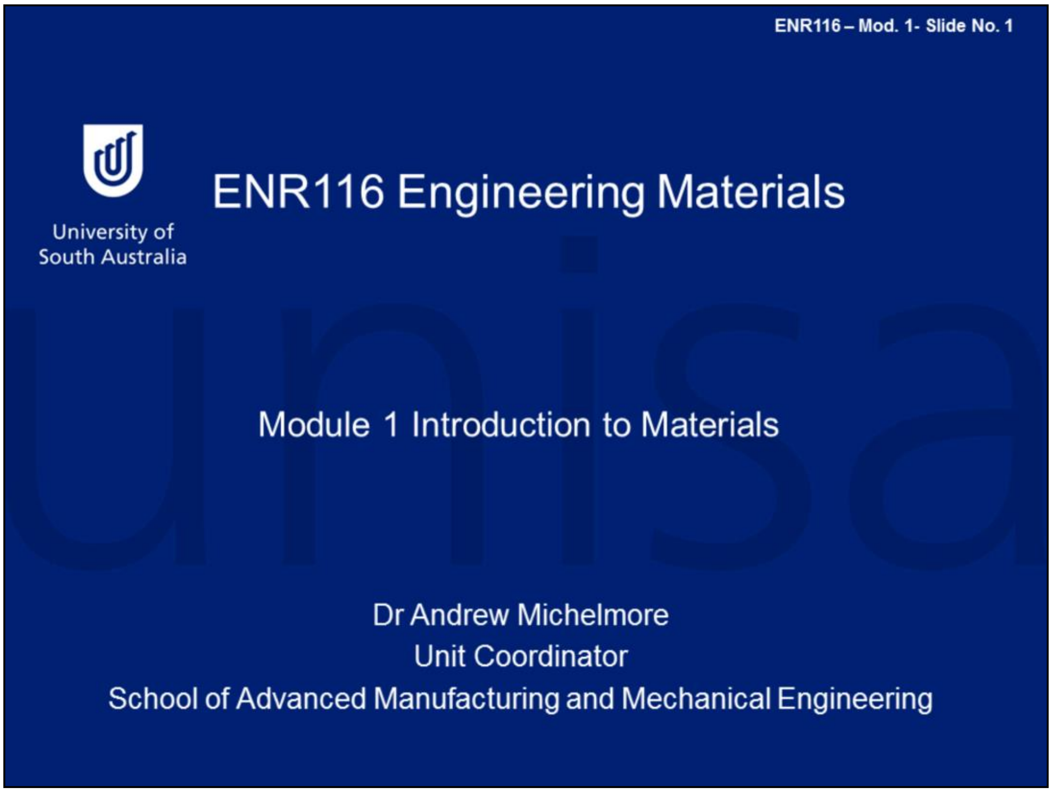

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ENR116 Engineering Materials

Module 1 Introduction to Materials

Dr Andrew Michelmore
Unit Coordinator
School of Advanced Manufacturing and Mechanical Engineering

Welcome to ENR116 Engineering Materials Module 1

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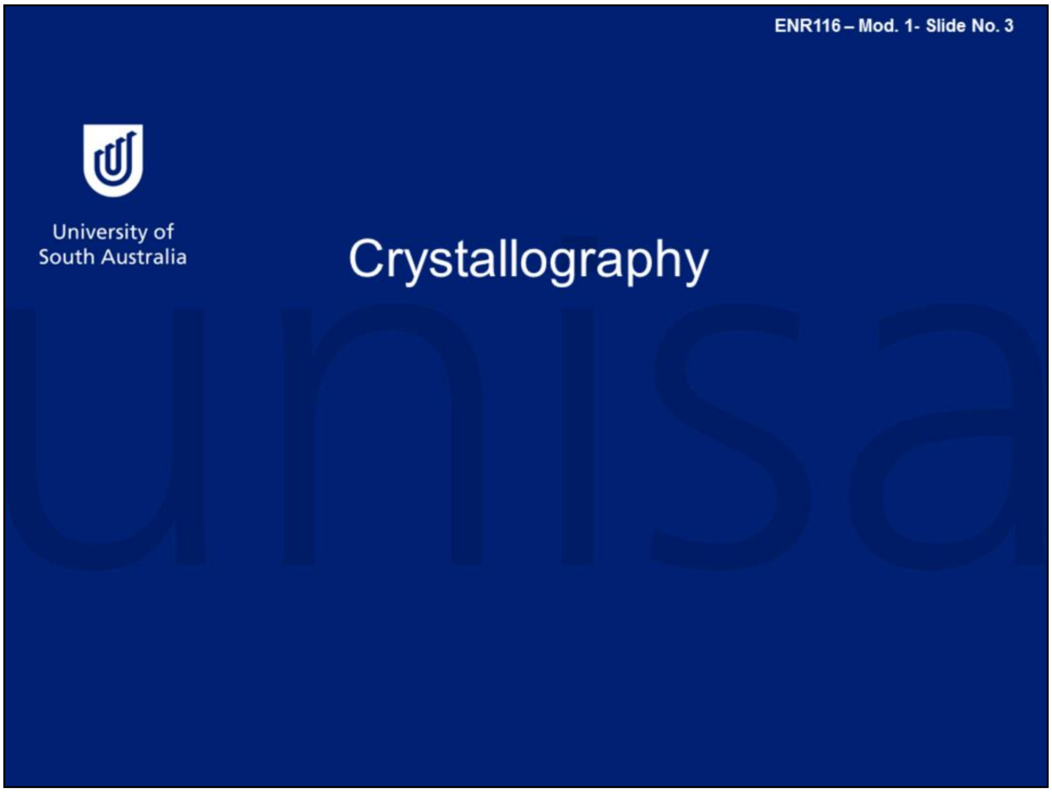

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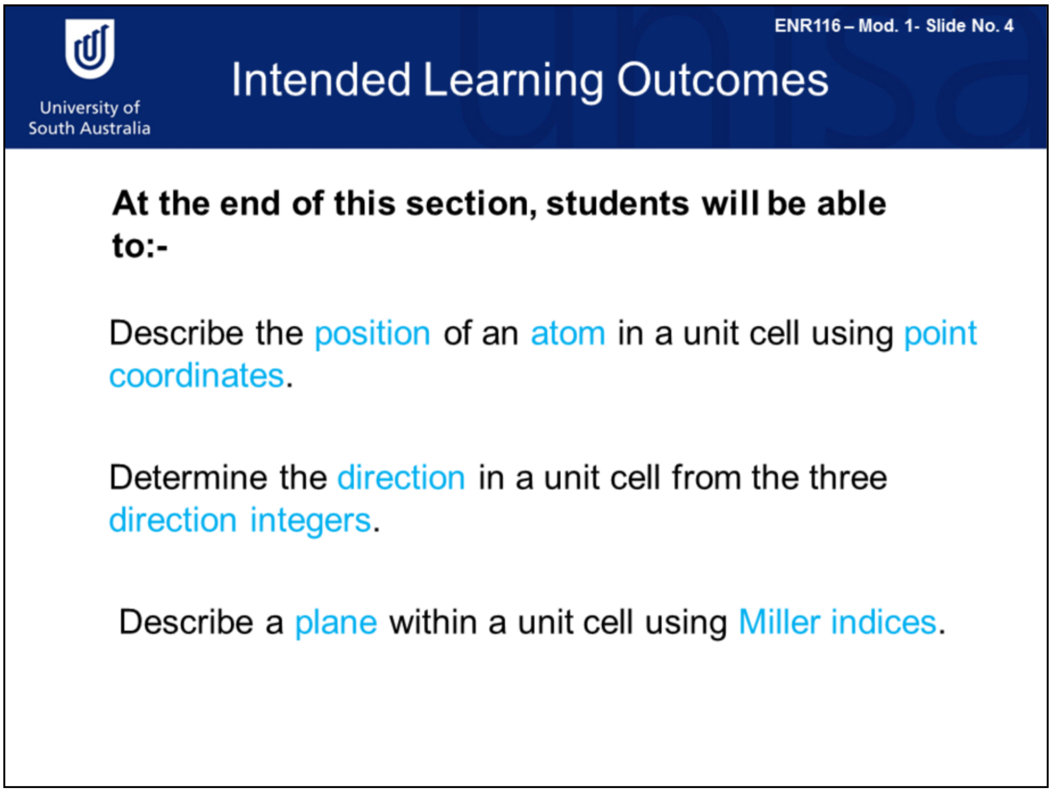
Crystallography

Crystallography



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Intended Learning Outcomes

At the end of this section, students will be able to:-

Describe the position of an atom in a unit cell using point coordinates.

