Unit 4: Defect Evolution & Transport

ME 5203 – Nuclear Materials

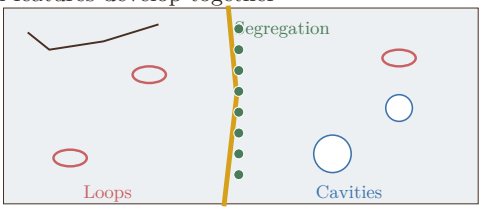
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After the displacement cascade

Several features develop together



- Some vacancies and interstitials survive cascade cooling.
- Mobile defects recombine, reach sinks or join clusters.
- Loops, cavities and local composition changes can develop.

This unit

How do the surviving defects change the material?

Unit 4: Learning Objectives

Motion and removal

- Interpret Fick's laws separately.
- Connect atomic jumps to diffusivity.
- Explain radiation-enhanced diffusion.
- Calculate sink removal rates and lifetimes.

Microstructure

- Explain defect binding and loop formation.
- Calculate swelling from cavity size and density.
- Explain the roles of temperature and helium.
- Describe segregation near grain boundaries.

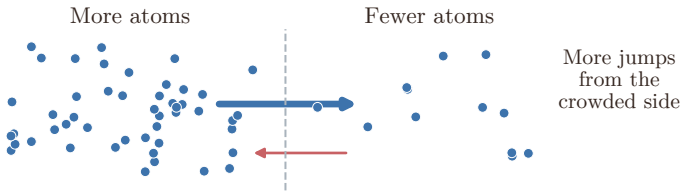
Defect processes act over different times

Process	What controls its time?	Useful description
Cascade cooling	Collision and energy-transfer processes	Atomistic molecular dynamics
Defect migration	Temperature and migration barriers	Atomic jumps, random walks
Capture or recombination	Mobility, defect spacing and sink structure	Kinetic Monte Carlo, rate equations
Cluster and cavity evolution	Defect supply, absorption and emission	Cluster dynamics, rate theory

Note

A migration time is not a universal number. A defect may be almost immobile at one temperature and mobile at another.

Random jumps can produce a net flux

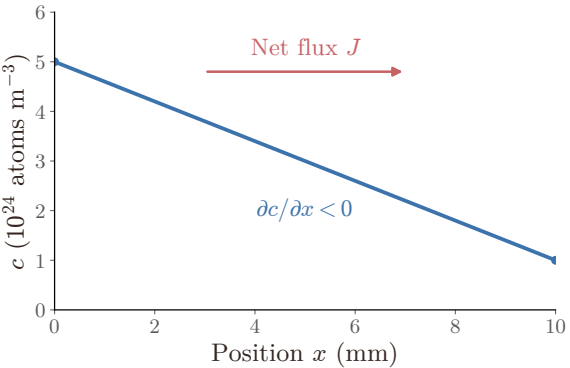


Atoms jump in both directions. More atoms on the left give more opportunities for left-to-right jumps.

Net transport

With concentration as the only driving force, the net flux is toward lower concentration.

Fick's first law gives the flux



Definition: Diffusion flux

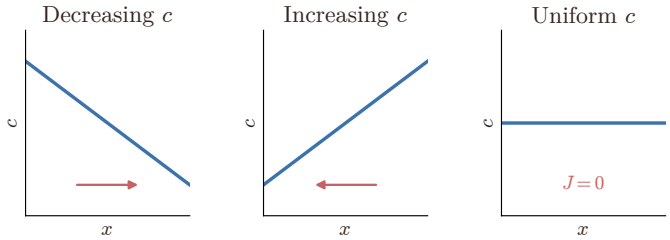
$$J = -D\frac{\partial c}{\partial x}$$

- J: atoms crossing unit area per second, atoms m^{-2} s^{-1}.
- D: diffusivity, m^2 s^{-1}.
- c: atoms per unit volume, atoms m^{-3}.

Note

The first law can apply during both steady and changing concentration profiles.

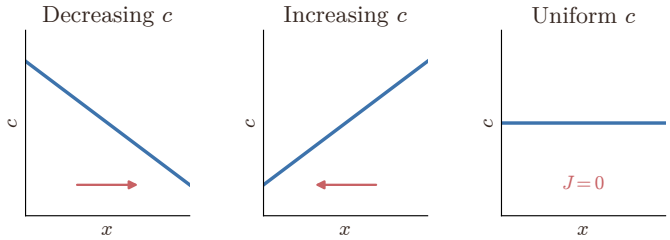
The minus sign gives the direction



Question

Which profile produces flux toward the left?

The minus sign gives the direction



Question

Which profile produces flux toward the left?

Answer

The middle profile. Concentration increases with x, so J is negative. A uniform profile gives zero net flux in this model.

Worked example: diffusion flux

Example: Given

$c_L = 5 \times 10^{24}$ and $c_R = 1 \times 10^{24}\,\text{atoms}\,\text{m}^{-3}$, separated by $L = 1\,\text{mm}$.
$D = 10^{-12}\,\text{m}^2\,\text{s}^{-1}$. Assume a linear profile, with x increasing to the right.

Question

What is the flux, and which way does it point?

Worked example: diffusion flux

Example: Given

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Question

What is the flux, and which way does it point?

$$\frac{\Delta c}{L} = \frac{1 \times 10^{24} - 5 \times 10^{24}}{10^{-3}} = -4 \times 10^{27}\,\text{atoms}\,\text{m}^{-4}$$

Worked example: diffusion flux

Example: Given

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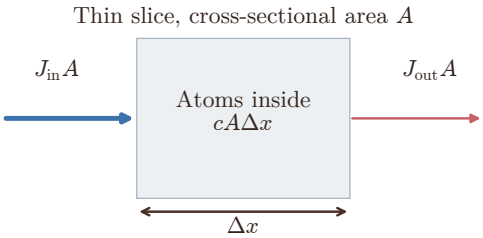
$$\frac{\Delta c}{L} = \frac{1 \times 10^{24} - 5 \times 10^{24}}{10^{-3}} = -4 \times 10^{27}\,\text{atoms}\,\text{m}^{-4}$$

Result

$$J = -(10^{-12})(-4 \times 10^{27}) = 4 \times 10^{15}\,\text{atoms}\,\text{m}^{-2}\,\text{s}^{-1}$$

Positive flux means net transport to the right.

Conservation connects flux to accumulation



No internal sources or sinks:
Change inside = flow in − flow out.

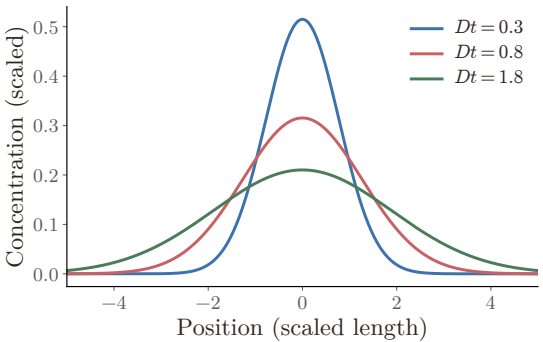
$$\frac{\partial c}{\partial t} A\Delta x = J_{\text{in}}A - J_{\text{out}}A$$

Divide by $A\Delta x$ and let the slice become thin:

$$\frac{\partial c}{\partial t} = -\frac{\partial J}{\partial x}$$

If more atoms enter than leave, c increases.

Fick's second law gives the change with time



Insert $J = -D\,\partial c/\partial x$ into conservation:

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x}\left(D\frac{\partial c}{\partial x}\right).$$

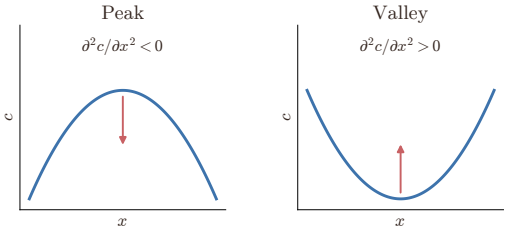
For constant D:

Definition: Second law

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2}$$

A narrow concentration peak spreads and becomes lower.

Curvature determines whether concentration rises or falls

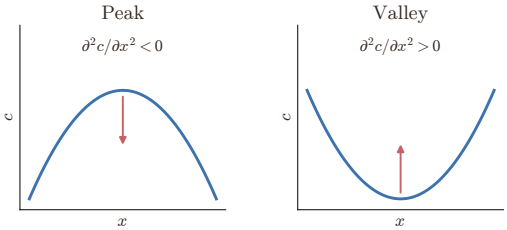


Constant $D > 0$; no sources or sinks.

