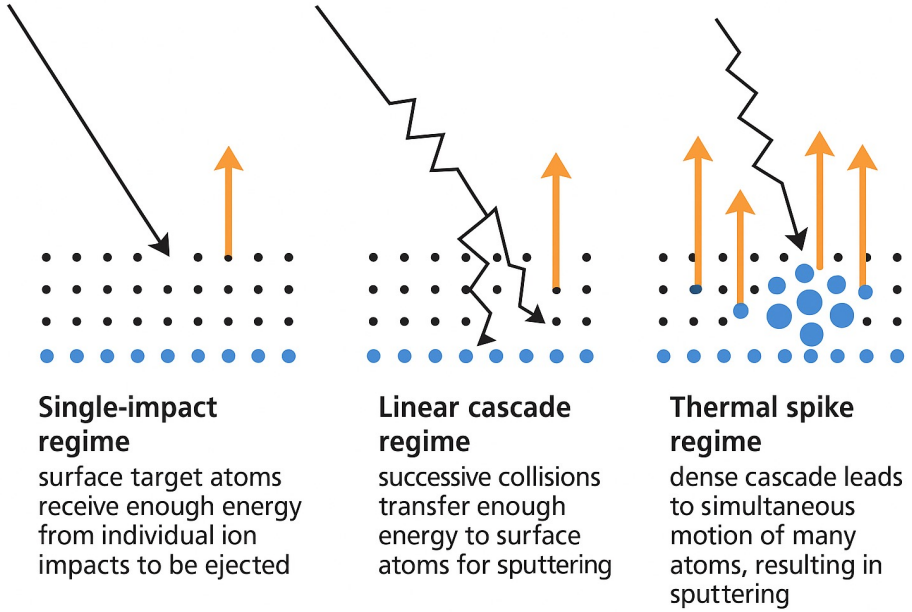

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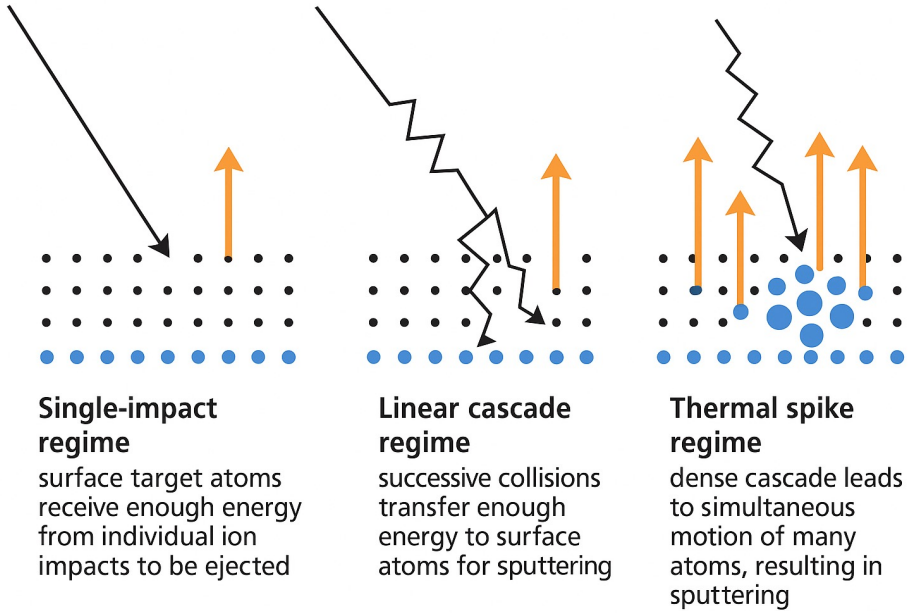
- Sputtering yield:

$$Y = \frac{Number\ of\ sputtered\ atoms}{Number\ of\ incident\ ions}$$



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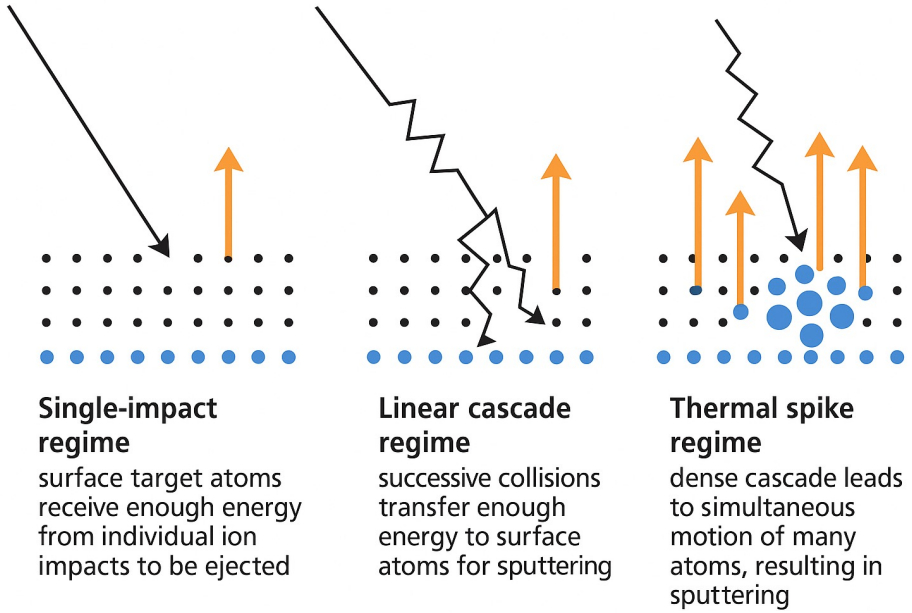
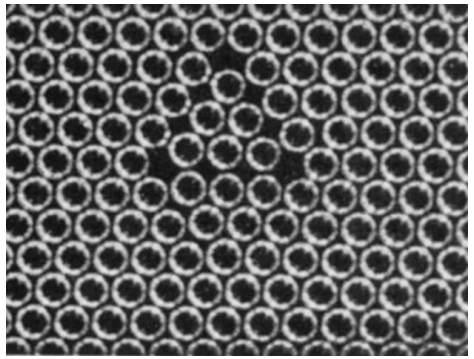
- Consequences of sputtering on implantation profiles
  - An initially Gaussian profile at low fluence broadens, and a plateau corresponding to a maximum concentration appears when the sputtered thickness equals $\overline{R_P}$; the maximum (plateau) concentration is approximately $C_m \sim \frac{1}{Y}$.



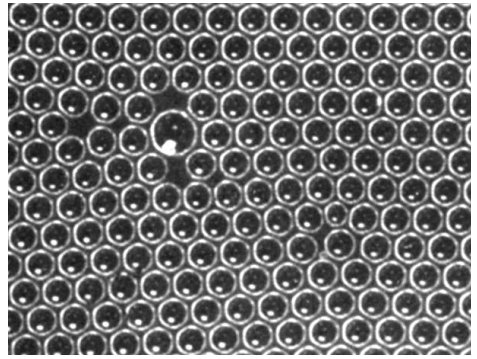
Production of point defects

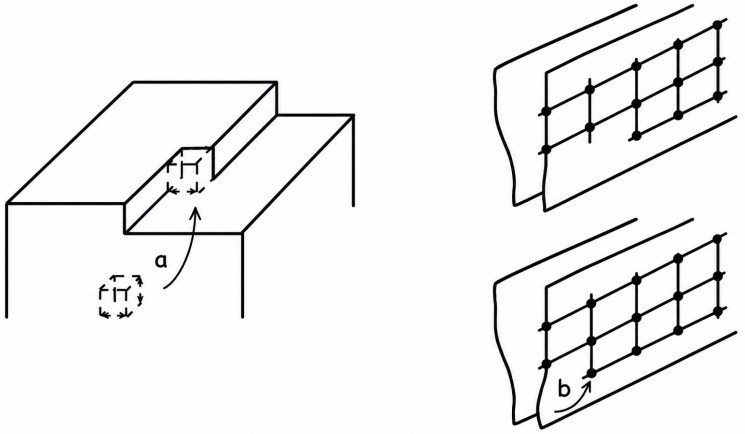
- **Vacancy**
  - Missing atom from its lattice site
  - Very frequent – one of the primary defects