Determine the direction in a unit cell from the three direction integers.

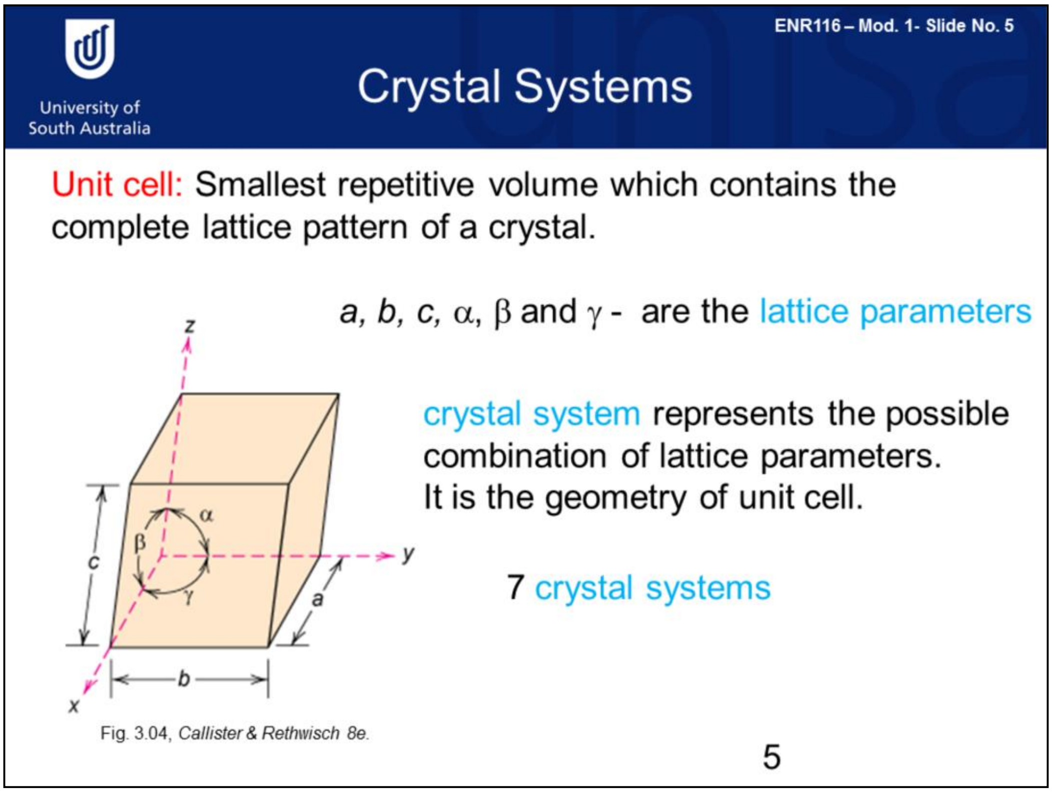
Describe a plane within a unit cell using Miller indices.

The intended learning outcomes from this lecture summary are that students will be able to:

Describe the position of an atom in a unit cell using point coordinates.

Determine the direction in a unit cell from the three direction integers.

Describe a plane within a unit cell using Miller indices.



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Crystal Systems

Unit cell: Smallest repetitive volume which contains the complete lattice pattern of a crystal.

a, b, c, α, β and γ - are the lattice parameters

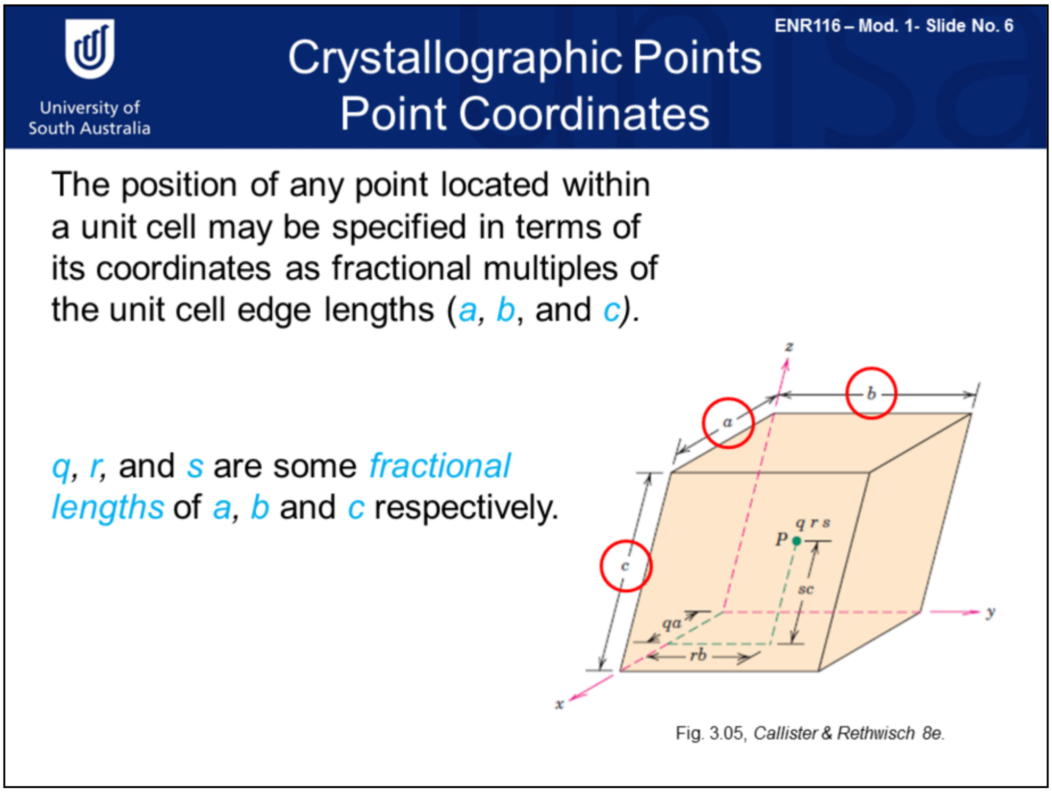
crystal system represents the possible combination of lattice parameters.
It is the geometry of unit cell.

7 crystal systems

Fig. 3.04, *Callister & Rethwisch 8e.*

5

Crystal systems. In the last lecture summary, we learnt that the unit cell is the smallest repetitive volume which contains the complete lattice pattern of a crystal. And we learnt that the lattice parameters are a, b and c for the edge lengths, and alpha, beta and gamma for the interaxial angles.
The crystal system therefore represents the possible combination of these lattice parameters, and defines the geometry of the unit cell.



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Crystallographic Points
Point Coordinates

The position of any point located within a unit cell may be specified in terms of its coordinates as fractional multiples of the unit cell edge lengths (*a*, *b*, and *c*).