Question

At the centre of a concentration peak, does concentration increase or decrease?

Curvature determines whether concentration rises or falls



Constant $D > 0$; no sources or sinks.

Question

At the centre of a concentration peak, does concentration increase or decrease?

Answer

It decreases. The curvature is negative, so $\partial c/\partial t < 0$. At a valley, the positive curvature makes concentration rise.

Fick's laws answer different questions

Definition: First law

$$J = -D\frac{\partial c}{\partial x}$$

How much material crosses a surface per second?

Definition: Second law

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2}$$

How does the concentration at a position change?

Question

With constant D and no sources or sinks, a linear profile carries a flux. Must its concentration change with time?

Fick's laws answer different questions

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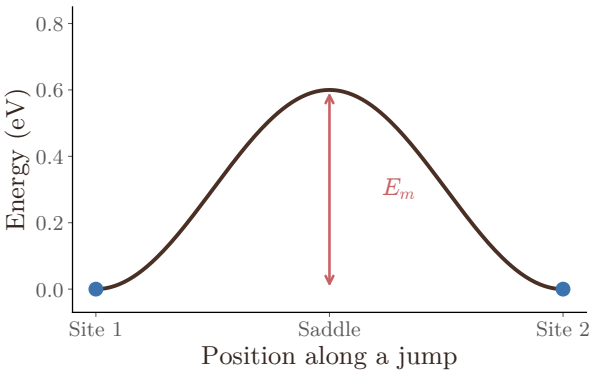
Question

With constant D and no sources or sinks, a linear profile carries a flux. Must its concentration change with time?

Answer

No. Equal flux enters and leaves each slice. The slope is nonzero, but the curvature is zero. Fixed boundary concentrations can maintain this state.

Migration requires crossing an energy barrier



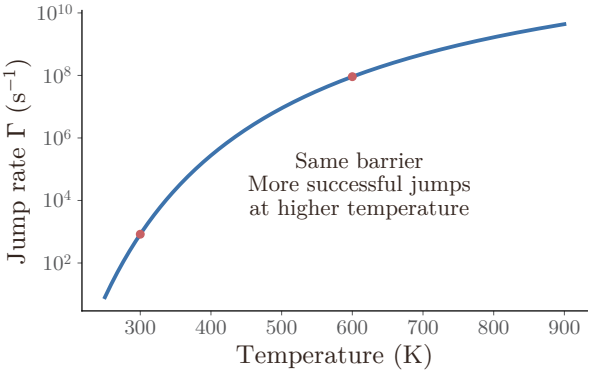
Illustrative barrier: $E_m = 0.60$ eV.

- A stable site is an energy minimum.
- The atom passes through a higher-energy arrangement during a jump.
- E_m is the migration barrier from the initial site to the saddle.

Different energies

Formation energy creates a defect. Migration energy moves an existing defect.

Temperature changes the jump rate



$$\Gamma = \Gamma_0 \exp\left(-\frac{E_m}{k_\mathrm{B} T}\right)$$

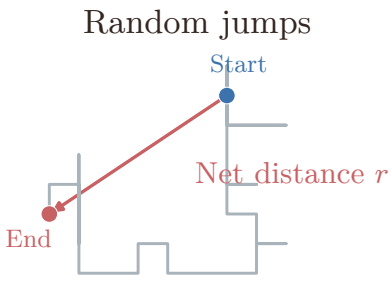
- Γ: total successful jumps per second.
- Γ_0: attempt-rate prefactor, s^{-1}, summed over directions.
- $k_\mathrm{B} = 8.617 \times 10^{-5}\,\mathrm{eV\,K^{-1}}$.
- T: temperature in kelvin.

Note

At higher temperature, more attempts cross the barrier.

Calculated example: $E_m = 0.60$ eV; $\Gamma_0 = 10^{13}$ s^{-1}.

A random walk connects jumps to diffusion



For uncorrelated jumps of length ℓ (path shown in 2D):

$$\langle r^2 \rangle = n\ell^2 = \Gamma t \ell^2.$$

For isotropic diffusion in three dimensions:

$$\langle r^2 \rangle = 6Dt.$$

$$D = \frac{\ell^2 \Gamma}{6}$$

Longer jumps and more jumps per second increase D.

The prefactor and activation energy

Definition: Arrhenius form

$$D = D_0 \exp\left(-\frac{Q}{k_\mathrm{B} T}\right)$$

D_0: prefactor

Units: $\mathrm{m}^2\ \mathrm{s}^{-1}$. It includes jump geometry and attempt frequency. In the simple random-walk model:

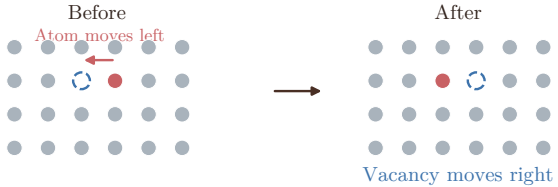
$$D_0 = \frac{\ell^2 \Gamma_0}{6}.$$

Q: activation energy

For an existing mobile defect, Q is its migration energy.

For equilibrium vacancy-mediated atomic diffusion, Q includes formation and migration energies.

Vacancy motion is atom motion in the opposite direction

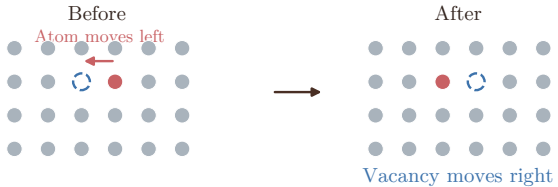


An atom fills the empty site. Its old site becomes the new vacancy.

Question

Did the vacancy move without any atom moving?

Vacancy motion is atom motion in the opposite direction



An atom fills the empty site. Its old site becomes the new vacancy.

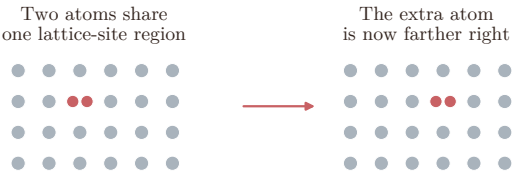
Question

Did the vacancy move without any atom moving?

Answer

No. One vacancy jump and one atom jump describe the same exchange, in opposite directions.

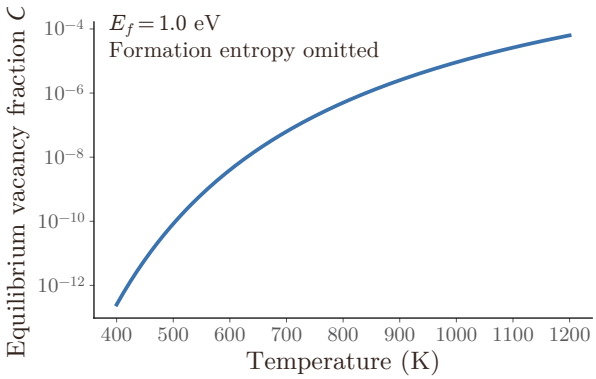
A self-interstitial can move by interstitialcy



Schematic interstitialcy step; nearby atoms also relax

- A self-interstitial is an extra atom of the host material.
- Its motion can involve several atoms pushing and exchanging positions.
- Small solutes such as H or C may hop between interstitial sites by a different mechanism.

Equilibrium vacancies must first be formed



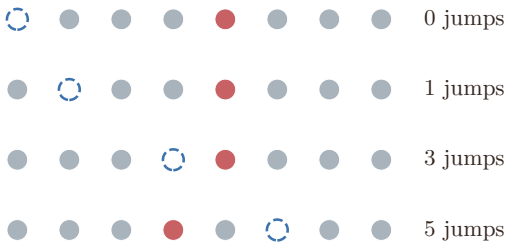
$$C_v^{\text{eq}} = \exp\left(\frac{S_f}{k_\text{B}}\right)\exp\left(-\frac{E_f}{k_\text{B}T}\right)$$

- C_v^{eq}: fraction of lattice sites that are vacant at equilibrium.
- E_f: vacancy formation energy.
- S_f: formation entropy.

Note

Heating increases the equilibrium vacancy population as well as the jump rate.

