Unit 2: Crystallography and Materials Science Fundamentals

ME 5203 – Nuclear Materials

P. Sharma, Ph.D.

Department of Mechanical Engineering
School of Energy Resources
University of Wyoming

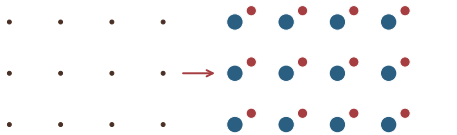
Fall 2026

What crystal structure tells us

- Where atoms normally sit.
- Which directions and planes we need to describe.
- Where defects can form and how dislocations move.

Nuclear materials

These are the starting points for understanding radiation damage.



Unit 2: Outline

Part	Topics
1	Lattices, unit cells, BCC, FCC and HCP
2	Directions, planes and diffraction
3	Ceramic structures and point defects
4	Dislocations, boundaries and stacking faults

By the end

Draw and label a structure, use its geometry, and identify its defects.

Crystalline and amorphous solids

- A crystal has a repeating atomic arrangement over long distances.
- An amorphous solid has local order but no long-range periodicity.
- The drawings show a two-dimensional comparison.



periodic



no long-range periodicity

Lattice + basis = crystal structure

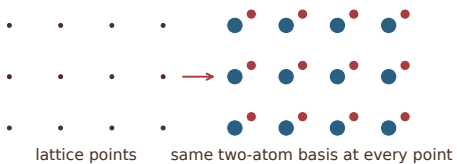
Lattice

A periodic set of equivalent points.

Basis

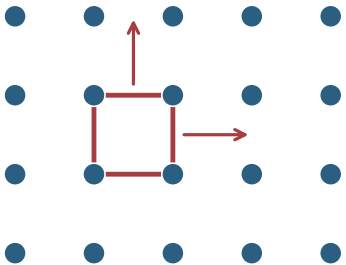
The same atom or group of atoms placed at every lattice point.

Both the positions and the species matter.



A unit cell repeats through space

- Translate the cell along its edge vectors to build the crystal.
- A primitive cell contains one lattice point.
- A conventional cell can be larger so its symmetry is easier to see.

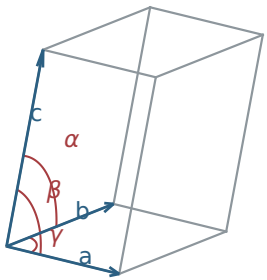


repeat the cell by translation

Six quantities describe a unit cell

$$a,\ b,\ c; \qquad \alpha,\ \beta,\ \gamma$$

- a, b, c: edge lengths.
- α: angle between b and c.
- β: angle between a and c.
- γ: angle between a and b.



Cubic cell

$a = b = c$ and all three angles are 90°.

The seven crystal systems

System	Conventional cell metric
Cubic	$a = b = c$; all angles 90°
Tetragonal	$a = b \neq c$; all angles 90°
Orthorhombic	a, b, c independent; all angles 90°
Hexagonal	$a = b$; $\alpha = \beta = 90^\circ$, $\gamma = 120^\circ$
Trigonal	Rhombohedral axes: $a = b = c$, $\alpha = \beta = \gamma$
Monoclinic	$\alpha = \gamma = 90^\circ$; β independent
Triclinic	Lengths and angles independent

Trigonal crystals can also use hexagonal axes. Symmetry defines the system.

The fourteen Bravais lattices

Crystal system	Allowed centring	Count
Triclinic	P	1
Monoclinic	P, C	2
Orthorhombic	P, C, I, F	4
Tetragonal	P, I	2
Trigonal	R	1
Hexagonal	P	1
Cubic	P, I, F	3

Meaning of the letters

P: primitive; C: base-centred; I: body-centred; F: face-centred; R: rhombohedral.

BCC and FCC describe lattices. HCP is a hexagonal lattice with a two-atom basis.

Atoms on cell boundaries are shared

- Corner atom: shared by eight cubic cells, so count 1/8.
- Face atom: shared by two cells, so count 1/2.
- Interior atom: count the whole atom.

What we count

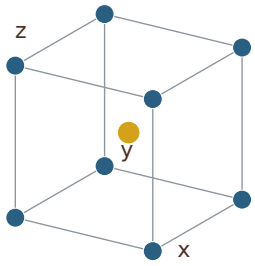
The net number of atoms assigned to one cell.



BCC: corners and one body centre

$$n = 8\left(\frac{1}{8}\right) + 1 = 2$$

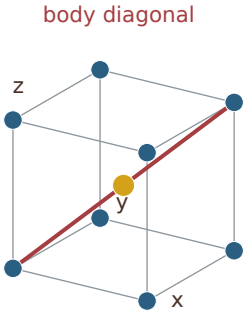
- Two atoms per conventional cubic cell.
- Each atom has eight nearest neighbours.
- Examples: α-Fe, Cr, Mo and W.



BCC atoms touch along the body diagonal

- The diagonal length is $\sqrt{3}a$.
- Follow a corner, the centre and the opposite corner.
- The centre-to-centre distances add to $4r$.

$$\sqrt{3}a = 4r$$



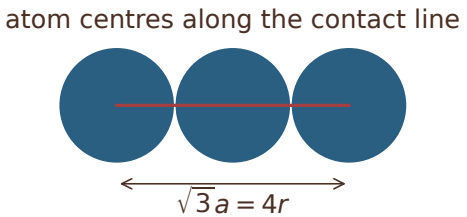
BCC: from atomic radius to cell edge

$$a = \frac{4r}{\sqrt{3}}$$

Symbols

a: cubic cell edge. r: hard-sphere atomic radius.

The contact model describes ideal geometry. Real atoms do not have sharp surfaces.



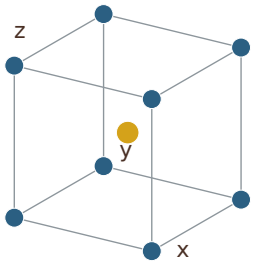
Atomic packing factor counts occupied volume

$$\mathrm{APF} = \frac{n(4\pi r^3/3)}{V_{\mathrm{cell}}}$$

- n: atoms assigned to the cell.
- $4\pi r^3/3$: volume of one sphere.
- $V_{\mathrm{cell}} = a^3$ for a cubic cell.

BCC result

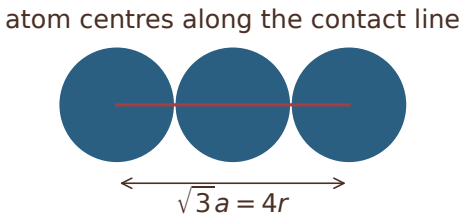
Insert $n = 2$ and $a = 4r/\sqrt{3}$:
$\mathrm{APF} = \pi\sqrt{3}/8 \approx 0.680$.



BCC geometry: a short calculation

Question

Assume a BCC material has $r = 0.125$ nm. What is a?

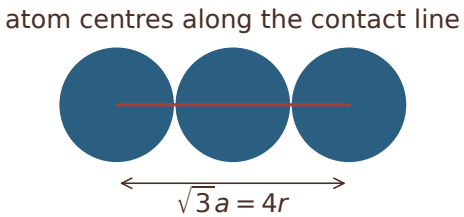


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$$a = \frac{4(0.125)}{\sqrt{3}} \text{ nm}$$



BCC geometry: a short calculation

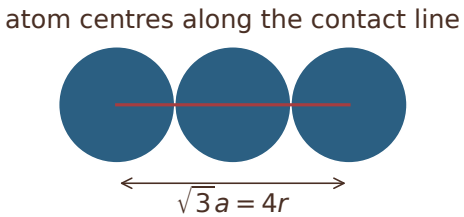
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Answer

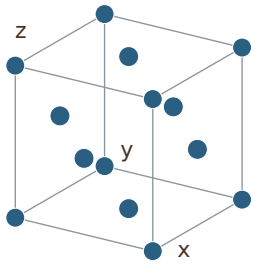
$a = 0.289$ nm. The cell edge exceeds the atomic diameter.