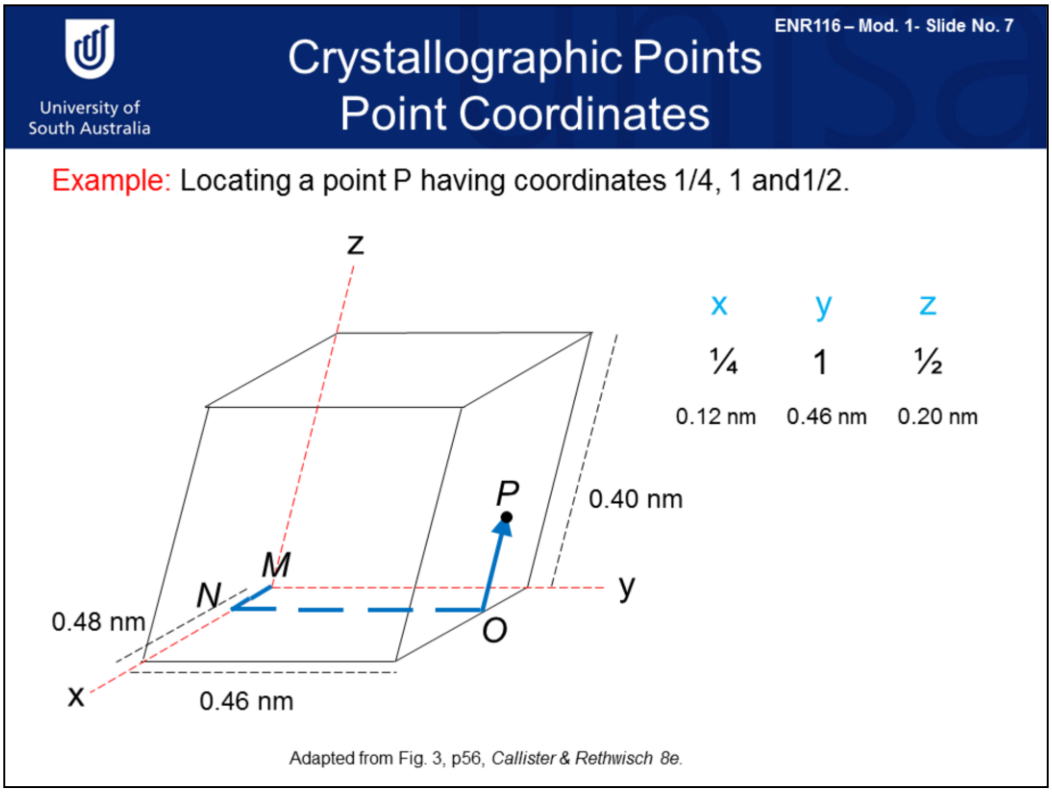
q, *r*, and *s* are some *fractional lengths* of *a*, *b* and *c* respectively.

Fig. 3.05, *Callister & Rethwisch 8e.*

Crystallographic points and point coordinates. The position of any point located within a unit cell may be specified in terms of its coordinates as fractional multiples of the unit cell edge lengths, *a, b*, and *c.*

For example, where q, r and s are some fractional lengths of a, b and c respectively.

q,r , and s are fractional lengths of the unit cell edge lengths a, b and c



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Crystallographic Points
Point Coordinates

Example: Locating a point P having coordinates 1/4, 1 and1/2.

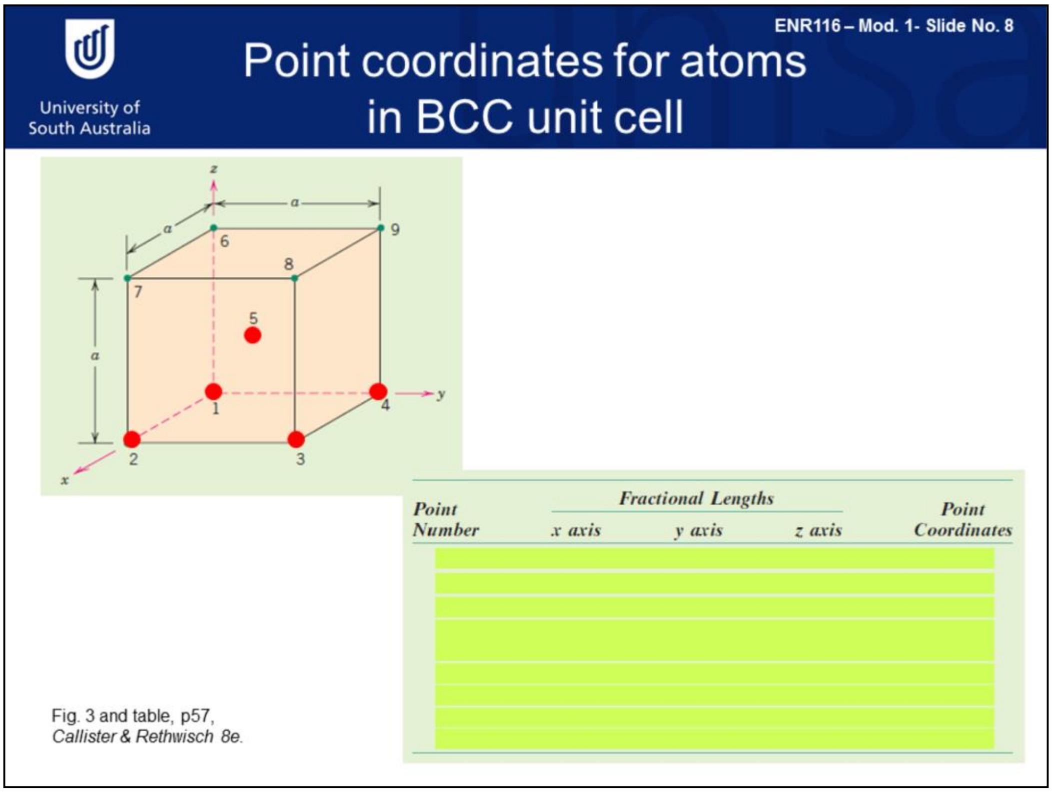
x	y	z
¼	1	½
0.12 nm	0.46 nm	0.20 nm

Adapted from Fig. 3, p56, *Callister & Rethwisch 8e.*

So lets do an example. Lets determine the position of point P, having coordinates ¼, 1 and ½ . How do we do this? We start at the centre of the coordinated system. We know that the fractional length in the x direction is a quarter of a, or 0.12nm. So we move from point M to point N in the x direction.

Then we know that the fractional length in the y direction is 1, or 0.46nm. So from point N we move 0.46nm in the y direction to point O.

Finally, we know that the fractional length in the z direction is 0.5, or 0.2nm, so we finally move from point O up in the z direction, 0.2nm to point P.