One vacancy moves more often than one particular atom



One vacancy: 5 jumps
Marked atom: 1 jump

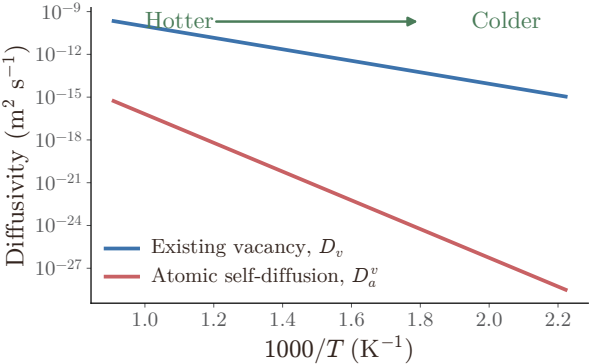
$$D_a^v \simeq f C_v D_v \quad \text{(dilute vacancies)}$$

- D_v: vacancy diffusivity.
- D_a^v: atomic self-diffusivity.
- C_v: vacant-site fraction.
- f: correlation factor.

Physical reason

One vacancy exchanges with many atoms. A marked atom moves when a vacancy reaches it.

Vacancy and atomic diffusivity have different slopes



Existing vacancy

$$D_v = D_{v0} e^{-E_m/(k_B T)}$$

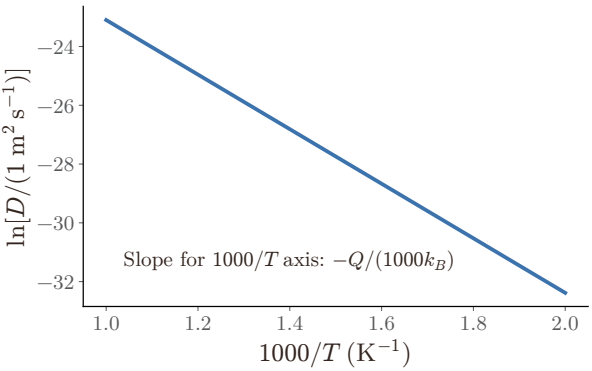
Equilibrium atomic diffusion

$$D_a^v \propto e^{-(E_f+E_m)/(k_B T)}$$

Right means colder: the horizontal axis is $1000/T$. Atomic diffusion falls faster because vacancies also become scarce.

Calculated example: $E_m = 0.8$ eV, $E_f = 1.2$ eV, $f = 0.78$, $S_f = 0$.

Reading an Arrhenius plot



$$\ln D = \ln D_0 - \frac{Q}{k_\mathrm{B}}\frac{1}{T}$$

- On a $1/T$ axis, slope $= -Q/k_\mathrm{B}$.
- On a $1000/T$ axis, slope $= -Q/(1000k_\mathrm{B})$.
- D_0 sets the extrapolated intercept at $1/T = 0$.

Note

A steeper negative slope means a larger activation energy.

Calculated example: $Q = 0.8$ eV; $D_0 = 10^{-6}$ m^2/s.

Worked example: defect diffusivity

Example: Illustrative parameters

$D_0 = 10^{-6}\,\mathrm{m^2\,s^{-1}}$, $E_m = 0.60\,\mathrm{eV}$, $T = 600\,\mathrm{K}$.

Question

What is the diffusivity of this existing defect?

Worked example: defect diffusivity

Example: Illustrative parameters

$D_0 = 10^{-6}\,\mathrm{m^2\,s^{-1}}$, $E_m = 0.60\,\mathrm{eV}$, $T = 600\,\mathrm{K}$.

Question

What is the diffusivity of this existing defect?

$$D = 10^{-6} \exp\left[-\frac{0.60}{(8.617 \times 10^{-5})(600)}\right]$$

Worked example: defect diffusivity

Example: Illustrative parameters

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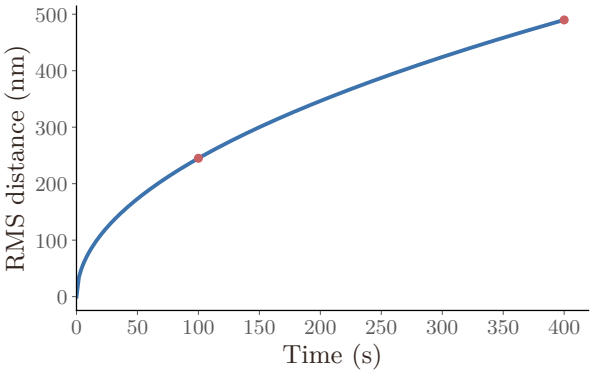
$$D = 10^{-6} \exp\left[-\frac{0.60}{(8.617 \times 10^{-5})(600)}\right]$$

Result

$$D = 9.12 \times 10^{-12}\,\mathrm{m^2\,s^{-1}}$$

This is defect diffusivity. Atomic self-diffusion also depends on the defect population and correlation.

Worked example: how far can a defect spread?



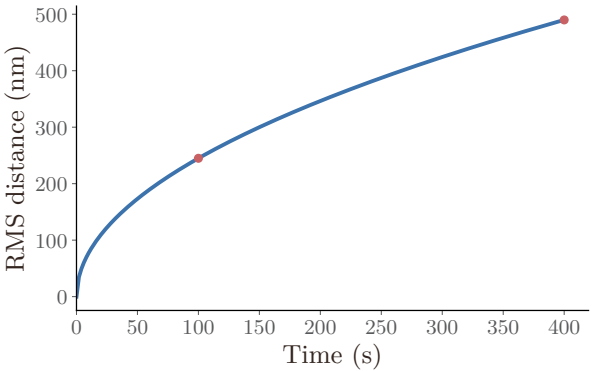
$$r_{\mathrm{rms}} = \sqrt{\langle r^2 \rangle} = \sqrt{6Dt}$$

Take $D = 10^{-16}\,\mathrm{m^2\,s^{-1}}$ and $t = 100\,\mathrm{s}$.

Question

What is the RMS distance? What if time becomes four times longer?

Worked example: how far can a defect spread?



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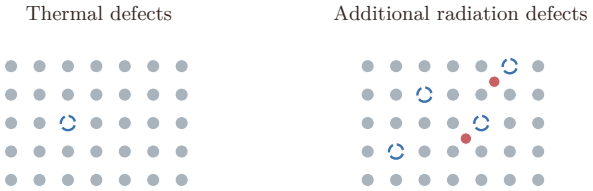
Question

What is the RMS distance? What if time becomes four times longer?

Answer

$r_{\mathrm{rms}} = 245\,\mathrm{nm}$.
At 400 s it is 490 nm, twice as far.

Irradiation supplies additional mobile defects



Same temperature; more defects available for transport

At the same temperature

More mobile vacancies and interstitials can provide more opportunities for atoms to move.

- The defects must survive and remain mobile.
- More defect production does not automatically mean more retained damage.

Radiation-enhanced diffusion depends on mobility and population

Definition: Simple self-diffusion estimate

$$D_a \simeq \underbrace{f_v D_v C_v}_{\text{vacancy contribution}} + \underbrace{f_i D_i C_i}_{\text{interstitial contribution}}$$

How fast?

D_v, D_i: defect diffusivities, $\mathrm{m}^2\ \mathrm{s}^{-1}$.

f_v, f_i: dimensionless correlation and mechanism factors.

How many?

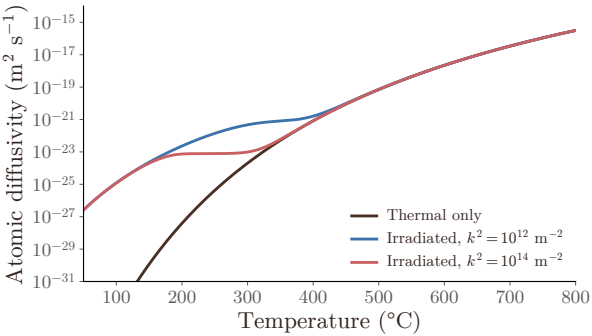
C_v, C_i: mobile defect fractions.

Irradiation can raise these above their thermal values.

Note

Solute diffusion requires species-specific jump rates and coupling. The same expression is not an exact formula for every alloying element.

A calculated example of radiation-enhanced diffusion



- Temperature increases to the right.
- Atomic diffusivity uses a logarithmic scale.
- Irradiation raises diffusion above the thermal curve.
- Stronger sinks reduce the enhancement.

Note

10 s vacancy-only model; constant production and sink absorption; no recombination.

Diffusion under irradiation changes with temperature

Temperature	Physical limitation	Expected consequence
Low	Some defects make very few thermal jumps	Defect-mediated transport can be slow even when defects exist
Intermediate	Radiation supplies mobile defects above equilibrium	Radiation-enhanced diffusion can be substantial
High	Thermal defects and thermal transport become more important	Relative radiation enhancement can become smaller

Note

Collision cascades can also relocate atoms directly. This displacement mixing differs from later thermally activated diffusion.