Vacancy



Interstitial





Production of point defects

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  - Missing atom from its lattice site
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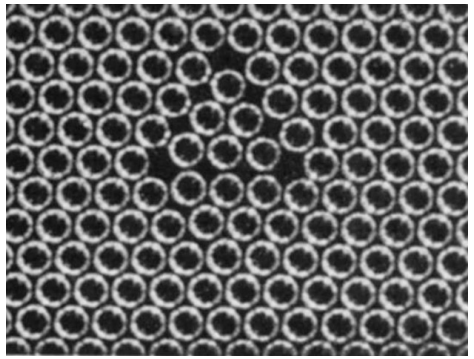

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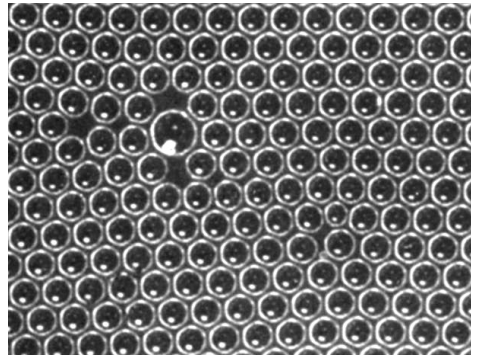

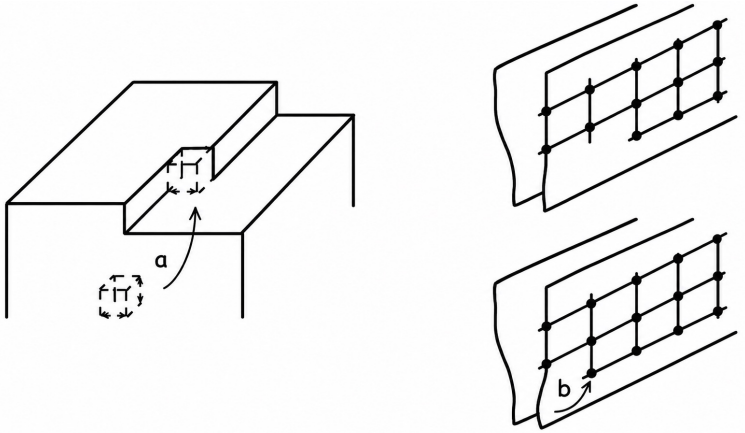

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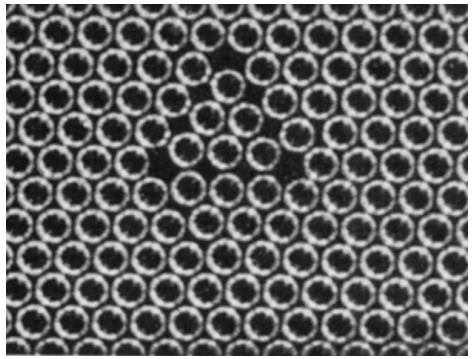

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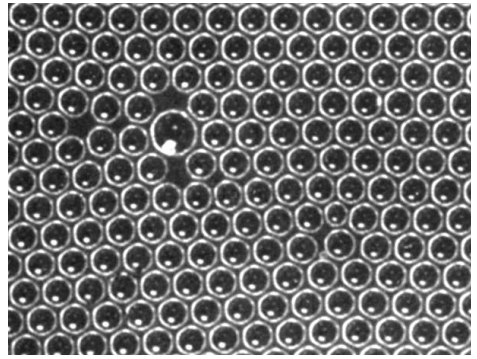