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Point coordinates for atoms in BCC unit cell

Point Number	Fractional Lengths			Point Coordinates
	x axis	y axis	z axis	

Fig. 3 and table, p57, *Callister & Rethwisch 8e.*

Understanding the point coordinate system for the unit is an important concept for the rest of this lecture summary. So lets do some more examples to make sure we understand it

We'll determine the coordinates for each atom in a body centred cubic system. For atom 1, we have coordinates of 000

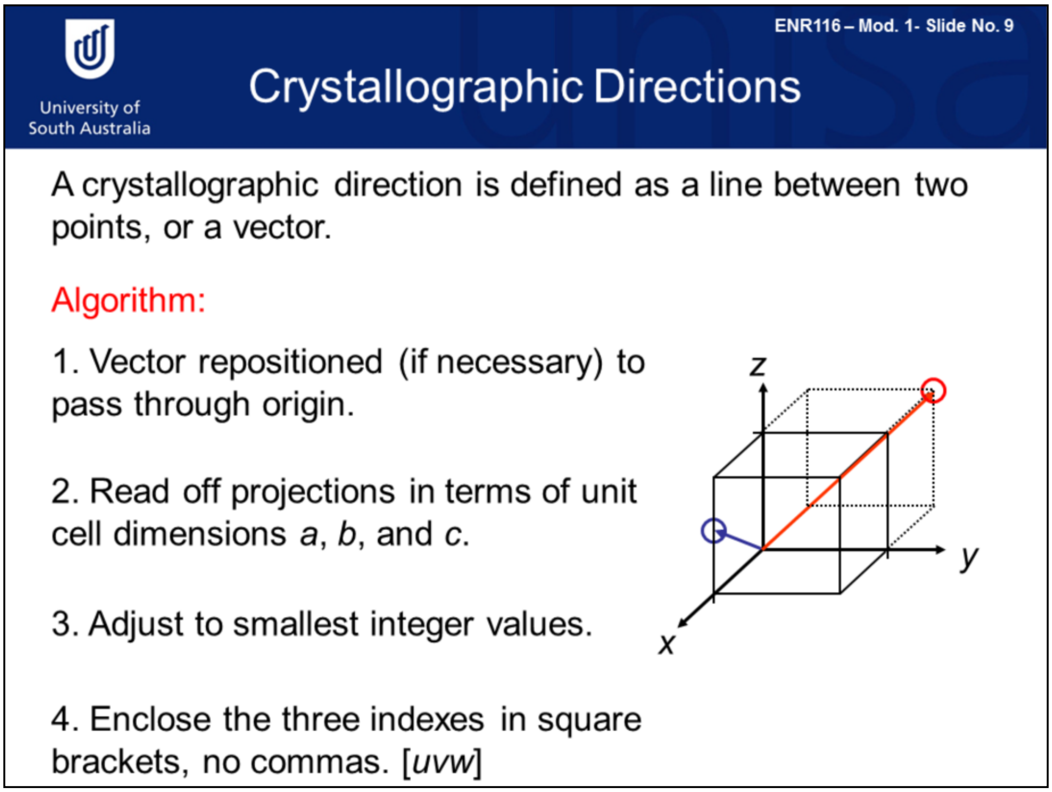
If we now look at atom 2, we have coordinates of 1 in the x direction, 0 in the y direction and 0 in the z direction.

Atom 3, we have 1 in the x direction, 1 in the y direction and 0 in the z direction.

For atom four we have 1 in the x direction, 0 in the y direction and 0 in the z direction

Now lets look at atom 5. Atom five we go a ½ in the x direction, a ½ in the y direction and a ½ in the z direction.

I'll let you go through points 6, 7,8 and 9, but it is important that you understand this before you move on. Please contact your tutor or place message in the content forum if you'd like some help.



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Crystallographic Directions

A crystallographic direction is defined as a line between two points, or a vector.

Algorithm:

1. Vector repositioned (if necessary) to pass through origin.

2. Read off projections in terms of unit cell dimensions *a*, *b*, and *c*.

3. Adjust to smallest integer values.

4. Enclose the three indexes in square brackets, no commas. [*uvw*]

Crystallographic directions. A crystallographic direction is defined as a line between two points, or a vector.

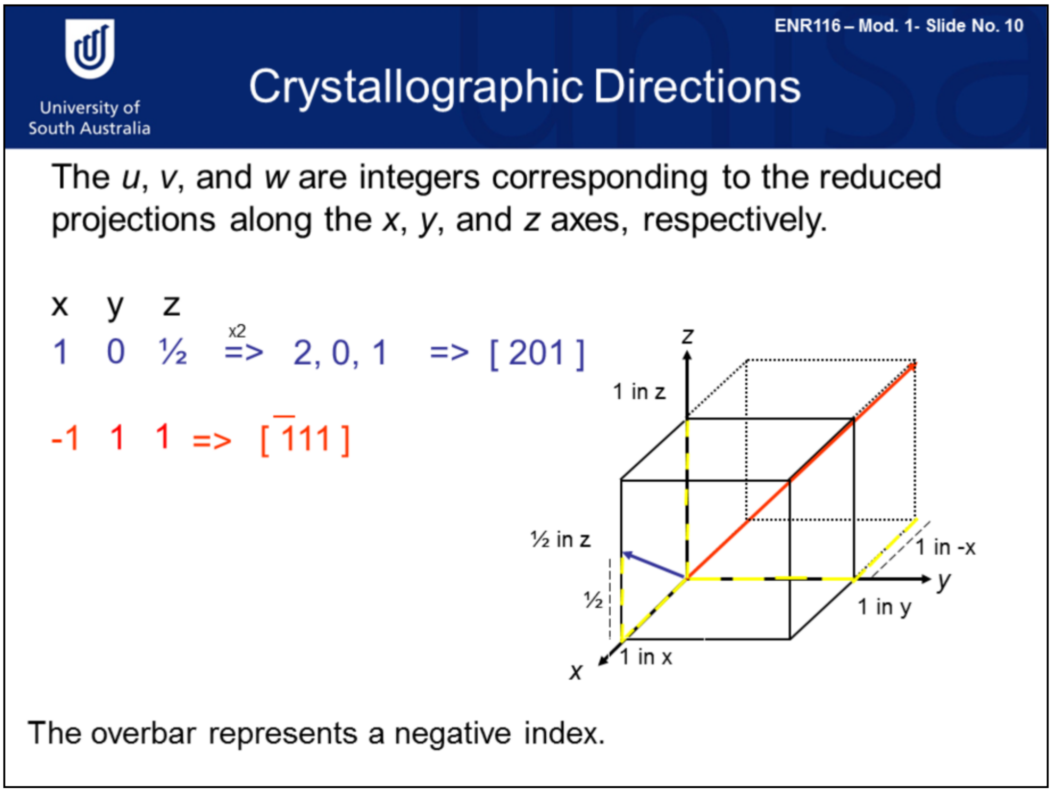
The algorithm for determining crystallographic directions is as follows:

First of all, reposition the vector such that it starts at the origin.

Secondly, read off the projections in terms of the unit cell dimensions a, b and c.

Thirdly, Adjust to the smallest integer values.

Finally, enclose the three indexes in square brackets, without commas.



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Crystallographic Directions

The *u*, *v*, and *w* are integers corresponding to the reduced projections along the *x*, *y*, and *z* axes, respectively.

x y z

1 0 ½ $\overset{x2}{=>}$ 2, 0, 1 => [201]

-1 1 1 => [$\bar{1}$11]

The overbar represents a negative index.