FCC: corners and six face centres

$$n = 8\left(\frac{1}{8}\right) + 6\left(\frac{1}{2}\right) = 4$$

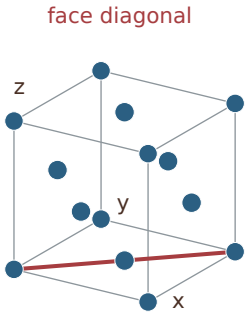
- Four atoms per conventional cubic cell.
- Each atom has twelve nearest neighbours.
- Examples: Cu, Ni, Al and austenitic steel matrices.



FCC atoms touch along a face diagonal

- The face diagonal has length $\sqrt{2}a$.
- It passes through one face-centre atom.
- The contact distance is again $4r$.

$$\sqrt{2}a = 4r$$



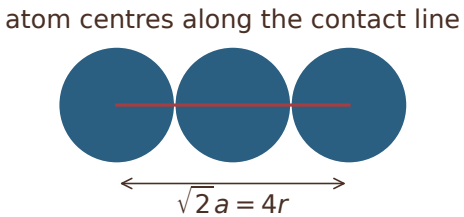
FCC packing factor

$$a = 2\sqrt{2}r$$

$$\text{APF} = \frac{4(4\pi r^3/3)}{(2\sqrt{2}r)^3} = \frac{\pi}{3\sqrt{2}} \approx 0.740$$

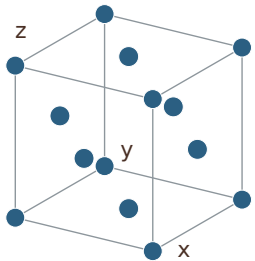
Physical meaning

Equal spheres occupy about 74% of the cell volume.



Question

FCC packs more efficiently than BCC. Must every FCC metal be denser than every BCC metal?



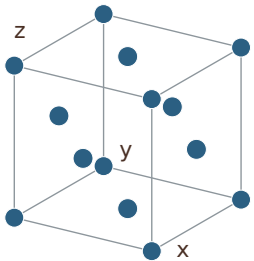
Packing factor and mass density

Question

FCC packs more efficiently than BCC. Must every FCC metal be denser than every BCC metal?

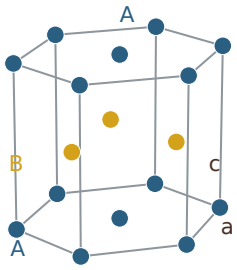
Answer

No. Density also depends on atomic mass and cell size. Packing factor alone is insufficient.



HCP: close-packed layers repeat ABAB

- The B layer sits in hollows of the A layer.
- The third layer returns to the A positions.
- Two lengths describe the structure: a and c.
- Ideal nearest-neighbour count: 12.



HCP: why you see both two and six atoms

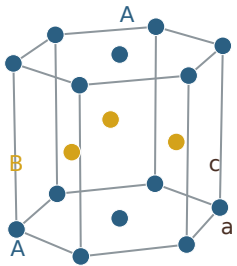
Small hexagonal cell

A primitive parallelepiped with a two-atom basis contains 2 atoms.

Large hexagonal prism shown here

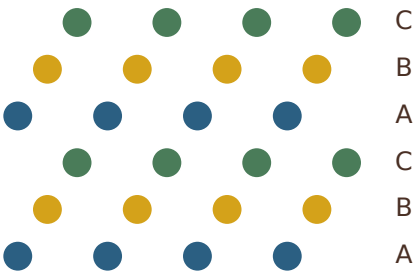
$12(1/6) + 2(1/2) + 3 = 6$ atoms.

The prism contains three primitive cells. State which cell you use.

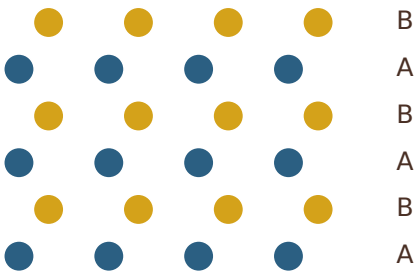


FCC and HCP differ in layer stacking

FCC: ABCABC



HCP: ABABAB



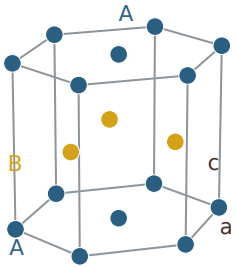
Same ideal packing fraction

Both reach 0.740, but the stacking sequence differs.

Ideal HCP geometry

$$a = 2r, \qquad \frac{c}{a} = \sqrt{\frac{8}{3}} \approx 1.633$$

- The ideal ratio follows from touching equal spheres.
- Real metals can deviate from this ratio.
- The basal plane and c direction are not equivalent.



Zirconium example

With $a \approx 0.323$ nm and $c \approx 0.515$ nm, $c/a \approx 1.59$.

Three structures: useful comparisons

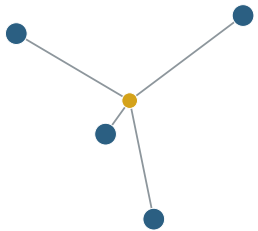
Quantity	BCC	FCC	Ideal HCP
Atoms in stated cell	2 (cube)	4 (cube)	6 (large prism)
Nearest neighbours	8	12	12
Packing fraction	0.680	0.740	0.740
Dense planes	{110}	{111}	(0001)
Close-packed planes	None	{111}	(0001)

Use with care

Crystal structure influences properties. Composition, temperature and microstructure also matter.

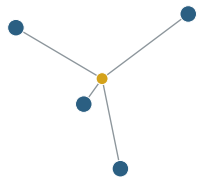
Interstitial sites are spaces between atoms

- An interstitial site is a geometric position between normal atom sites.
- It can be empty in a perfect crystal.
- An interstitial defect exists when an extra atom occupies an interstitial configuration.

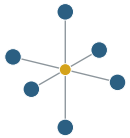


Tetrahedral and octahedral coordination

Four surrounding atoms



Six surrounding atoms



Gold marker

A possible interstitial position. The blue atoms show its local coordination.

Counting interstitial sites

Conventional cubic cell	Tetrahedral	Octahedral
FCC	8	4
BCC	12	6

Geometry versus energy

BCC sites are distorted. The largest geometric hole does not always give the lowest defect energy.

Self-interstitial atoms often form split configurations, such as dumbbells, after relaxation.

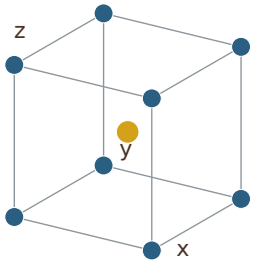
Density comes from one cell

$$\rho = \frac{nM}{N_A V_{\text{cell}}}$$

- ρ: mass density.
- n: atoms per cell; M: molar mass.
- N_A: Avogadro constant.
- V_{cell}: volume of that same cell.

Units

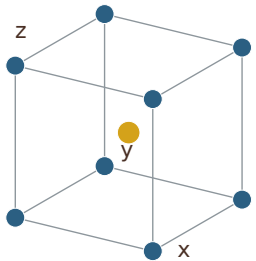
Use M in g/mol and V in cm^3 to obtain g/cm^3.