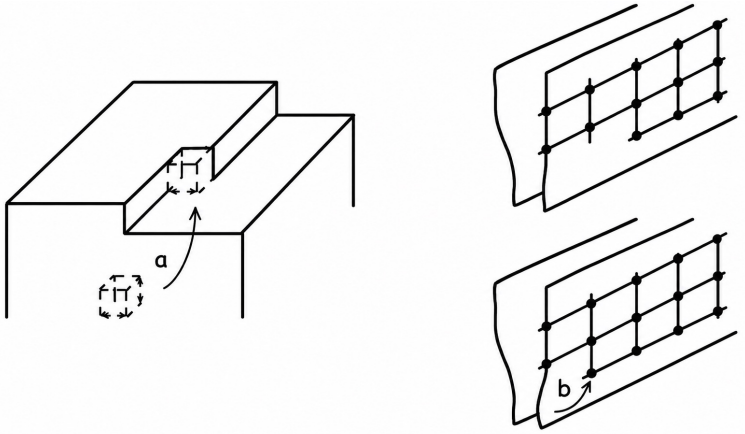

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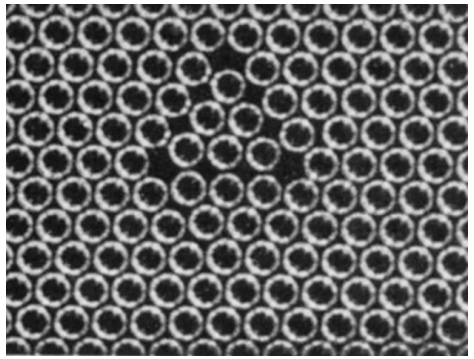

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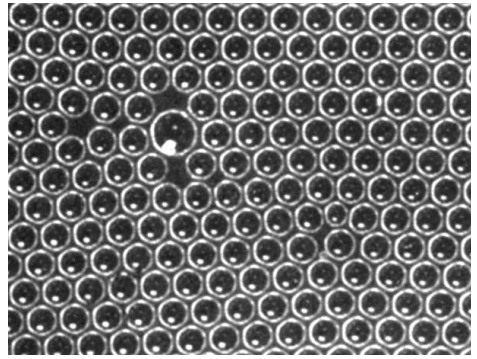

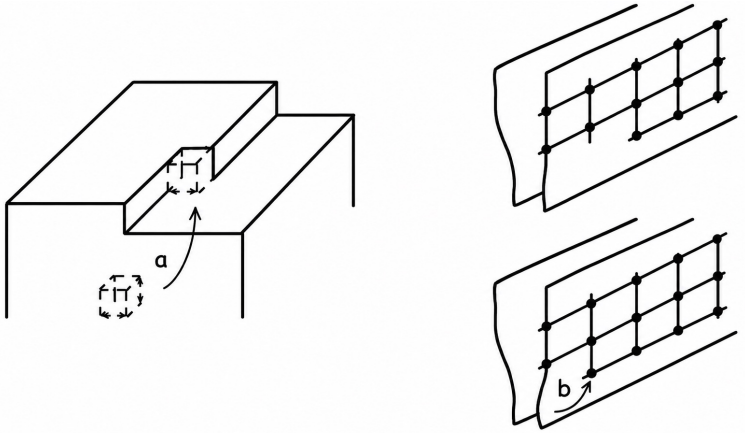

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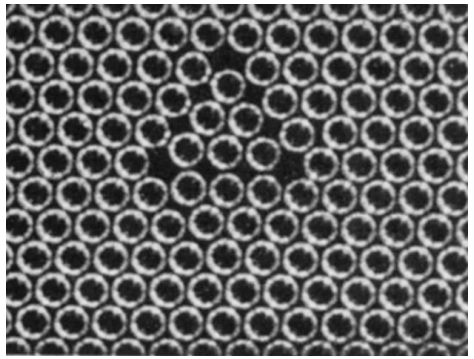

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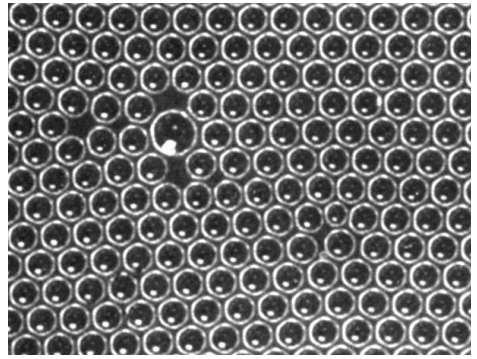