The defect balance is a count of gains and losses



Net increase: $6 - 2 - 1 = 3$ vacancies

Rate of change = production − recombination − sink removal

- Rate theory tracks average concentrations.
- Each loss term describes a specific physical process.

Concentration and rate: the units matter

Definition: Site fractions used from here onward

$$C_v = \frac{N_v}{N_{\text{sites}}}, \qquad C_i = \frac{N_i}{N_{\text{sites}}}$$

Symbol	Meaning	Units
C_v, C_i	Mobile defects per lattice site	Dimensionless
G	Mobile defects produced per site per second	s^{-1}
dC/dt	Change in defect fraction per second	s^{-1}
Ω	Atomic volume	m^3 per atom

Note

Number density and site fraction are related by $c = C/\Omega$.

The source term counts mobile defects

Definition: Effective source term

$$G = \xi \dot{d}$$

- $\dot{d}$: specified displacement dose rate, commonly NRT-dpa s^{-1}.
- ξ: effective fraction supplying the mobile defects represented by the model.
- Defects that recombine promptly or enter immobile clusters do not all enter this source term.

Question

If $\dot{d} = 10^{-7}\,\mathrm{s}^{-1}$ and $\xi = 0.3$, what is G?

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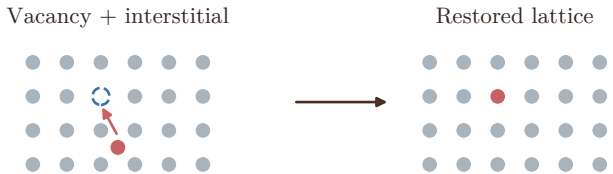
Question

If $\dot{d} = 10^{-7}\,\mathrm{s}^{-1}$ and $\xi = 0.3$, what is G?

Answer

$G = 3 \times 10^{-8}\,\mathrm{s}^{-1}$. The value of ξ must match the chosen dose definition and defect model.

Recombination restores an occupied lattice site



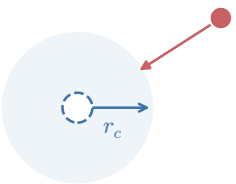
One event

One interstitial and one vacancy disappear when the extra atom fills the empty site.

- The atom remains in the material.
- The defect count falls because the lattice arrangement is restored.

Recombination depends on encounters

An encounter can remove both defects



Relative mobility: $D_i + D_v$

$$R_{iv} = K_{iv} C_i C_v$$

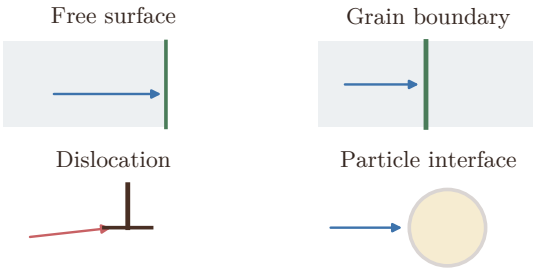
For dilute defects in a continuum capture model:

$$K_{iv} \simeq \frac{4\pi r_c (D_i + D_v)}{\Omega}$$

- r_c: effective capture radius, m.
- $D_i + D_v$: relative diffusivity, m^2/s.
- Ω: atomic volume, m^3.

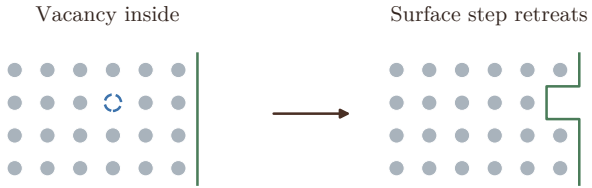
Here K_{iv} and R_{iv} have units s^{-1}.

Sinks remove defects from the mobile population



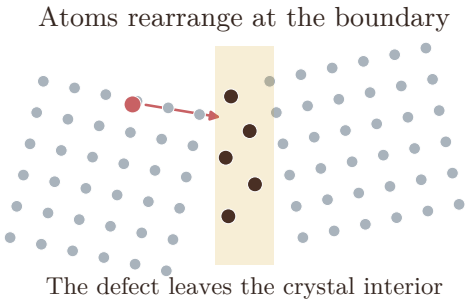
Capture changes the sink structure or stores the defect there. An atom does not disappear.

A free surface can absorb a vacancy



- Atoms exchange with the vacancy until it reaches the surface.
- The free surface changes position locally, leaving a step.
- The vacancy is no longer a defect inside the crystal.

A grain boundary can accommodate defects

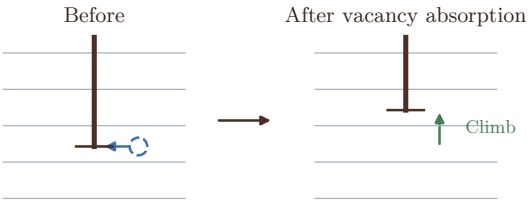


- A boundary separates crystals of different orientation.
- Its atomic structure differs from the regular crystal interior.
- Atoms can rearrange as vacancies or interstitials arrive.

Note

Capture efficiency depends on boundary structure, temperature and defect type.

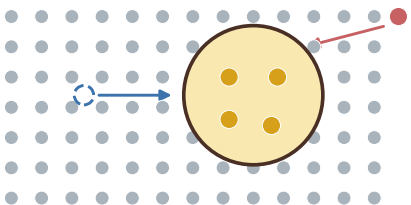
Defect absorption can move a dislocation by climb



- The thick line represents an extra half-plane ending at an edge dislocation.
- Absorbing vacancies removes atoms from the end of that half-plane.
- Its end changes position. This motion is called **climb**.

Particle interfaces can capture defects

Defect capture at the particle interface



- Sites at the interface differ from sites inside the matrix.
- It may trap defects or help vacancies and interstitials recombine.
- Capture depends on the interface structure and chemistry.

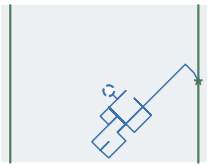
Materials choice

Check particle spacing and interface stability.

Sink strength measures how readily defects reach sinks

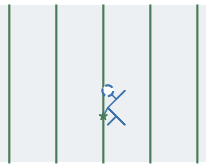
Where will a mobile defect usually survive longer?

Fewer sinks



Smaller k^2

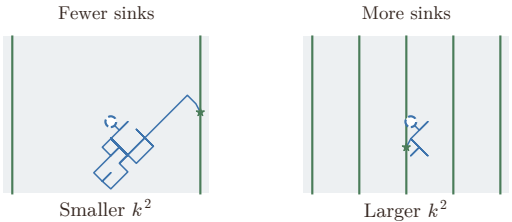
More sinks



Larger k^2

Sink strength measures how readily defects reach sinks

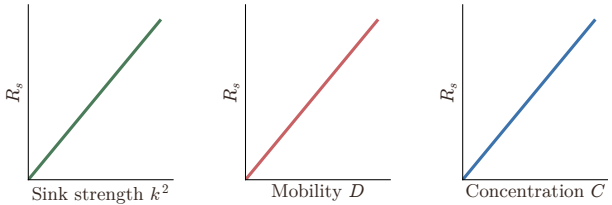
Where will a mobile defect usually survive longer?



Definition: Sink strength k^2

Larger k^2 means more effective capture. It depends on sink size, spacing and capture efficiency. Units: m^{-2}.

Sink removal combines strength, mobility and population

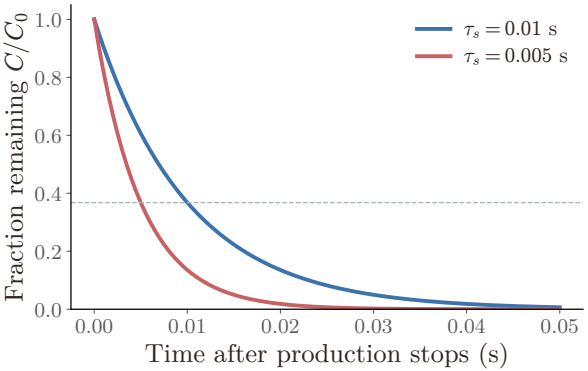


Forward absorption; thermal emission neglected.

$$R_s = k^2 D C$$

k^2	Sink strength	m^{-2}
D	Diffusivity of the mobile defect	m^2/s
C	Mobile defect fraction	Dimensionless
R_s	Defect fraction removed per second	s^{-1}

The sink lifetime is the inverse removal frequency



After production stops, with constant $k^2 D$ and sink removal only:

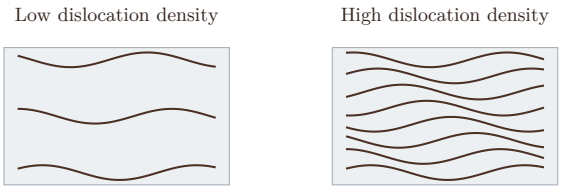
$$\frac{dC}{dt} = -k^2 D C$$

$$C(t) = C_0 e^{-t/\tau_s}$$

$$\tau_s = \frac{1}{k^2 D} \quad \text{(seconds)}$$

At $t = \tau_s$, about 37% remain. The lifetime is a statistical scale.