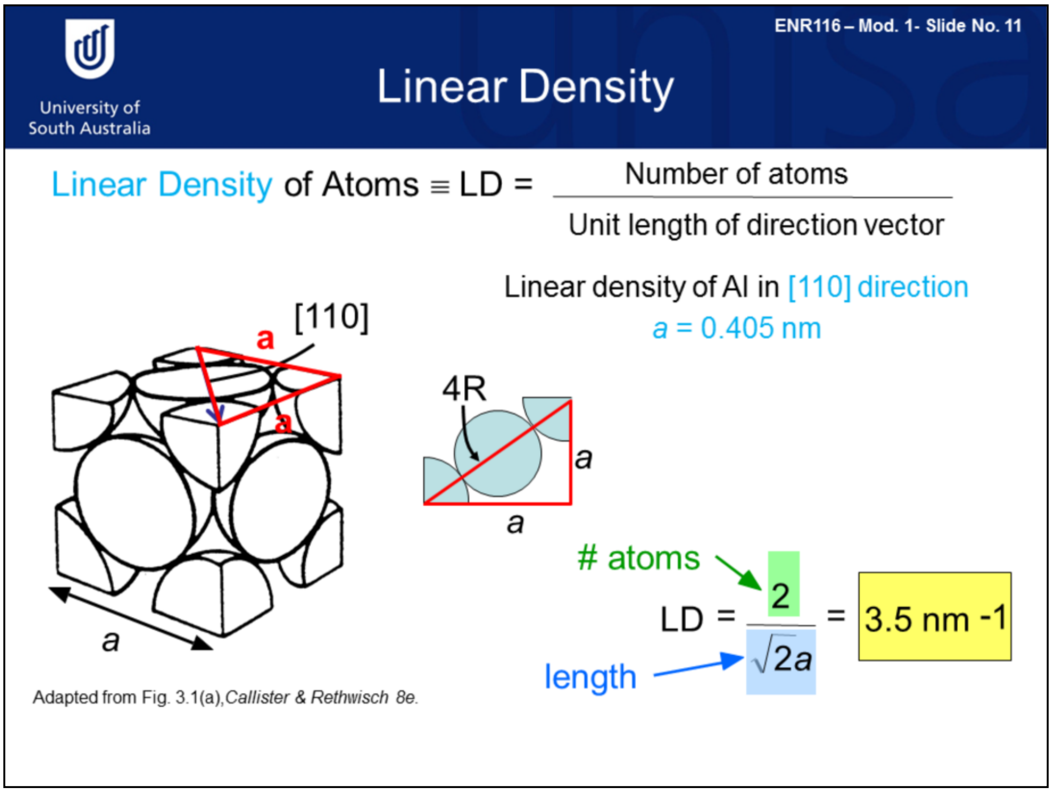
Lets go through some simple examples of crystallographic directions

U, v and w are integers corresponding to the reduced projections along the *x*, *y*, and *z* axes, respectively

Consider the vector shown here in blue. The projections are 1 in the x direction, 0 in the y direction and ½ in the z direction. Converting to integers we get 2, 0 and 1. And then finally, we enclose these numbers in brackets.

Now we'll look at this vector, shown in red. Here the projections are -1 in the x direction, 1 in the y direction and 1 in the z direction. These numbers are already integers, so we can just enclose these in brackets, with an overbar representing a negative value.

Note that, because of the symmetry of cubic crystals, it is possible to change the place and sign of the integers and have equivalent directions. Angle brackets are used to denote a *family* of directions which are equivalent due to symmetry operations.



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Linear Density

Linear Density of Atoms ≡ LD = $\frac{\text{Number of atoms}}{\text{Unit length of direction vector}}$

Linear density of Al in [110] direction

a = 0.405 nm

$$LD = \frac{2}{\sqrt{2}a} = \boxed{3.5\ \text{nm}^{-1}}$$

Adapted from Fig. 3.1(a), *Callister & Rethwisch 8e.*

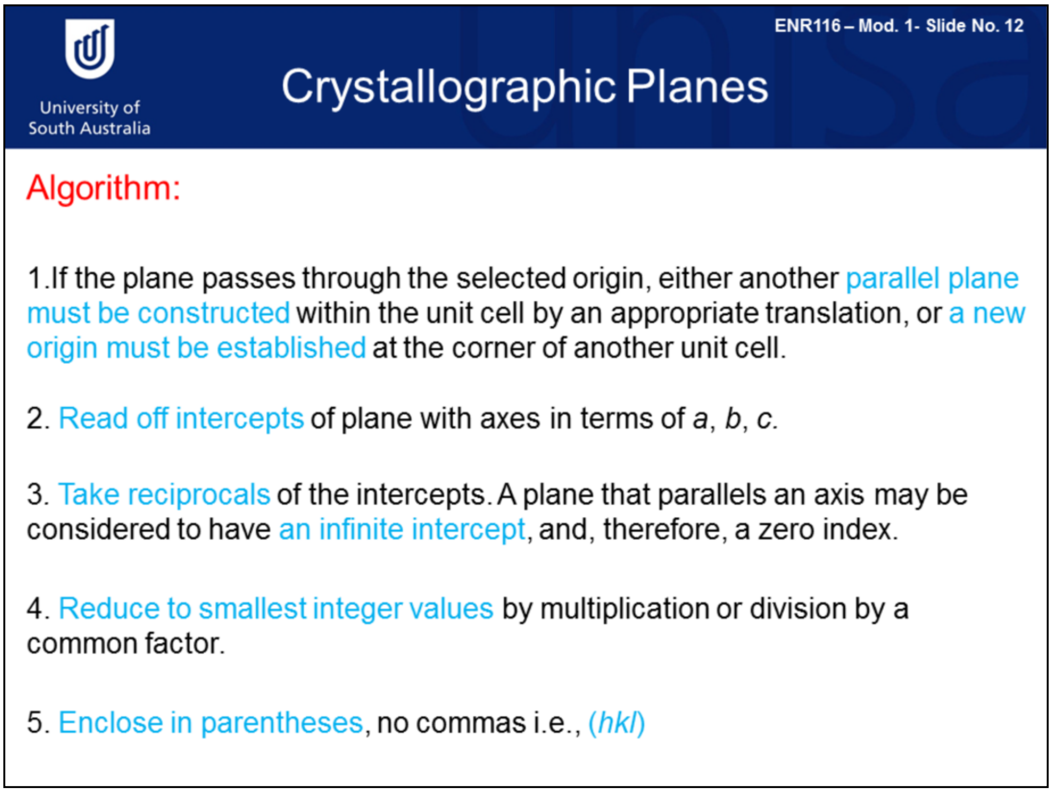
Now that we know about crystallographic directions, we can determine the linear density across a given direction in a crystal.

= number of atoms / unit length of vector. The linear density is given as the number of atoms along the direction of the vector, divided by the length of the vector.

In this example, we need to determine the linear density of aluminum in the [110] direction. We are given the unit cell edge length, a, as 0.405nm.

So to determine the linear density, we need to know the number of atoms in the direction of the vector. The number of atoms along the length of the direction in this case is 2.

We then divide by the length of the vector, which we can determine by Pythagoras theorem, as this direction forms a right angled triangle with two of the unit cell edge lengths. The length of the vector is root 2 a. When we work this out, we get 3.5 atoms per nm.



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Crystallographic Planes

Algorithm:

1.If the plane passes through the selected origin, either another parallel plane must be constructed within the unit cell by an appropriate translation, or a new origin must be established at the corner of another unit cell.

2. Read off intercepts of plane with axes in terms of *a*, *b*, *c*.

3. Take reciprocals of the intercepts. A plane that parallels an axis may be considered to have an infinite intercept, and, therefore, a zero index.

4. Reduce to smallest integer values by multiplication or division by a common factor.

5. Enclose in parentheses, no commas i.e., (*hkl*)

Now we can look at crystallographic planes.