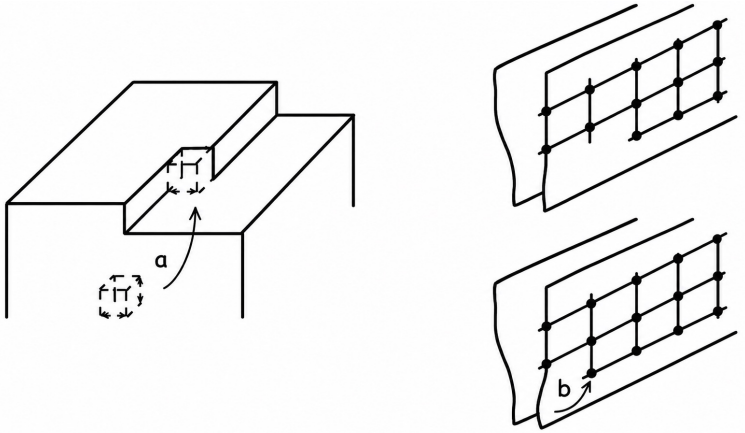

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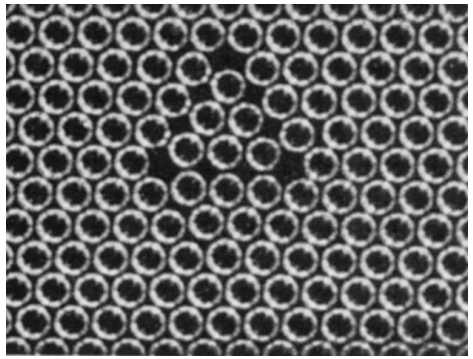

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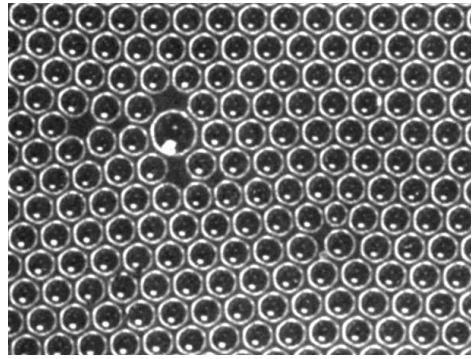

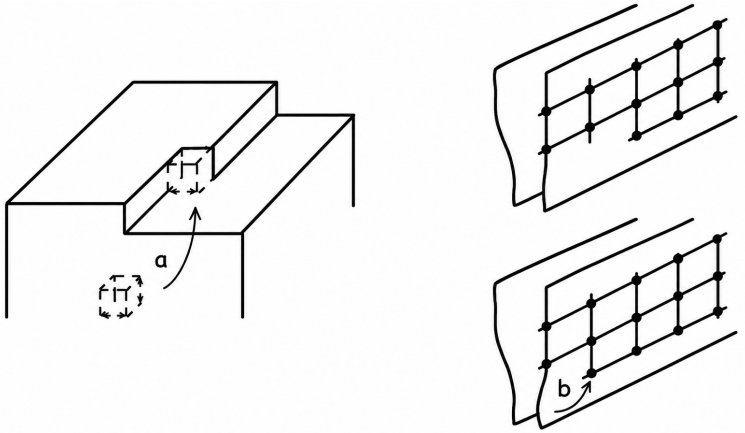

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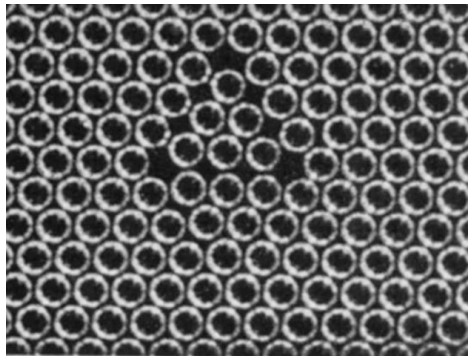
- **Defect clusters (e.g., vacancy clusters, interstitial loops)**
  - Aggregation of primary defects
  - Frequent at high dose or temperature

Vacancy



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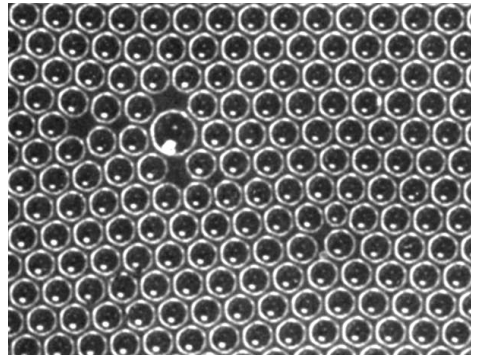