Dislocation sink strength increases with line density



$\rho_d =$ total dislocation length / material volume

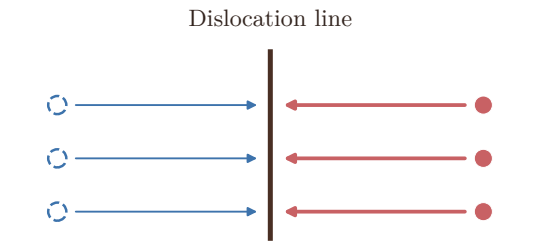
Definition

$$k_d^2 \simeq Z\rho_d$$

- ρ_d: total dislocation line length per unit volume, $\mathrm{m/m^3} = \mathrm{m^{-2}}$.
- Z: dimensionless capture factor for the specified defect.

Sink bias distinguishes vacancy and interstitial capture

$$k_{d,i}^2 = Z_i \rho_d, \qquad k_{d,v}^2 = Z_v \rho_d$$



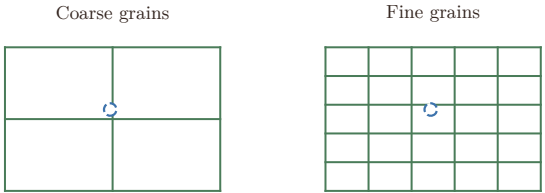
Capture factors can differ: $Z_i > Z_v$

- Dislocation strain fields interact with point defects.
- In the usual dislocation-bias model, $Z_i > Z_v$.
- Mobility and concentration also affect the actual capture rates.

Meaning of bias

At otherwise comparable conditions, capture efficiency differs between defect types.

Smaller grains shorten the distance to a boundary

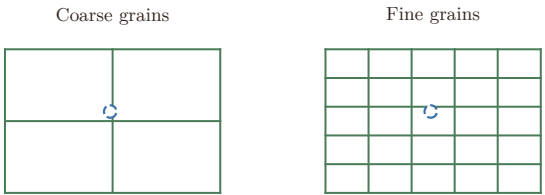


Similar grain shapes: $k_{\mathrm{GB}}^2 \propto 1/d_g^2$

Question

Halve the grain size. How does sink strength change if the boundary geometry and capture efficiency remain similar?

Smaller grains shorten the distance to a boundary



Similar grain shapes: $k^2_{\mathrm{GB}} \propto 1/d_g^2$

Question

Halve the grain size. How does sink strength change if the boundary geometry and capture efficiency remain similar?

Answer

About four times larger, because $k^2_{\mathrm{GB}} \propto 1/d_g^2$.

Several sink types can act together

Approximate rate-theory sum

$$k^2_{\text{total}} \simeq k^2_d + k^2_{\text{GB}} + k^2_{\text{cavity}} + k^2_{\text{interface}} + \cdots$$

Dilute spherical absorbers

$$k^2_{\text{cavity}} \simeq 4\pi r N$$

r: radius, m.
N: number per unit volume, m^{-3}.

Note: Physical interpretation

More absorbing objects increase capture. Larger radius also increases their ability to collect diffusing defects.

Compute strengths separately for vacancies and interstitials when capture differs.

The coupled vacancy and interstitial equations

Vacancies

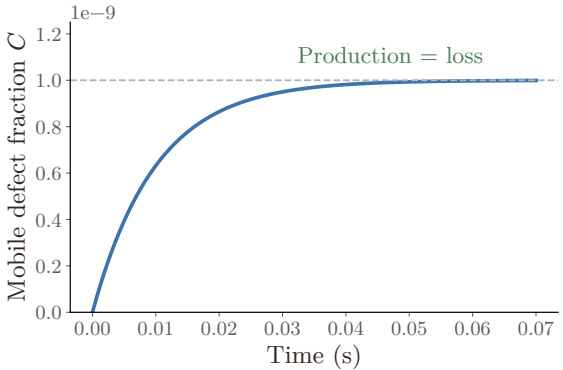
$$\frac{dC_v}{dt} = G - K_{iv}C_iC_v - k_v^2 D_v(C_v - C_v^{\mathrm{eq}})$$

Interstitials

$$\frac{dC_i}{dt} = G - K_{iv}C_iC_v - k_i^2 D_i C_i$$

- G adds mobile defects. The same source is assumed for both species here.
- Recombination removes one of each species.
- Sink terms remove mobile defects; the vacancy term includes an equilibrium emission contribution.

Steady concentration means production balances removal



Plot: $G = 10^{-7}$ s^{-1}, $k^2 D = 100$ s^{-1}, $C(0) = 0$.

With sink removal dominant and equilibrium defects negligible:

$$\frac{dC}{dt} = G - k^2 D C$$

At steady state, $dC/dt = 0$:

$$C_{\text{ss}} = \frac{G}{k^2 D} = G\tau_s$$

Defects still arrive and leave. Their average population stays constant.

Worked example: sink strength, lifetime and concentration

Example: Given

$\rho_d = 10^{14}\,\mathrm{m}^{-2}$, $Z = 1$, $D = 10^{-12}\,\mathrm{m}^2\,\mathrm{s}^{-1}$, $G = 10^{-7}\,\mathrm{s}^{-1}$.
Assume dislocations dominate, recombination is small and $C \gg C^{\mathrm{eq}}$.

Question

Find k^2, τ_s and C_{ss}.

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Assume dislocations dominate, recombination is small and $C \gg C^{\mathrm{eq}}$.

Question

Find k^2, τ_s and C_{ss}.

$$k^2 = Z\rho_d = 10^{14}\,\mathrm{m}^{-2}, \qquad k^2 D = 100\,\mathrm{s}^{-1}$$

Results

$$\tau_s = 0.01\,\mathrm{s}, \qquad C_{\mathrm{ss}} = \frac{10^{-7}}{100} = 10^{-9}$$

Doubling ρ_d halves both τ_s and C_{ss} under these assumptions.

Two limiting balances give different dose-rate dependence

Sink-dominated balance

$$G \simeq k^2 D C \quad \Rightarrow \quad C \propto G$$

Twice the production rate gives twice the concentration if k^2 and D remain fixed.

Recombination-only model

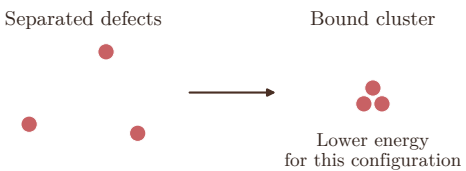
$$G \simeq K_{iv} C^2 \quad \Rightarrow \quad C \simeq \sqrt{G/K_{iv}}$$

This uses $C_i = C_v = C$. Four times the production rate gives twice the concentration.

Note

Equal production does not guarantee equal concentrations when vacancy and interstitial sink losses differ. Temperature alone does not identify the dominant balance.

Defects can bind into clusters

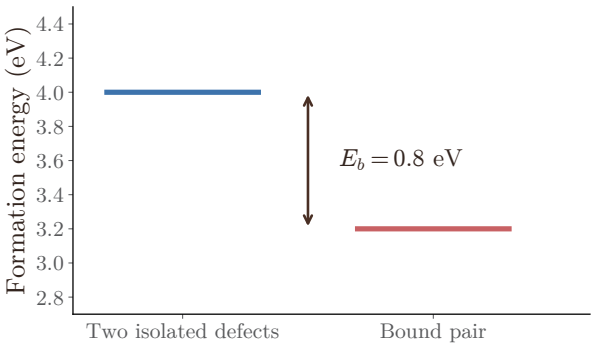


- A bound arrangement has lower energy than the same defects far apart.
- Mobile defects can meet by diffusion.
- Cascades can also produce clusters directly.

Note: Stability

A cluster can lose defects by thermal emission. Binding does not make it permanent.