Worked example: density of BCC iron

Question

Use $n = 2$, $M = 55.85$ g/mol and $a = 2.87$ Å. Find the density.

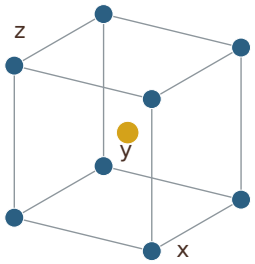


Worked example: density of BCC iron

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$$\rho = \frac{2(55.85)}{(6.022 \times 10^{23})(2.87 \times 10^{-8})^3}$$



Worked example: density of BCC iron

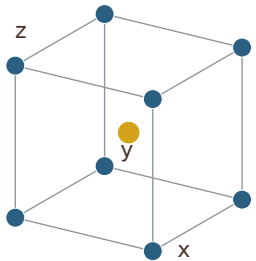
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$$\rho = \frac{2(55.85)}{(6.022 \times 10^{23})(2.87 \times 10^{-8})^3}$$

Answer

$\rho = 7.85$ g/cm^3 (rounded).



Four brackets, four meanings

Notation	Meaning	Example
$[uvw]$	One direction	$[110]$
$\langle uvw \rangle$	Symmetry-related directions	$\langle 110 \rangle$
(hkl)	Plane orientation / indexed planes	(111)
$\{hkl\}$	Symmetry-related plane orientations	$\{111\}$

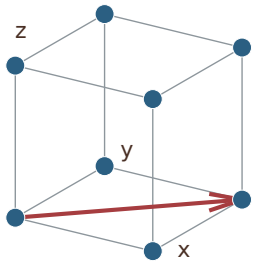
Negative index

A bar means negative: $[\bar{1}10]$ means $[-1, 1, 0]$.

A direction is an arrow in the crystal

- Subtract the start coordinates from the end coordinates.
- Express the displacement in cell-edge units.
- Clear fractions and reduce to the smallest integers.
- Write square brackets: $[uvw]$.

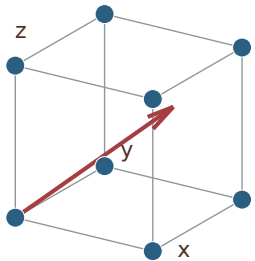
$$(0,0,0) \text{ to } (1,1,0) \quad \Rightarrow \quad [110]$$



Direction with fractional coordinates

Question

An arrow starts at the origin and ends at $(1/2, 1, 1/2)$ in cell units. What is its direction?



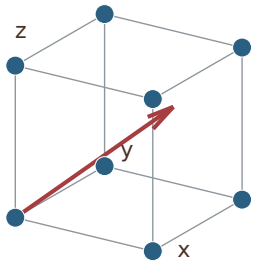
Direction with fractional coordinates

Question

An arrow starts at the origin and ends at $(1/2, 1, 1/2)$ in cell units. What is its direction?

Answer

Multiply by 2: [121].



Direction when the arrow starts elsewhere

Question

Start: $(1, 0, 0)$. End: $(0, 1, 0)$. What is the direction?

Direction when the arrow starts elsewhere

Question

Start: $(1, 0, 0)$. End: $(0, 1, 0)$. What is the direction?

$$\Delta = (0 - 1,\ 1 - 0,\ 0 - 0) = (-1, 1, 0)$$

Direction when the arrow starts elsewhere

Question

Start: $(1, 0, 0)$. End: $(0, 1, 0)$. What is the direction?

$$\Delta = (0 - 1,\ 1 - 0,\ 0 - 0) = (-1, 1, 0)$$

Answer

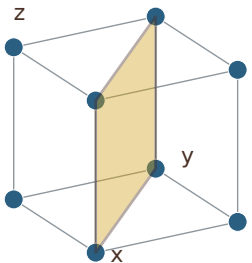
$[\bar{1}10]$. Reversing the arrow gives $[1\bar{1}0]$.

A plane is described by its intercepts

- Find intercepts in units of a, b, c.
- Take their reciprocals.
- Clear fractions to describe the orientation.
- Use parentheses: (hkl).

Parallel to an axis

An infinite intercept gives an index of zero.

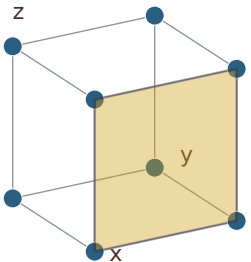


The (100) plane

intercepts: $(1, \infty, \infty)$

reciprocals: $(1, 0, 0)$

- It cuts the x axis at a.
- It is parallel to y and z.

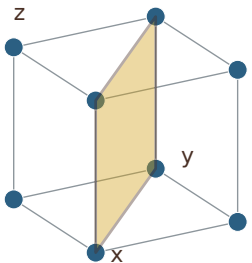


The (110) plane

intercepts: $(1, 1, \infty)$

reciprocals: $(1, 1, 0)$

- It cuts x and y.
- It remains parallel to z.

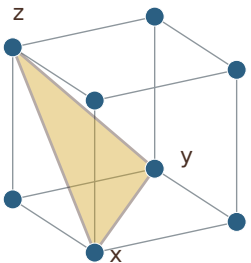


The (111) plane

intercepts: $(1, 1, 1)$

reciprocals: $(1, 1, 1)$

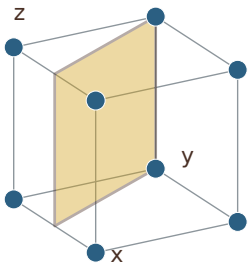
The triangular patch shows one part of an infinite plane.



Plane indexing: try the reciprocals

Question

A plane cuts x at $a/2$, cuts y at b, and is parallel to z. What are its indices?



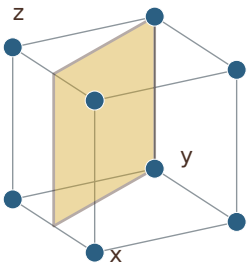
Plane indexing: try the reciprocals

Question

A plane cuts x at $a/2$, cuts y at b, and is parallel to z. What are its indices?

Answer

(210): reciprocals of $(1/2, 1, \infty)$ are $(2, 1, 0)$.

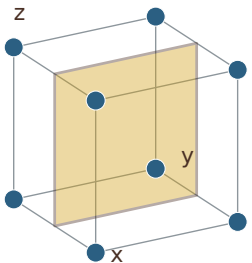


Parallel planes can have different spacing

- (100) and (200) have the same orientation.
- In a cubic crystal, $d_{100} = a$ and $d_{200} = a/2$.
- Keep the full indices when describing diffraction reflections.

If the plane passes through the origin

Use a parallel plane or move the origin before taking intercepts.



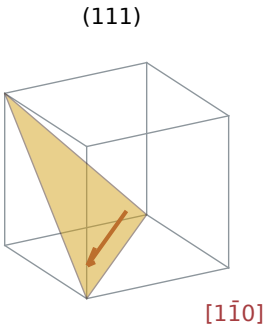
Plane normals and directions

- In cubic crystals, $[hkl]$ is normal to (hkl).
- A direction $[uvw]$ lies in (hkl) when $hu + kv + lw = 0$.

Example

$[1\bar{1}0]$ lies in (111) because $1 - 1 + 0 = 0$.

The same-index normal rule does not generally hold for noncubic crystals.



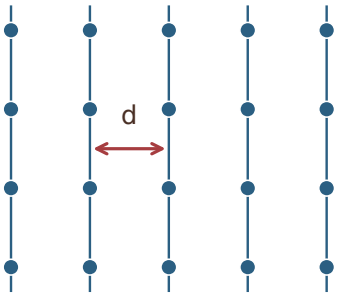
Spacing between cubic planes

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

- d_{hkl}: perpendicular distance between indexed planes.
- a: cubic lattice parameter.
- h, k, l: plane indices.