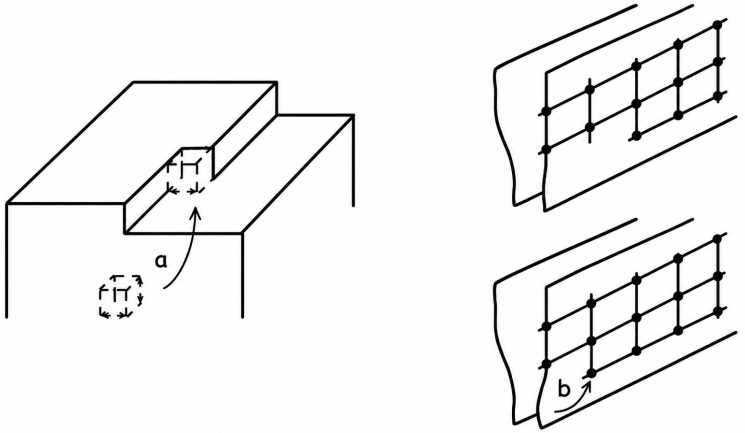

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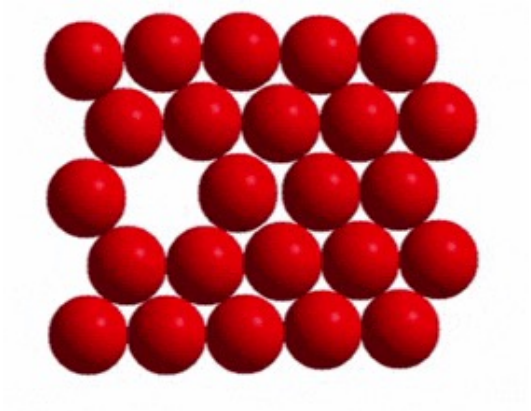

Always present at an equilibrium
(thermal agitation)

$$N_v = N \exp\left(-\frac{Q_f}{k_B T}\right)$$

Q_f: formation energy $\approx 1\ eV$
T: temperature
k_B: constant of Boltzmann
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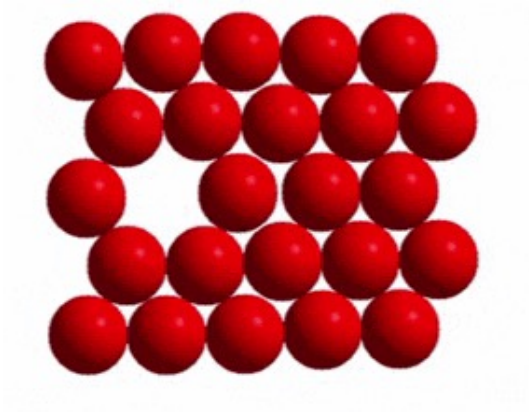
Production of point defects



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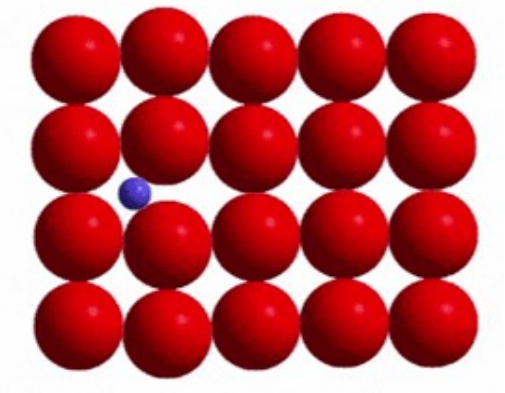

Varies with temperature
(thermal agitation)

$$N_i = N \exp\left(-\frac{Q_i}{k_B T}\right)$$

Q_i: formation energy
T: temperature
k_B: constant of Boltzmann
k_B = 1.381·10^{-23} J/K
N: number of atoms

Thanks for your listening!

If you need further information:

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Email: antoine.guitton@univ-lorraine.fr

Website: www.antoine-guitton.fr

LEM3 LABORATOIRE D'ÉTUDE DES MICROSTRUCTURES ET DE MÉCANIQUE DES MATÉRIAUX

UNIVERSITÉ DE LORRAINE

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