Binding energy measures the energy gained by joining



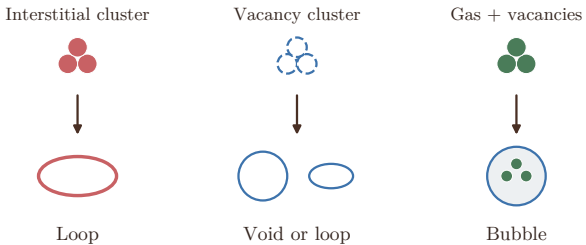
For two defects:

$$E_b = E_f(A) + E_f(B) - E_f(AB)$$

- $E_f(A), E_f(B)$: isolated-defect energies.
- $E_f(AB)$: pair formation energy.
- Positive E_b means favourable binding.

Separating this pair costs 0.8 eV.

Different clusters produce different structures



Note

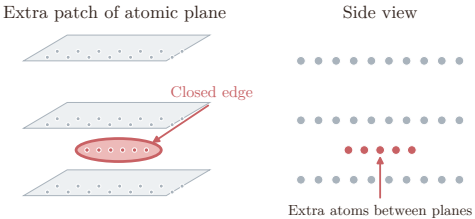
Vacancy clusters can form cavities, collapsed loops or stacking-fault tetrahedra. The outcome depends on crystal structure, energetics, gas and temperature.

Why an interstitial dislocation is a loop

Where is the dislocation line around an extra patch of plane?

Why an interstitial dislocation is a loop

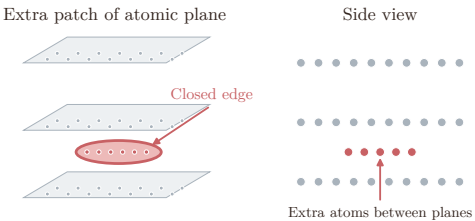
Where is the dislocation line around an extra patch of plane?



The dislocation is the perimeter of the patch

Why an interstitial dislocation is a loop

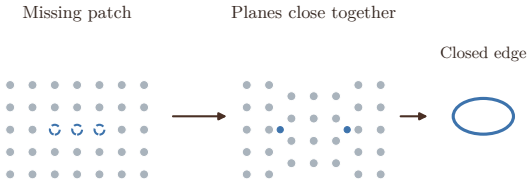
Where is the dislocation line around an extra patch of plane?



The dislocation is the perimeter of the patch

The dislocation is the edge of the extra patch. The edge closes on itself, forming a loop.

A vacancy loop forms when a missing patch collapses

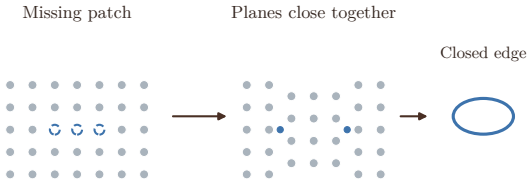


A collapsed vacancy loop differs from an open cavity

Question

Is a vacancy loop simply a small empty hole?

A vacancy loop forms when a missing patch collapses



A collapsed vacancy loop differs from an open cavity

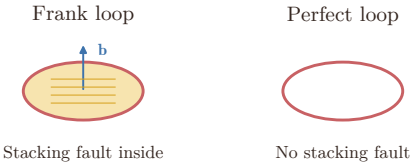
Question

Is a vacancy loop simply a small empty hole?

Answer

No. The planes close together and leave a dislocation around the edge. A void retains an open cavity.

Frank and perfect loops differ in their enclosed fault



FCC Frank loop

$\mathbf{b} = \frac{a}{3}\langle 111\rangle$ on a $\{111\}$ plane.
It encloses a stacking fault and cannot glide conservatively like a perfect dislocation.

FCC perfect loop

$\mathbf{b} = \frac{a}{2}\langle 110\rangle$.
It has no enclosed stacking fault. Its mobility depends on its geometry and obstacles.

a: lattice parameter. $\mathbf{b}$: Burgers vector.

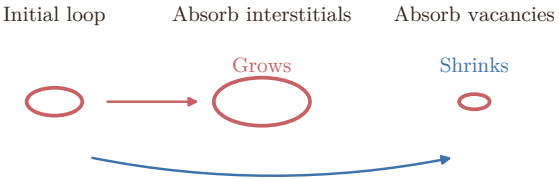
Loop type and mobility depend on crystal structure

Crystal	Common examples	Key point
FCC	Frank $a/3\langle 111\rangle$; perfect $a/2\langle 110\rangle$	Faulted loops can change character through dislocation reactions
BCC	$a/2\langle 111\rangle$ and $a\langle 100\rangle$ loops	Both occur; mobility and population depend on material and conditions
HCP	Several loop families	Basal and prismatic directions are not equivalent

Note

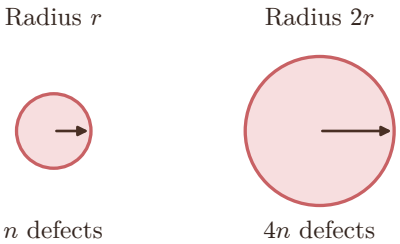
A closed dislocation line does not imply a freely moving loop. Pinning, solutes, other defects and loop character affect motion.

Absorption can grow or shrink an interstitial loop



- Adding interstitials increases the extra patch of plane.
- Adding vacancies removes part of that excess.
- Net growth depends on both incoming fluxes and defect emission.

Loop radius is related to the number of stored defects



For a circular planar loop:

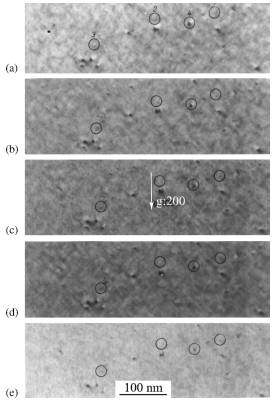
$$n\Omega = A|b_\perp| = \pi r^2 |b_\perp|$$

- n: number of excess or missing atoms.
- Ω: atomic volume.
- $b_\perp$: Burgers-vector component normal to the loop plane.

$$n \propto r^2$$

At fixed $b_\perp$, doubling radius requires four times as many stored defects.

Small loops appear through their TEM contrast



The same irradiated region under different diffraction conditions.

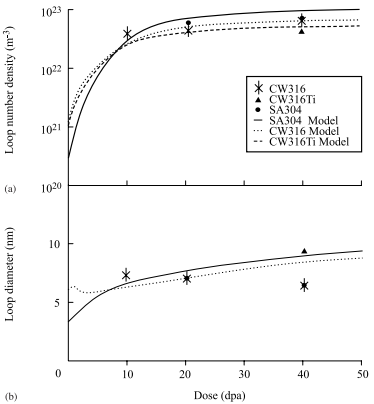
- The drawn circles mark defect locations. They are not the loop edges.
- Panels (a)–(e) show the same region under changing diffraction conditions.
- The central panel labels the $g = 200$ reflection.

Note

Diffraction contrast changes between panels. These are not successive stages of loop growth.

Was (2007), Fig. 7.44; Jenkins and Kirk (2001), Fig. 2.4.

Loop number density and size are different measurements



- Horizontal axis: irradiation dose in dpa.
- Upper panel: loop number density, m^{-3}, logarithmic scale.
- Lower panel: average loop diameter, nm.
- Symbols show measurements; curves show model calculations.

Interpretation

A nearly constant number of loops can coexist with increasing loop size. Read both panels.

Was (2007), Fig. 7.58.

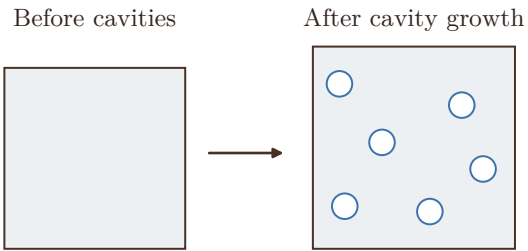
Loops can obstruct moving dislocations



Loops obstruct the motion of other dislocations

- Plastic deformation requires dislocations to move.
- Irradiation loops can obstruct that motion.
- Additional stress may be needed to overcome the obstacles, producing hardening.

Void swelling increases material volume

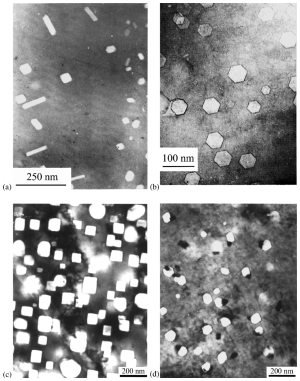


Definition: Void swelling

The material volume increases as cavities form and grow.