The algorithm for constructing crystallographic planes is as follows:

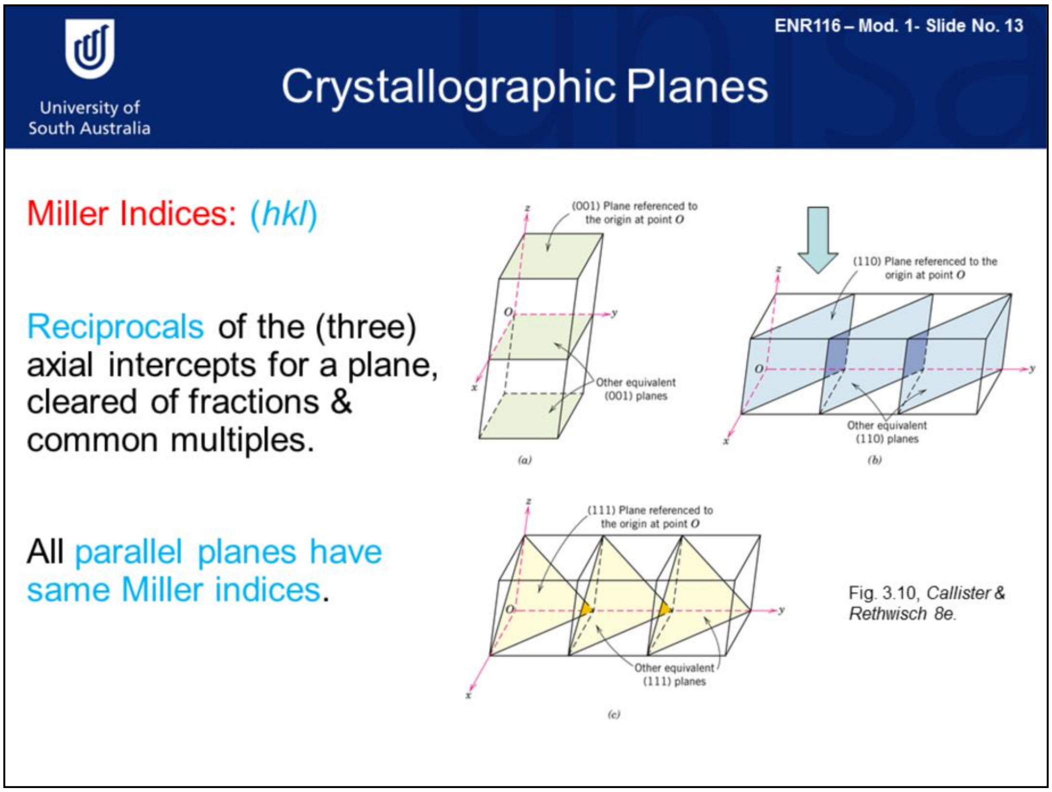
If the plane passes through the selected origin, either another parallel plane must be constructed within the unit cell by an appropriate translation, or a new origin must be established at the corner of another unit cell.

Read off intercepts of plane with axes in terms of *a*, *b*, *c.*

Take reciprocals of the intercepts. A plane that parallels an axis may be considered to have an infinite intercept, and, therefore, a zero index.

Reduce to smallest integer values by multiplication or division by a common factor.

Finally, enclose in parentheses without no commas



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Crystallographic Planes

Miller Indices: (*hkl*)

Reciprocals of the (three) axial intercepts for a plane, cleared of fractions & common multiples.

All parallel planes have same Miller indices.

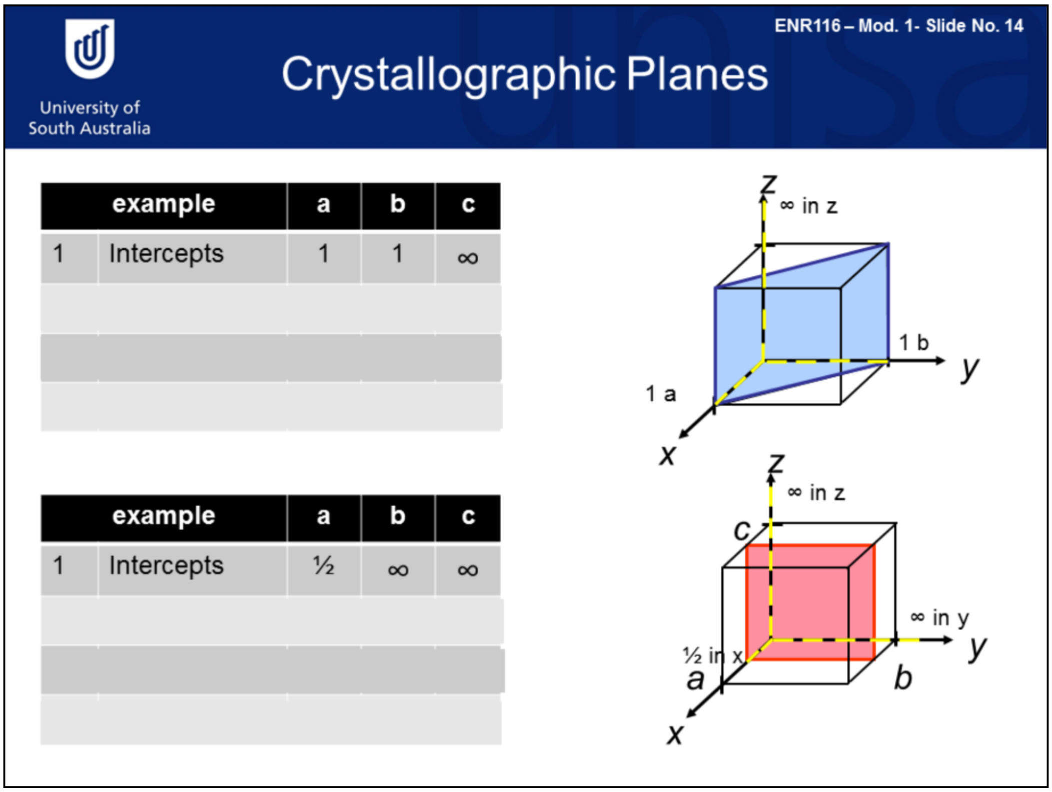
Fig. 3.10, *Callister & Rethwisch 8e.*

Crystallographic planes are described in in terms of their Miller Indices, given here as h k and l

Note that all parallel planes have the same Miller Indices

So, for example, all the blue planes here on the right are parallel, and therefore have the same Miller Indices, (110)

Parallel planes are equivolent



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Crystallographic Planes

example		a	b	c
1	Intercepts	1	1	∞

example		a	b	c
1	Intercepts	½	∞	∞

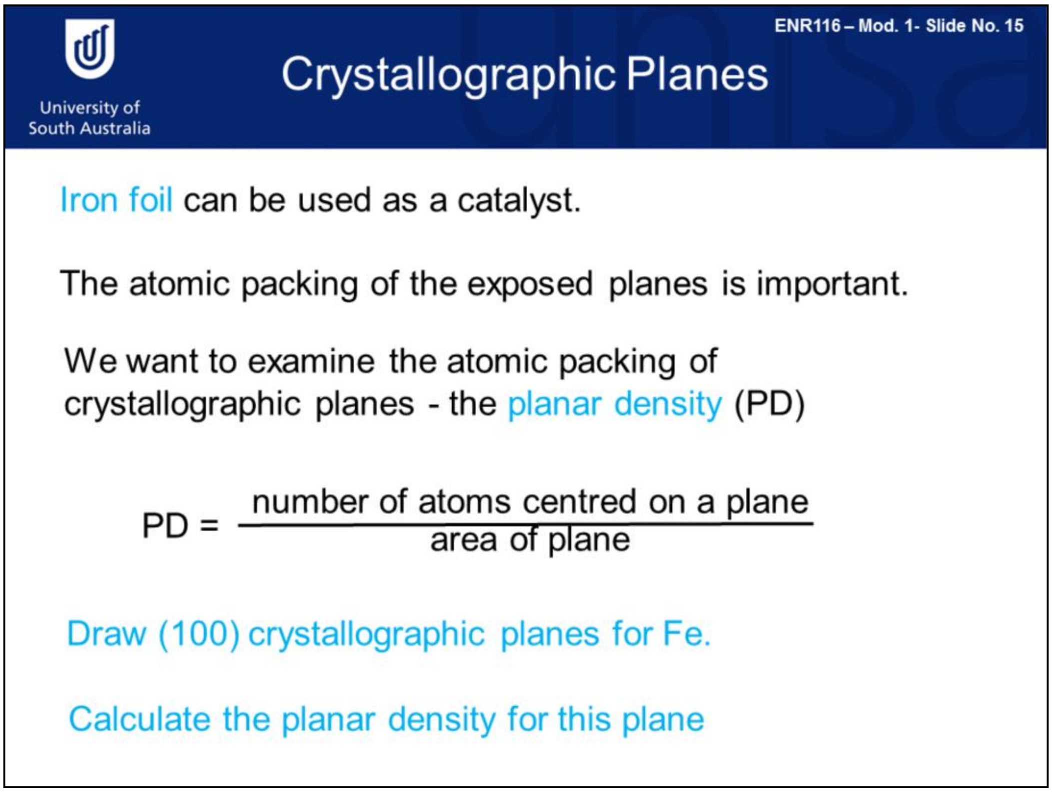
Lets do some simple examples of Miller Indices. First we'll look at the plane shown here in blue. Fist of all, we have to check that the plane does not pass through the origin, which it doesn't.