Examples

$d_{100} = a$, $d_{110} = a/\sqrt{2}$, $d_{111} = a/\sqrt{3}$.

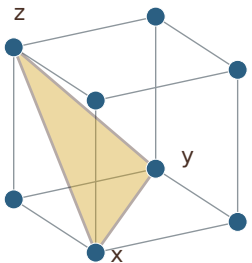


parallel planes

Plane spacing: a short calculation

Question

For a cubic crystal with $a = 0.360$ nm, find d_{111}.



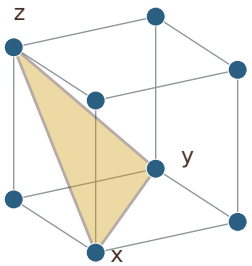
Plane spacing: a short calculation

Question

For a cubic crystal with $a = 0.360$ nm, find d_{111}.

Answer

$d_{111} = 0.360/\sqrt{3} = 0.208$ nm.



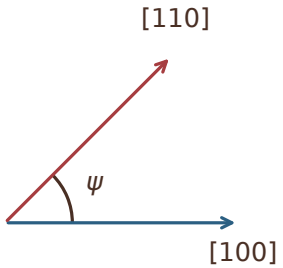
Angle between cubic planes

$$\cos\psi = \frac{h_1h_2 + k_1k_2 + l_1l_2}{\sqrt{h_1^2 + k_1^2 + l_1^2}\sqrt{h_2^2 + k_2^2 + l_2^2}}$$

- Calculate the angle between the plane normals.
- ψ: angle; the two index sets identify the planes.

Cubic example

Between (100) and (110): $\cos\psi = 1/\sqrt{2}$, so $\psi = 45°$.



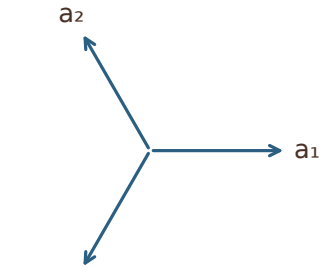
angle between normals

Hexagonal crystals use four-index notation

- Three basal axes, a_1, a_2, a_3, are 120° apart.
- The c axis is perpendicular to the basal plane.
- Planes: $(hkil)$, where $i = -(h + k)$.
- Directions: $[uvtw]$, where $t = -(u + v)$.

Common examples

Basal plane: (0001). c direction: [0001].

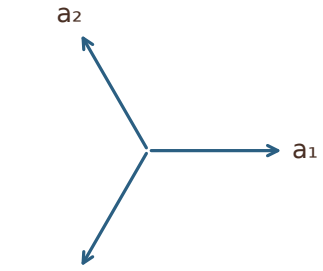


basal axes: 120° apart

Hexagonal notation: complete the index

Question

A plane is written $(10i0)$. What is i?



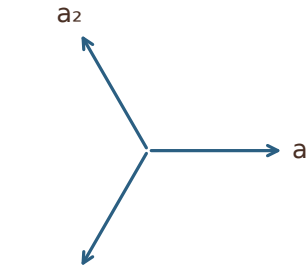
Hexagonal notation: complete the index

Question

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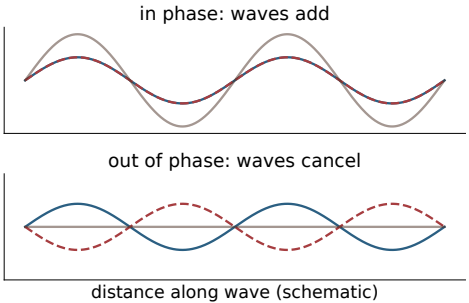
$i = -(1+0) = -1$. The plane is $(10\bar{1}0)$, a prismatic plane.



basal axes: 120° apart

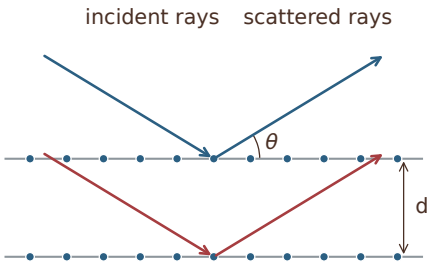
Diffraction begins with scattered waves

- Atoms scatter the incident X-rays.
- At some angles the scattered waves reinforce each other.
- At other angles their phases partly or fully cancel.



Bragg geometry compares two paths

- Consider rays scattered by adjacent parallel planes.
- d is the perpendicular plane spacing.
- θ is measured from the plane.
- The lower path has an extra distance $2d \sin\theta$.

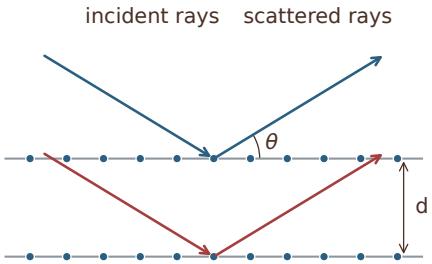


Bragg's law

$$n\lambda = 2d\sin\theta$$

Symbol	Meaning
n	Positive integer order
λ	X-ray wavelength
d	Plane spacing
θ	Bragg angle

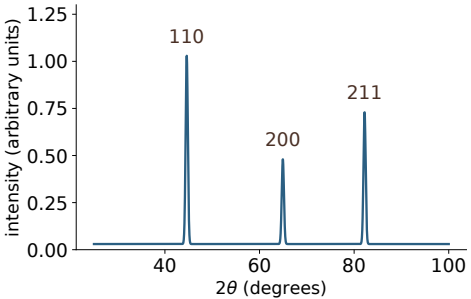
The extra path must equal a whole number of wavelengths.



What an XRD graph shows

- Horizontal axis: scattering angle 2θ in degrees.
- Vertical axis: detected intensity.
- Peak positions give plane spacings.
- Peak heights also depend on structure, texture and measurement conditions.

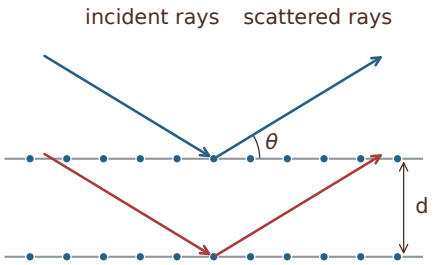
Calculated example: $a = 2.87$ Å, $\lambda = 1.5406$ Å. Heights and widths are illustrative.



The most common Bragg-law mistake

Question

A peak occurs at $2\theta = 44.67°$. Which angle belongs inside $\sin\theta$?



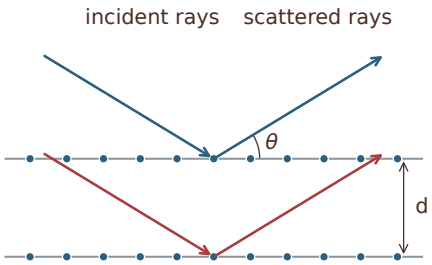
The most common Bragg-law mistake

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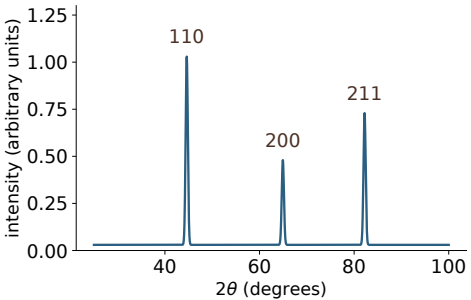
$\theta = 22.335°$. Halve the measured 2θ value.