- A void is a three-dimensional cavity.
- Swelling depends on the total volume of the cavities.
- Temperature, dose rate, alloy and microstructure all matter.

Cavities are visible in irradiated materials



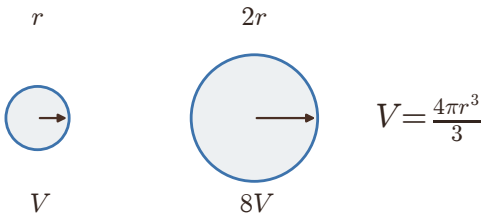
- The micrographs show cavity populations in different metals.
- Cavity shape and size differ between panels.
- Read each scale bar before comparing sizes.

Note

A 2D image alone does not directly give the total 3D cavity volume fraction. Quantification needs size and number-density information.

Was (2007), Fig. 8.1.

Swelling is controlled by cavity volume



For dilute spherical cavities of one radius:

$$S = \frac{\Delta V}{V_0} \simeq \frac{4\pi}{3} N r^3$$

- S: fractional swelling.
- N: cavities per unit volume, m^{-3}.
- r: cavity radius, m.

At fixed N, doubling r gives eight times the swelling.

Worked example: swelling from a cavity population

Example: Given

$N = 10^{21}\,\mathrm{m}^{-3}$ and $r = 5\,\mathrm{nm} = 5 \times 10^{-9}\,\mathrm{m}$.

Question

What is the fractional swelling? What is it as a percentage?

Worked example: swelling from a cavity population

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$$S = \frac{4\pi}{3}(10^{21})(5 \times 10^{-9})^3 = 5.24 \times 10^{-4}$$

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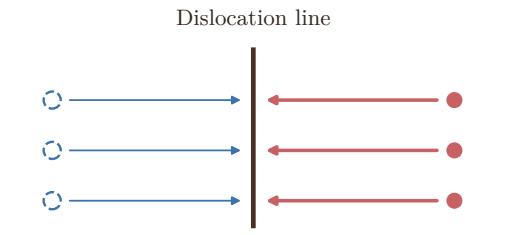
$$S = \frac{4\pi}{3}(10^{21})(5 \times 10^{-9})^3 = 5.24 \times 10^{-4}$$

Result

$$S = 0.0524\%$$

At $r = 10\,\mathrm{nm}$ with the same number density, $S = 0.419\%$.
Use radius, not diameter, in the formula.

Sink bias can leave vacancies available for cavity growth



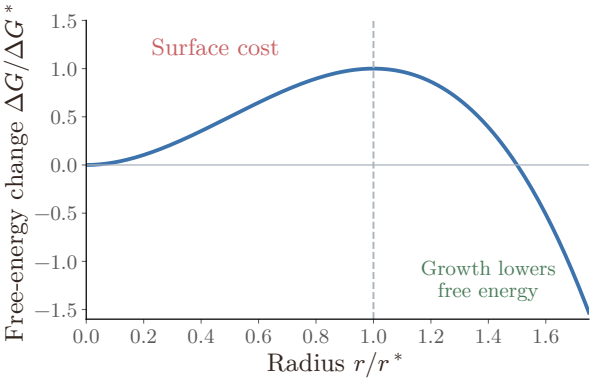
Capture factors can differ: $Z_i > Z_v$

1. Irradiation creates vacancy–interstitial pairs.
2. Dislocations can capture interstitials more efficiently.
3. Other sinks can then receive a net vacancy flux.
4. Net vacancy absorption can grow cavities.

Note

Equal production does not require equal capture at each sink.

Void nucleation competes with the cost of a new surface



- A cavity creates an internal surface, which costs energy.
- Vacancy supersaturation favours collecting vacancies into a cavity.
- In a simple model these effects create a nucleation barrier.

$$r^* = \frac{2\gamma\Omega}{k_\mathrm{B}T \ln S_v}, \qquad S_v = \frac{C_v}{C_v^{\mathrm{eq}}} > 1$$

Classical spherical model; gas and stress omitted.
γ: surface energy (J/m^2). Ω: atomic volume. r^*: critical radius.

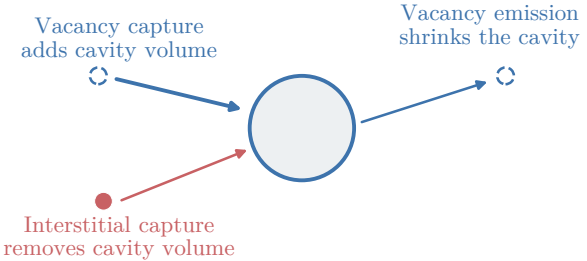
Helium can stabilize small cavities



- Nuclear reactions can generate helium in the material.
- Helium has very low solubility in many metals and can bind to vacancy clusters.
- Gas can help stabilize cavities and affect their nucleation and growth.

A cavity grows when its vacancy gain exceeds its losses

$$\frac{dV_c}{dt} = \Omega \left(\dot{N}_v - \dot{N}_i - \dot{N}_{\text{em}} \right)$$



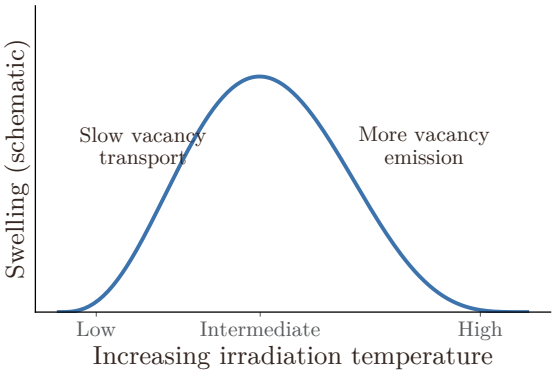
- V_c: cavity volume.
- $\dot{N}_v$: vacancy capture rate.
- $\dot{N}_i$: interstitial capture rate.
- $\dot{N}_{\text{em}}$: vacancy emission rate.

Each $\dot{N}$ counts defects per second.

Note

For a spherical cavity, $dV_c/dt = 4\pi r^2 \, dr/dt$.

Swelling often peaks over an intermediate temperature range

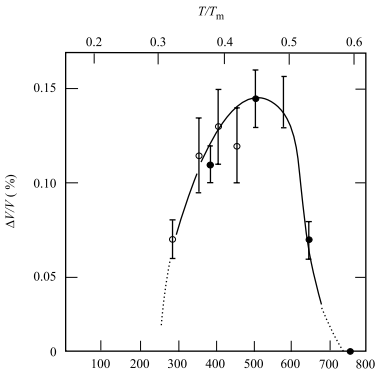


- Low temperature: slow vacancy transport limits growth.
- Intermediate: vacancies can reach and grow cavities.
- High temperature: emission and lower supersaturation can limit growth.

Note

The peak depends on the material and irradiation conditions.

An experimental example of a swelling temperature peak



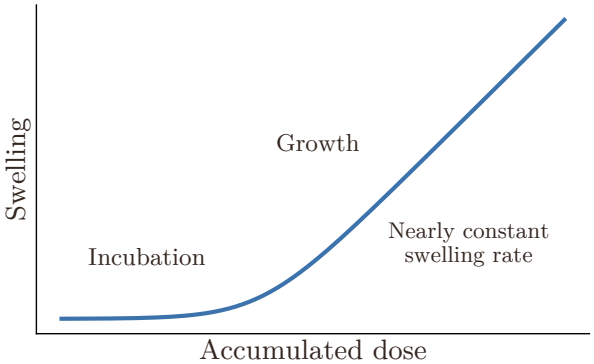
- Bottom axis: irradiation temperature, °C.
- Top axis: T/T_m, with both temperatures in kelvin.
- Vertical axis: volume swelling, percent.

Reading the curve

For this exposure, swelling is largest near the middle of the temperature range. It falls on either side.

Was (2007), Fig. 8.16.

Swelling can continue after the mobile defect population stabilizes



- Incubation: little measurable swelling while nuclei develop.
- Growth: cavities collect vacancies and increase in volume.
- A nearly straight region means an approximately constant swelling rate per dose.

Two different statements

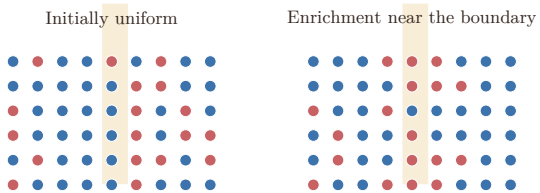
Constant mobile defect concentration does not mean constant cavity volume.