Secondly, we read off the intercepts in terms of a, b and c. The intercept in the x direction is 1. You can see the intercept in the y direction is also 1, and the plane runs parallel to the z axis, that is, there is no intercept in this direction, and that's denoted as infinite.

We then take the reciprocals of these values, giving us a reduction of 110, and the miller indices are therefore 110, in brackets.

Moving on to the second example, here in red. As before, it doesn't pass through the origin, so no translation is required. The x intercept is ½ . The plane runs parallel to the y axis, giving us infinity for that direction, and also parallel to z, giving us infinity there too.

Taking reciprocals, we get 2, 0 and 0 and as these are all integers, a reduction of 2 00. The miller plane is 200 in brackets.



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Crystallographic Planes

Iron foil can be used as a catalyst.

The atomic packing of the exposed planes is important.

We want to examine the atomic packing of crystallographic planes - the planar density (PD)

$$PD = \frac{\text{number of atoms centred on a plane}}{\text{area of plane}}$$

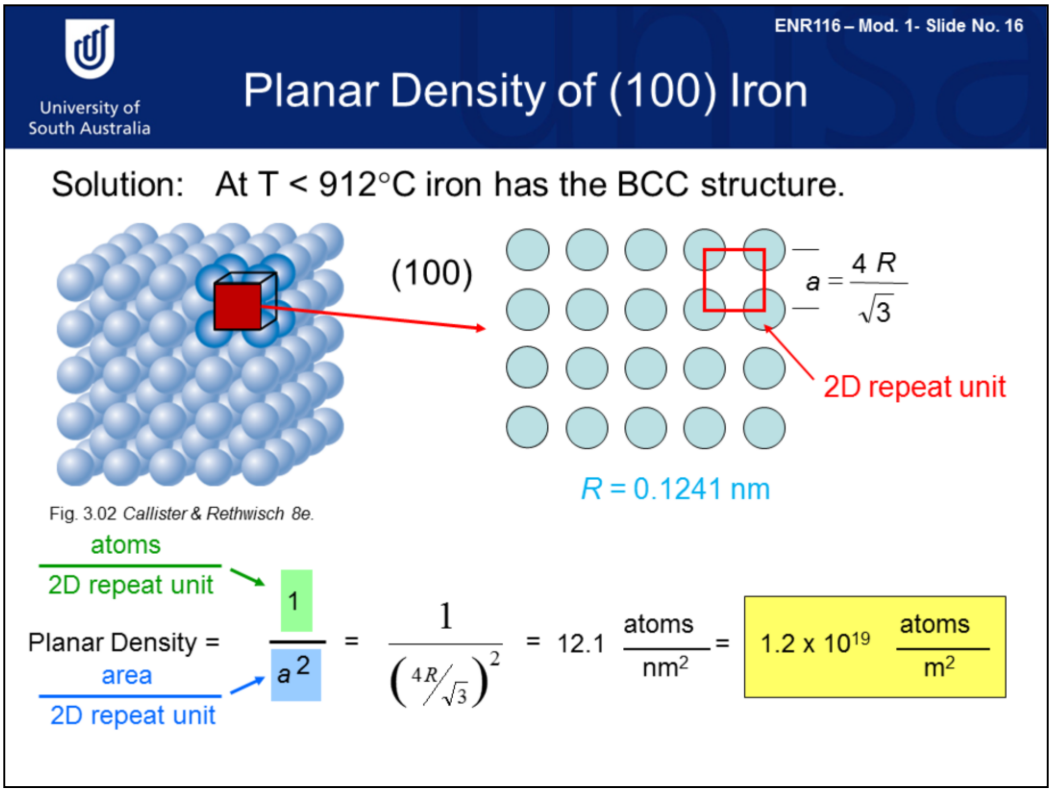
Draw (100) crystallographic planes for Fe.

Calculate the planar density for this plane

So lets go through an example of why crystallographic planes are of interest. Iron foil can be used as a catalyst and therefore the atomic packing of the exposed

planes is important. In this example, we want to examine the atomic packing for crystallographic planes, or the planar density. The planar density is given by the number of atoms centred on a plane, divided by the area of that plane.

To do this, we'll draw the (100) crystallographic plane for Fe, and then calculate the planar density for this plane.



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Planar Density of (100) Iron

Solution: At T < 912°C iron has the BCC structure.

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

$R = 0.1241$ nm

Fig. 3.02 *Callister & Rethwisch 8e.*

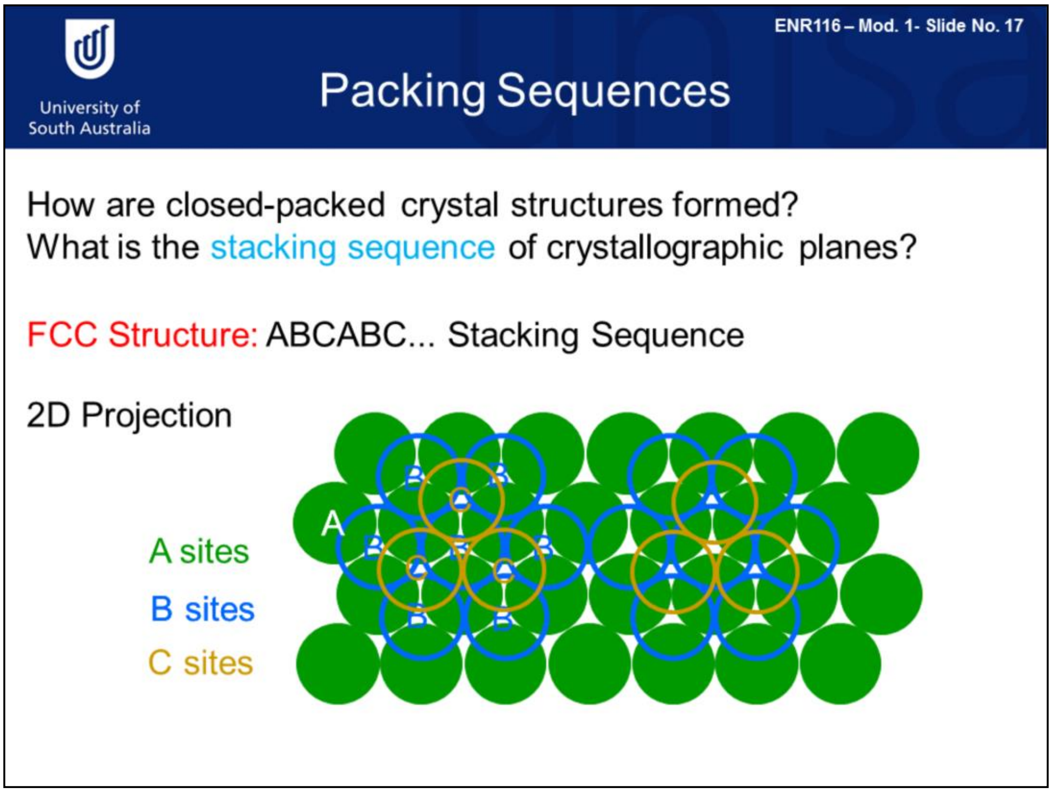
$$\text{Planar Density} = \frac{\dfrac{\text{atoms}}{\text{2D repeat unit}}}{\dfrac{\text{area}}{\text{2D repeat unit}}} = \frac{1}{a^2} = \frac{1}{\left(\frac{4R}{\sqrt{3}}\right)^2} = 12.1\ \frac{\text{atoms}}{\text{nm}^2} = \boxed{1.2 \times 10^{19}\ \frac{\text{atoms}}{\text{m}^2}}$$

The crystal structure of iron, when it's processed below 912C, is BCC.