Worked example: peak position to spacing

Question

Use $2\theta = 44.67°$, $\lambda = 1.5406$ Å and $n = 1$. Find d.

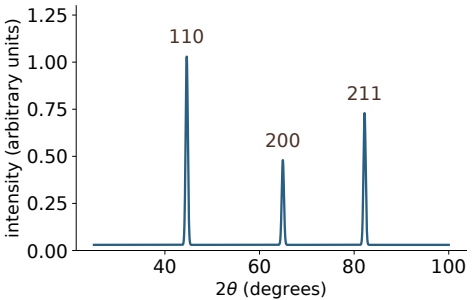


Worked example: peak position to spacing

Question

Use $2\theta = 44.67^\circ$, $\lambda = 1.5406$ Å and $n = 1$. Find d.

$$d = \frac{1.5406}{2\sin(22.335^\circ)} \text{ Å}$$



Worked example: peak position to spacing

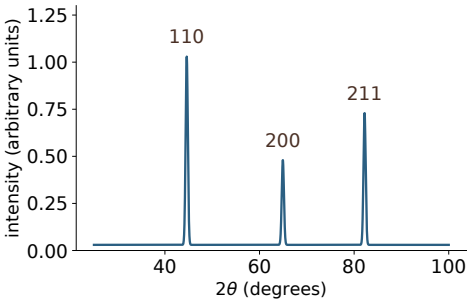
Question

Use $2\theta = 44.67^\circ$, $\lambda = 1.5406$ Å and $n = 1$. Find d.

$$d = \frac{1.5406}{2\sin(22.335^\circ)} \text{ Å}$$

Answer

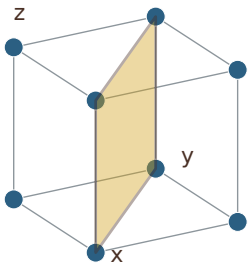
$d \approx 2.027$ Å.



Worked example: spacing to lattice parameter

Question

The peak is indexed as BCC (110). Use $d_{110} = 2.027$ Å to find a.

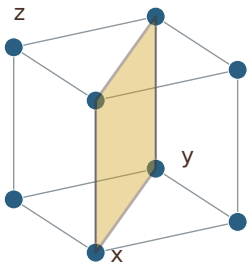


Worked example: spacing to lattice parameter

Question

The peak is indexed as BCC (110). Use $d_{110} = 2.027$ Å to find a.

$$d_{110} = \frac{a}{\sqrt{1^2 + 1^2 + 0^2}}$$



Worked example: spacing to lattice parameter

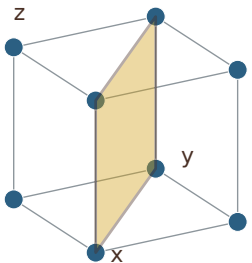
Question

The peak is indexed as BCC (110). Use $d_{110} = 2.027$ Å to find a.

$$d_{110} = \frac{a}{\sqrt{1^2 + 1^2 + 0^2}}$$

Answer

$a = d_{110}\sqrt{2} \approx 2.867$ Å.



Why some reflections are absent

$$F_{hkl} = \sum_j f_j \exp[2\pi i(hx_j + ky_j + lz_j)]$$

- F_{hkl}: net scattering amplitude from the cell.
- f_j: scattering factor of atom j.
- x_j, y_j, z_j: fractional coordinates.
- If the terms cancel, that reflection is absent.

Structure factor

The basis controls how waves from atoms inside a cell add.

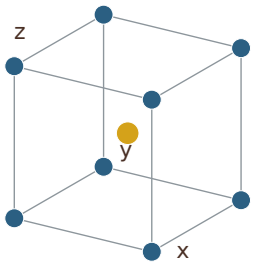
BCC: the two contributions can cancel

$$F_{hkl} = f\left[1 + (-1)^{h+k+l}\right]$$

- Assume identical atoms at corner and centre.
- Even $h + k + l$: terms add, so $F = 2f$.
- Odd $h + k + l$: terms cancel, so $F = 0$.

Allowed examples

(110), (200), (211). The (100) reflection is absent.



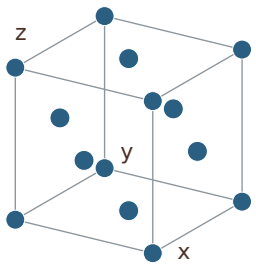
FCC: all even or all odd

- Add the corner and three independent face-site contributions.
- A reflection is allowed when h, k, l are all even or all odd.
- Mixed parity gives cancellation.

Examples

(111), (200), (220): allowed.
(100), (110): absent.

These rules describe the conventional FCC lattice. A multi-atom basis can add further absences.



Selection rules: compare BCC and FCC

Question

Which of (110), (111), (200) are allowed for elemental BCC and FCC?

Selection rules: compare BCC and FCC

Question

Which of (110), (111), (200) are allowed for elemental BCC and FCC?

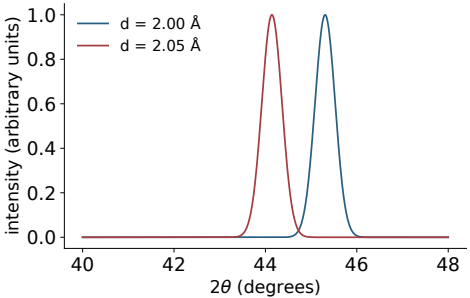
Answer

BCC: (110), (200).
FCC: (111), (200).

When the lattice expands, where does the peak move?

Question

Keep the wavelength fixed and increase d. Does 2θ increase or decrease?



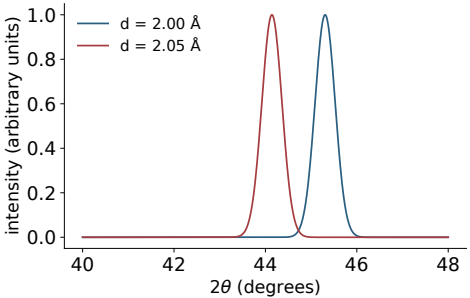
When the lattice expands, where does the peak move?

Question

Keep the wavelength fixed and increase d. Does 2θ increase or decrease?

Answer

It decreases. Larger d requires smaller $\sin\theta$ in $2d\sin\theta = \lambda$.

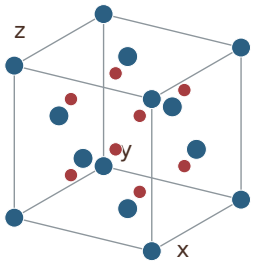


Ceramics require species and site occupancies

- Identify which sublattice each species occupies.
- Count each species separately.
- Check the chemical formula and charge balance.

Radius ratio

A hard-sphere geometric guide. Bonding and energy also determine the stable structure.

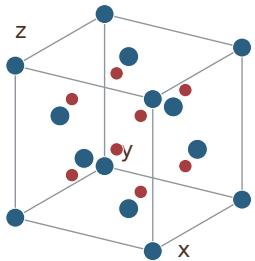


Fluorite: UO_2 as the example

- U atoms form an FCC sublattice.
- O atoms occupy all eight tetrahedral sites.
- The cubic cell contains 4 U and 8 O atoms.
- The ratio is 1 : 2, giving UO_2.

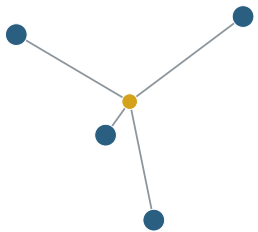
Colour key

Blue: uranium. Red: oxygen.



Fluorite has two coordination numbers

- Each uranium has eight oxygen neighbours.
- Each oxygen has four uranium neighbours.
- Here: O at the gold centre, U at the blue corners.