Swelling resistance depends on how defects are handled

Possible change	**Intended effect**	**What must also be checked?**
Grain refinement	Shorter paths to boundaries	Boundary stability, segregation and gas accumulation
Stable particle interfaces	Capture and recombination sites	Interface efficiency and thermal stability
Dislocation structure	Changes defect capture rates	Vacancy–interstitial bias and recovery
Alloy chemistry	Changes mobility, trapping and clustering	Phase stability and mechanical properties

The defect balance and the location of retained damage determine whether the change improves performance.

Radiation-induced segregation changes local composition



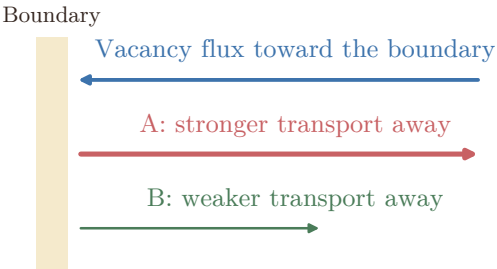
Local composition changes while the overall alloy composition is conserved

Definition: RIS

Defect transport couples to the transport of alloying elements, changing their concentrations near sinks.

- The change is local.
- A boundary can become enriched in one element and depleted in another.

The inverse Kirkendall mechanism couples opposite fluxes



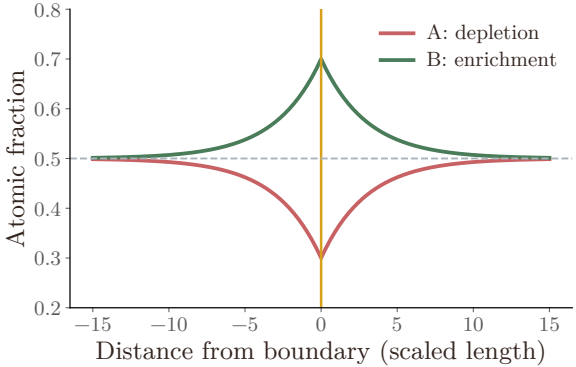
A becomes depleted; B becomes enriched relative to A

1. Vacancies flow toward a sink.
2. Atoms exchange with vacancies, moving in the opposite direction.
3. If A is transported away more strongly than B, A becomes depleted near the sink.

Note

This is a simplified vacancy-mediated explanation. Real alloys can have several competing transport contributions.

Enrichment and depletion are measured relative to the bulk

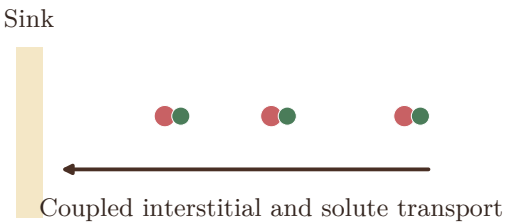


- Boundary position is $x = 0$.
- A falls below its bulk atomic fraction near the boundary.
- B rises above its bulk fraction.
- Far from the boundary, both approach their bulk values.

Binary illustration

$$C_A(x) + C_B(x) = 1$$

Interstitial transport can also carry solutes toward sinks

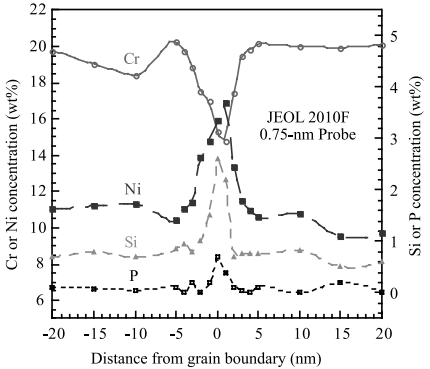


- Some solutes bind to, or move with, interstitial configurations.
- Transport toward a sink can then enrich those solutes near it.
- Vacancy-mediated and interstitial-mediated contributions can compete.

Note

The direction of segregation must be established for the particular alloy and conditions.

Measured segregation in irradiated stainless steel



- x: distance from boundary, nm.
- Left y: Cr and Ni, wt%.
- Right y: Si and P, wt%.
- Here Cr is depleted. Ni, Si and P are enriched.

Note

Chromium depletion can reduce corrosion resistance.

Was (2007), Fig. 6.1.

Temperature changes the competition that produces RIS

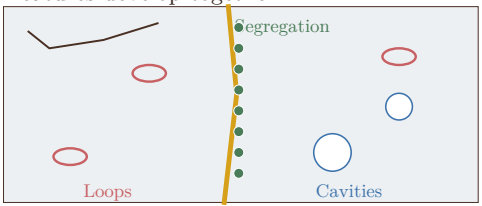
Condition	Transport behaviour	Effect on segregation
Low mobility	Few jumps; limited defect and solute transport	RIS may develop slowly
Mobile defects	Sustained defect fluxes couple to unequal solute fluxes	Significant segregation can develop
Thermal diffusion	Diffusion reduces local composition gradients	Can oppose radiation-induced segregation

Note

RIS often peaks at intermediate temperatures. Its size and direction depend on the alloy, dose rate, dose and sink.

Several microstructural changes occur together

Several features develop together

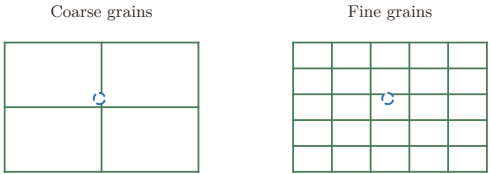


- Loops can obstruct plastic flow.
- Cavities can cause swelling.
- Grain-boundary segregation changes local chemistry.
- Gas can accumulate at cavities and interfaces.

Connection to Unit 5

Properties depend on defect type, size, number and location.

Class discussion: are finer grains always better?

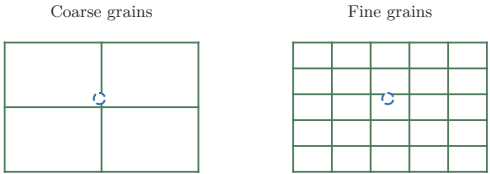


Similar grain shapes: $k_{\mathrm{GB}}^2 \propto 1/d_g^2$

Question

At the same composition, temperature and dose rate, what is one benefit and one concern of finer grains?

Class discussion: are finer grains always better?



Similar grain shapes: $k^2_{\mathrm{GB}} \propto 1/d_g^2$

Question

At the same composition, temperature and dose rate, what is one benefit and one concern of finer grains?

Answer

Benefit: shorter paths to sinks. Concern: boundaries can collect solutes or helium, and the grains may coarsen.

Summary of Equations

Question	Equation
How much crosses a unit area?	$J = -D\,\partial c/\partial x$
How does concentration change locally?	$\partial c/\partial t = D\,\partial^2 c/\partial x^2$
How fast does a defect move?	$D = D_0 e^{-Q/(k_{\mathrm{B}}T)}$
How fast do sinks remove defects?	$R_s = k^2 DC$
How long does a mobile defect survive?	$\tau_s = 1/(k^2 D)$ in the sink-only model
What population balances production?	$C_{\mathrm{ss}} = G/(k^2 D)$ in the sink-dominated limit
How much volume do cavities add?	$S \simeq (4\pi/3)Nr^3$ for dilute equal-sized spheres

Unit 4 review

1. Diffusion requires both accessible jumps and mobile defects.
2. Recombination and sink absorption remove defects from the mobile population.
3. Sink strength describes capture geometry and efficiency; diffusivity sets the time scale.
4. Bound clusters can become loops or cavities, with different physical effects.
5. Defect fluxes can change alloy composition near sinks.

Final question

Why can two samples at the same dpa have different microstructures?

Unit 4 review

1. Diffusion requires both accessible jumps and mobile defects.
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Final question

Why can two samples at the same dpa have different microstructures?

Temperature, dose rate, initial sinks, alloy chemistry and gas production change what happens to the defects after they are created.

References

1. G. S. Was, *Fundamentals of Radiation Materials Science: Metals and Alloys*. Springer, 2007. Chs. 4–8 and 12. DOI: 10.1007/978-3-540-49472-0.

2. K. L. Murty and I. Charit, *An Introduction to Nuclear Materials: Fundamentals and Applications*. Wiley-VCH, 2013. Ch. 6.

3. M. L. Jenkins and M. A. Kirk, *Characterization of Radiation Damage by Transmission Electron Microscopy*. Institute of Physics Publishing, 2001. Fig. 2.4, p. 13.