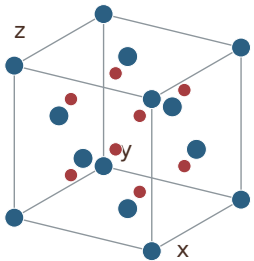
Consistency check

$4\ \mathrm{U} \times 8 = 8\ \mathrm{O} \times 4 = 32$ U–O neighbour pairs per cell.

UO_2: formula units in one cell

Question

The cell contains 4 U and 8 O atoms. How many UO_2 formula units are present?



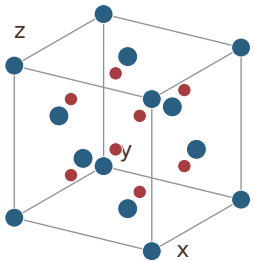
UO_2: formula units in one cell

Question

The cell contains 4 U and 8 O atoms. How many UO_2 formula units are present?

Answer

Four formula units. Use $4M_{UO_2}$ in the density numerator.

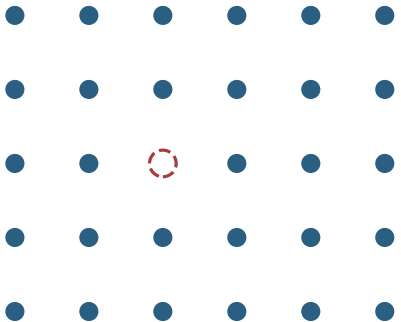


Nonstoichiometry changes defect populations

- UO_{2-x} has less oxygen than ideal UO_2.
- UO_{2+x} has more oxygen than ideal UO_2.
- Oxygen defects and uranium charge states adjust to maintain charge balance.

Simple starting picture

Oxygen deficiency can involve O vacancies. Oxygen excess can involve O interstitials and defect clusters.

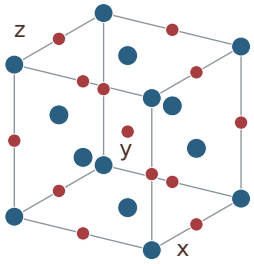


Rock salt: two interpenetrating FCC sublattices

- One species forms an FCC sublattice.
- The other occupies all octahedral sites.
- The conventional cell contains 4 + 4 atoms.
- Each species has six unlike nearest neighbours.

Examples

NaCl structure type. UC and UN have this structure.



Fluorite and rock salt: compare occupancies

Feature	Fluorite	Rock salt
Formula	MX_2	MX
Reference sublattice	FCC	FCC
Occupied sites of X	All tetrahedral	All octahedral
Species counts	4 M + 8 X	4 M + 4 X
Coordination of M / X	8 / 4	6 / 6

Question to ask

Which site occupancy changes the formula from MX to MX_2?

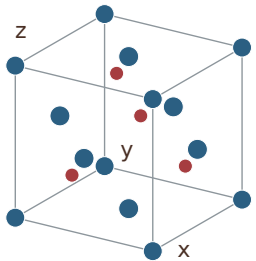
Other ceramic structure types

Structure	Arrangement / example
Antifluorite	M_2X; species roles reversed from fluorite; Li_2O
Zinc blende	Half the tetrahedral sites occupied; cubic SiC
Wurtzite	Hexagonal tetrahedral structure; a SiC polytype
Perovskite	ABX_3; e.g. $SrTiO_3$
Spinel	AB_2X_4; e.g. $MgAl_2O_4$

SiC has multiple polytypes. Its stacking sequence must be specified.

Zinc blende fills half the tetrahedral sites

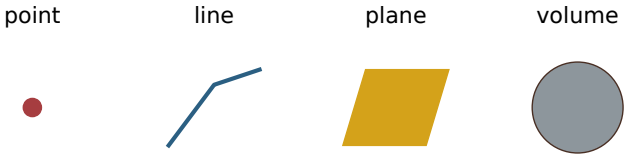
- Start with an FCC sublattice of one species.
- Occupy four of its eight tetrahedral positions with the second species.
- Both species have four unlike neighbours.



Compare with fluorite

Half occupation gives MX. Full occupation gives MX_2.

Real crystals contain defects



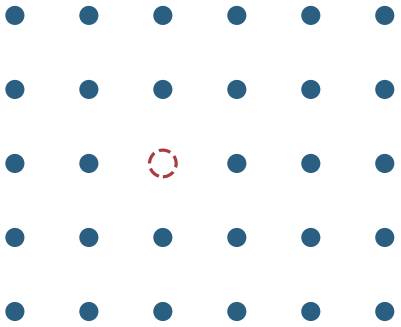
Dimension	Example
Point	Vacancy or interstitial
Line	Dislocation
Planar	Grain boundary or stacking fault
Volume	Void or precipitate

A vacancy is one missing atom

- The normal lattice site remains identifiable.
- Neighbouring atoms relax around the empty site.
- A vacancy can move when a neighbour jumps into it.

Drawing convention

A dashed circle marks the missing atom. It is not a separate particle.



Atom and vacancy move in opposite directions



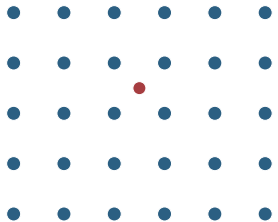
Each exchange

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

The same vacancy can move repeatedly through exchanges with different atoms.

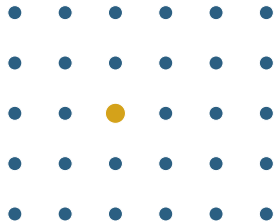
Interstitial and substitutional atoms

Interstitial



Extra atom between normal sites.

Substitutional



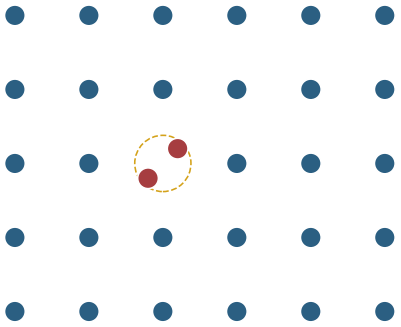
Different species on a normal site.

A self-interstitial can form a dumbbell

- Two atoms share the region around one normal lattice site.
- The nearby lattice relaxes.
- The preferred orientation depends on material and conditions.

BCC iron

A ⟨110⟩ dumbbell is a common example. Other BCC metals can favour different configurations.

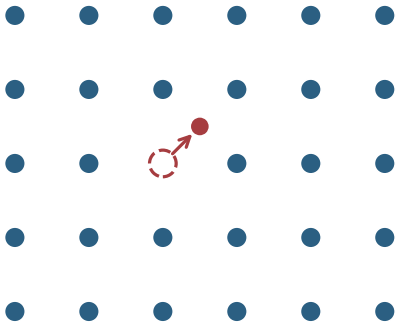


A Frenkel pair conserves atom count

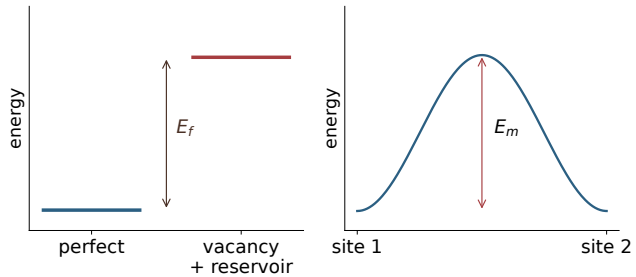
- An atom leaves a normal site.
- It becomes a self-interstitial.
- One vacancy and one interstitial remain.

Radiation connection

A sufficiently energetic collision can create this pair.



Formation energy and migration energy differ



Two separate questions

E_f: energy cost to create a defect, with atom bookkeeping specified.
E_m: barrier for an existing defect to make a jump.

Equilibrium vacancy fraction

$$C_v^{\text{eq}} \simeq \exp\left(\frac{S_f}{k_B}\right)\exp\left(-\frac{H_f}{k_B T}\right)$$

- $C_v^{\text{eq}} = N_v/N_s$: vacant sites / total sites.
- H_f, S_f: formation enthalpy and entropy.
- T: kelvin; k_B: Boltzmann constant.

Approximation

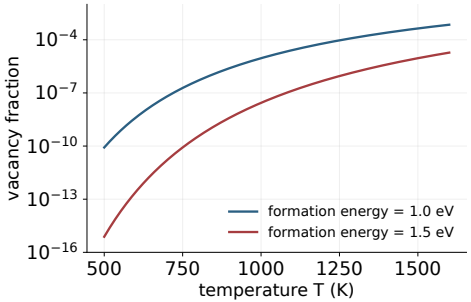
Ignore the entropy prefactor and use E_f for H_f: $C_v^{\text{eq}} \approx e^{-E_f/(k_B T)}$.

Heating increases the equilibrium vacancy fraction

- Horizontal axis: temperature in kelvin.
- Vertical axis: vacancy fraction on a log scale.
- Higher formation energy gives fewer vacancies at the same temperature.

Model shown

$C_v = \exp[-E_f/(k_B T)]$; entropy prefactor set to 1.



Worked example: one vacancy in how many sites?

Question

Use $E_f = 1.0$ eV, $T = 1000$ K and $k_B = 8.617 \times 10^{-5}$ eV/K.

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Answer

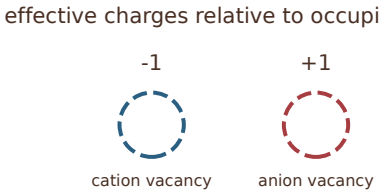
$C_v \approx 9.12 \times 10^{-6}$: about one vacancy per 1.10×10^{5} sites.

Schottky defects preserve the compound ratio

- Remove a stoichiometric set of ions from the interior to a reservoir such as the surface.
- The resulting vacancies preserve charge neutrality overall.

For a monovalent MX crystal

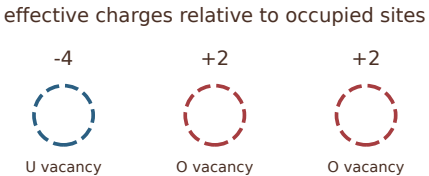
One cation vacancy and one anion vacancy form a neutral set.



Schottky bookkeeping in UO_2

Question

If one U^{4+} site is vacant, how many O^{2-} vacancies make a neutral Schottky set?



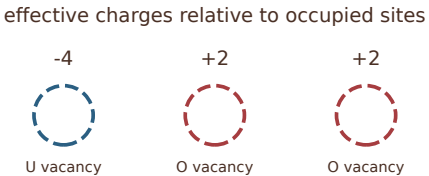
Schottky bookkeeping in UO_2

Question

If one U^{4+} site is vacant, how many O^{2-} vacancies make a neutral Schottky set?

Answer

Two. Effective vacancy charges: $-4 + 2(+2) = 0$. A Schottky set need not contain only two vacancies.

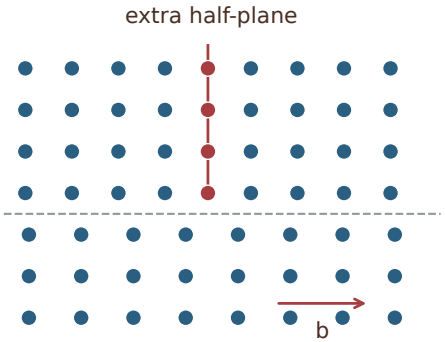


Dislocations allow slip one region at a time

- A dislocation is a line defect.
- Its motion advances the boundary between slipped and unslipped regions.
- Atoms rearrange locally as the line moves.

Why this matters

Plastic deformation can occur at much lower stress than shifting an entire perfect plane at once.

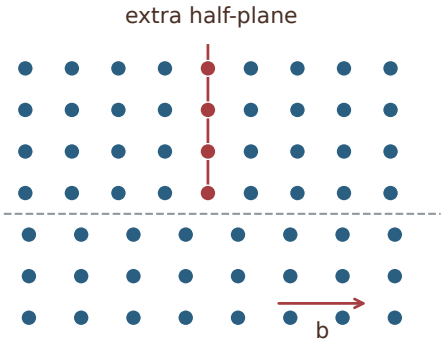


Edge dislocation: the extra half-plane ends

- The extra half-plane terminates inside the crystal.
- Its edge is the dislocation line.
- The view looks along that line.

$$\mathbf{b} \perp \boldsymbol{\xi}$$

b: Burgers vector; $\boldsymbol{\xi}$: line direction.

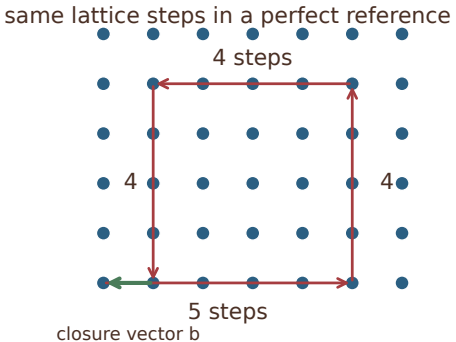


The Burgers vector measures closure failure

- Trace a closed path in lattice steps around the dislocation.
- Repeat the same steps in a perfect reference crystal.
- The reference path fails to close. Its closure vector gives the Burgers vector, with a stated sign convention.

Physical meaning

b gives the magnitude and direction of the lattice displacement carried by the dislocation.

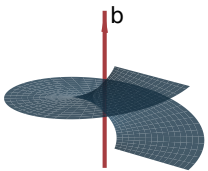


Screw dislocation: planes form a ramp

- A circuit around the line changes the height by one Burgers vector.
- The sketch shows the resulting helical ramp.

$$\mathbf{b} \parallel \boldsymbol{\xi}$$

Cross-slip can occur between allowed slip planes containing the screw segment.

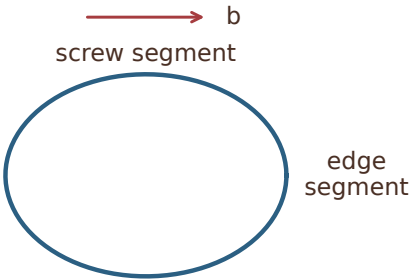


One dislocation can have mixed character

- The line direction changes along a curved dislocation.
- The Burgers vector stays constant along a line without a junction.
- Local character depends on the angle between **b** and the line.

On the drawn loop

Horizontal tangent: screw character.
Vertical tangent: edge character.



Common perfect-dislocation Burgers vectors

Structure	Vector family	Magnitude
BCC	$\frac{a}{2}\langle 111\rangle$	$a\sqrt{3}/2$
FCC	$\frac{a}{2}\langle 110\rangle$	$a/\sqrt{2}$
HCP a-type	$\frac{1}{3}\langle 11\bar{2}0\rangle$	a

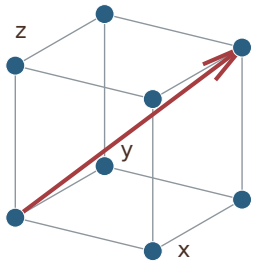
Magnitude and direction

The indices give direction. The prefactor gives the actual translation length. For HCP, the vector uses the hexagonal lattice basis.

Burgers-vector magnitude in BCC

Question

A BCC metal has $a = 0.287$ nm and $\mathbf{b} = (a/2)[111]$. Find $|\mathbf{b}|$.



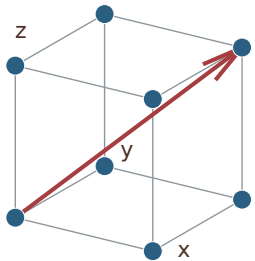
Burgers-vector magnitude in BCC

Question

A BCC metal has $a = 0.287$ nm and $\mathbf{b} = (a/2)[111]$. Find $|\mathbf{b}|$.

Answer

$|\mathbf{b}| = (0.287/2)\sqrt{3} = 0.249$ nm.

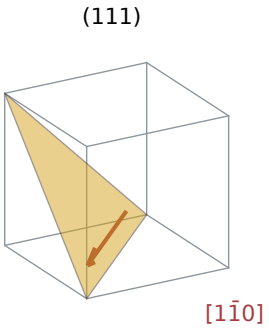


A slip system needs a plane and a direction

- The slip direction lies inside the slip plane.
- The Burgers vector is along the slip direction.
- FCC example: $(111)[1\bar{1}0]$.

Geometry check

$1(1) + 1(-1) + 1(0) = 0$, so this direction lies in the plane.



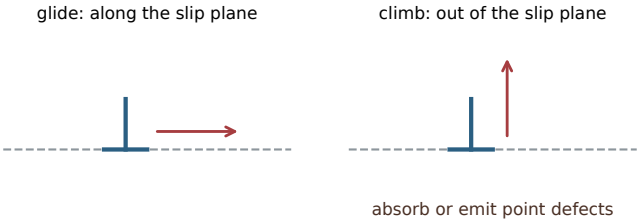
Slip systems: availability and ease are different

Structure	Common slip families	Slip behaviour
FCC	$\{111\}\langle 110\rangle$	12 geometric systems
BCC	$\{110\}, \{112\}, \{123\}\langle 111\rangle$	No close-packed plane
HCP	Basal, prismatic, pyramidal	Activation is material-dependent

Ductility

Count alone is insufficient. Mobility, resolved stress and temperature determine which systems operate.

Glide and climb move an edge dislocation differently



What enables motion

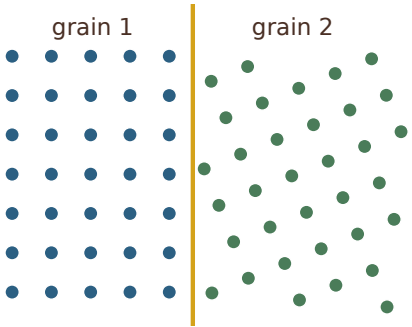
Glide advances slip within the slip plane. Climb changes the half-plane by absorbing or emitting point defects.

Grain boundaries separate different orientations

- Each grain has its own crystal orientation.
- The boundary joins the two atomic arrangements.
- Boundaries can block dislocations and absorb mobile point defects.

Radiation response

Their effect depends on boundary structure, stability and defect capture.

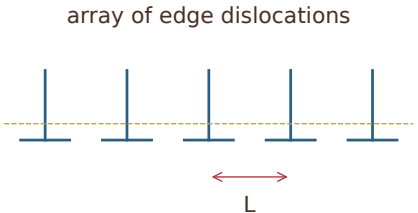


Low-angle boundaries can be dislocation arrays

$$\theta \approx \frac{b}{L} \qquad (\theta \text{ in radians})$$

- b: relevant Burgers-vector magnitude.
- L: spacing between dislocations.
- Closer dislocations give a larger small misorientation.

This relation describes a simple low-angle tilt boundary.

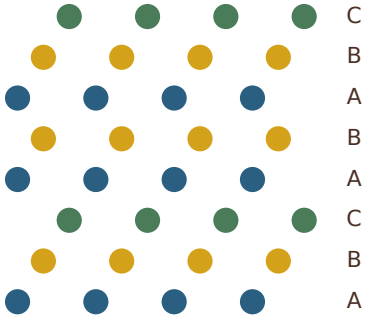


A stacking fault changes the layer sequence

- Perfect FCC stacking is ABCABC.
- A local interruption creates a planar fault.
- A fault can be bounded by partial dislocations.

Read from bottom to top

The drawn sequence is ABCABABC. The local ABAB segment differs from perfect FCC stacking.

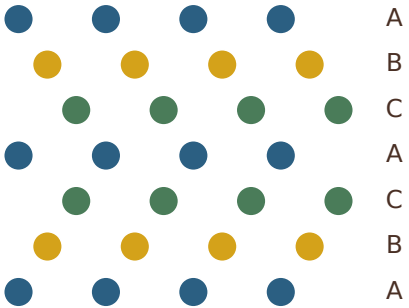


A twin reverses the stacking sequence

- The crystal orientations on either side are related by a twin operation.
- For the illustrated coherent FCC twin, the stacking reverses across the central plane.

Read from bottom to top

ABCACBA. The sequence mirrors around the central A layer.



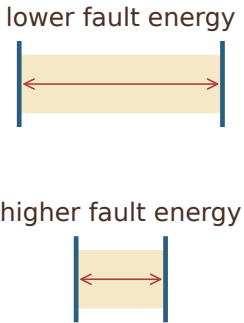
Stacking-fault energy affects partial separation

$$\gamma_{\mathrm{SF}} = \frac{\text{excess energy}}{\text{fault area}}$$

- Units: $\mathrm{J/m^2}$, often $\mathrm{mJ/m^2}$.
- Fault energy favours a narrower ribbon.
- Elastic repulsion between the partials favours separation.

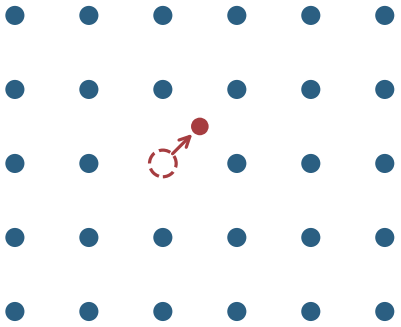
For otherwise comparable conditions

Lower fault energy generally gives wider partial separation.



Crystal structure sets the starting geometry

- It defines normal sites, possible defects and slip geometry.
- Radiation response also depends on defect energies and mobility.
- Sinks, solutes, temperature and irradiation conditions affect what survives.



Connection to Unit 3

Next: how energetic particles create defects and displacement cascades.

Closing check: three short explanations

Question

1. Why does one corner atom count as 1/8?
2. Why can an XRD reflection be absent?
3. How does a Frenkel pair change atom count?

Closing check: three short explanations

Question

1. Why does one corner atom count as 1/8?
2. Why can an XRD reflection be absent?
3. How does a Frenkel pair change atom count?

Answer

1. Eight cells share it.
2. Scattered waves cancel for that reflection.
3. Atom count is unchanged.

Practice after class

- For FCC with $r = 0.128$ nm, calculate a and APF.
- Index a plane with intercepts $(1, 2, \infty)$.
- Calculate d for $2\theta = 50°$, $\lambda = 1.5406$ Å.
- Estimate C_v for $E_f = 1.0$ eV at 1200 K.

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- Calculate d for $2\theta = 50°$, $\lambda = 1.5406$ Å.
- Estimate C_v for $E_f = 1.0$ eV at 1200 K.

Answers

$a = 0.362$ nm; APF $= 0.740$. Plane (210).
$d = 1.823$ Å. Vacancy fraction $\approx 6.31 \times 10^{-5}$.