The (100) plane is shown here in red. If we zoom in on this area, we get the structure shown here. From the body centred cubic structure, we have a – the length of the unit cell edge – as 4 x R divided by root 3 and we are given the radius of iron.

So to determine the planar density, we need the number of atoms in the 2D repeat unit. If you look at the illustration again, you will see that there are four quarter atoms within the red square, so the number of atoms centered of the plane is one. We then we divide this by the area of the repeat unit, which is given by a squared.

If we do this we get 12.1 atoms per nm squared, or 1.2 x 10 to the 19 atoms per metres squared.



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Packing Sequences

How are closed-packed crystal structures formed?
What is the stacking sequence of crystallographic planes?

FCC Structure: ABCABC... Stacking Sequence

2D Projection

A sites
B sites
C sites

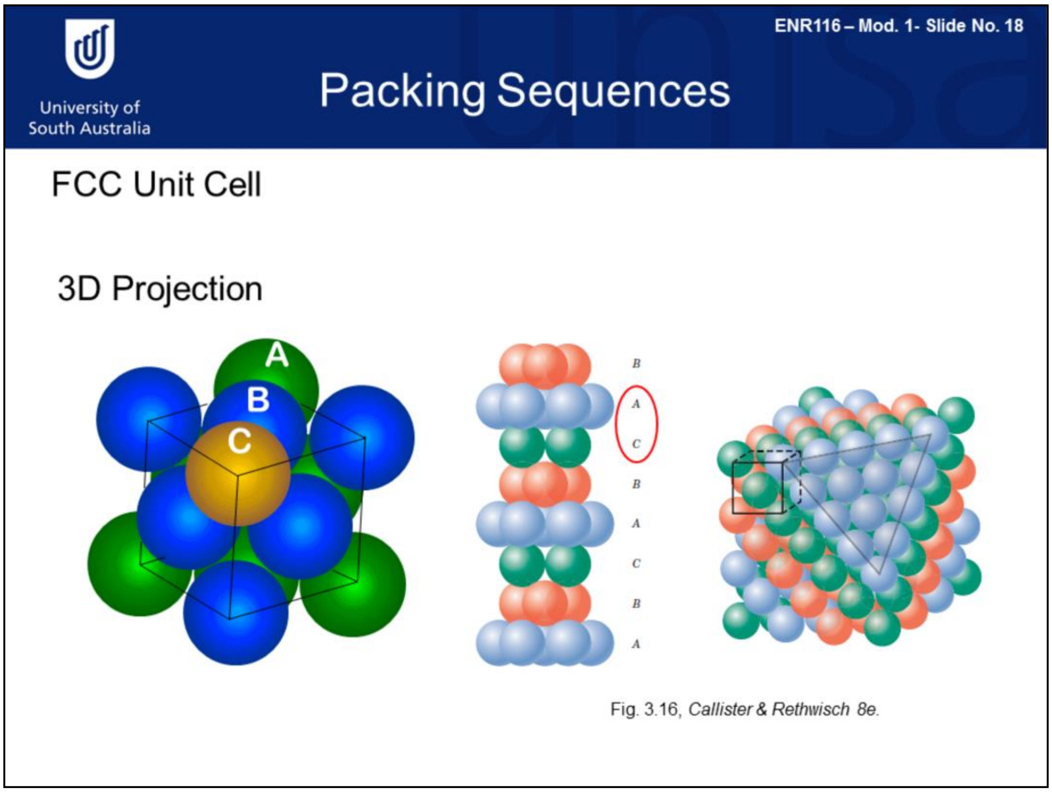
Packing sequences. How are closed-packed crystal structures formed? And what is the stacking sequence of crystallographic planes?

Remember that face centred cubic and hexagonal close packed structures have the highest atomic packing factors of 0.74.

For face centred cubic's crystal structure, the packing structure is ABC,ABC etc.

The second layer then sits with the atoms directly above these voids, as shown with plane B.

The important point for the face centred cubic structure is where the next layer, C, is located. This layer sits in voids which are not directly above plane A.



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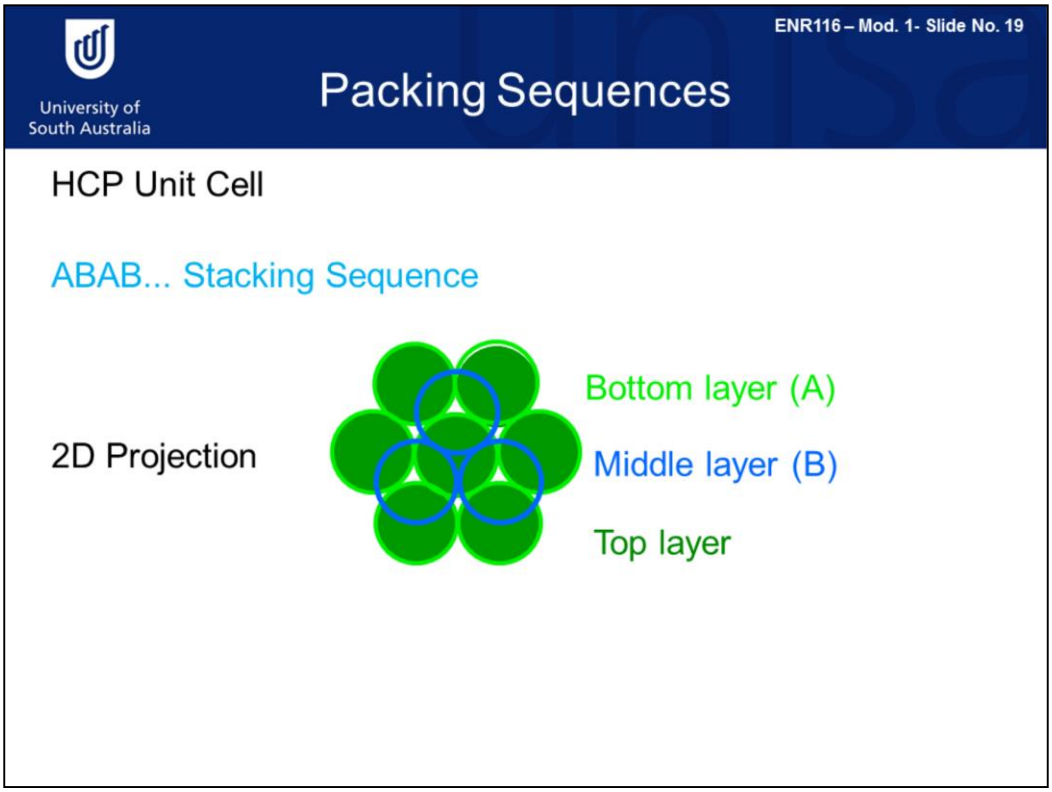
Packing Sequences

FCC Unit Cell

3D Projection

Fig. 3.16, *Callister & Rethwisch 8e.*

Here we can see some 3D projections of the face centred cubic crystal structure. Note in the central diagram that planes A and C are offset from each other.



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Packing Sequences

HCP Unit Cell

ABAB... Stacking Sequence

2D Projection

Bottom layer (A)

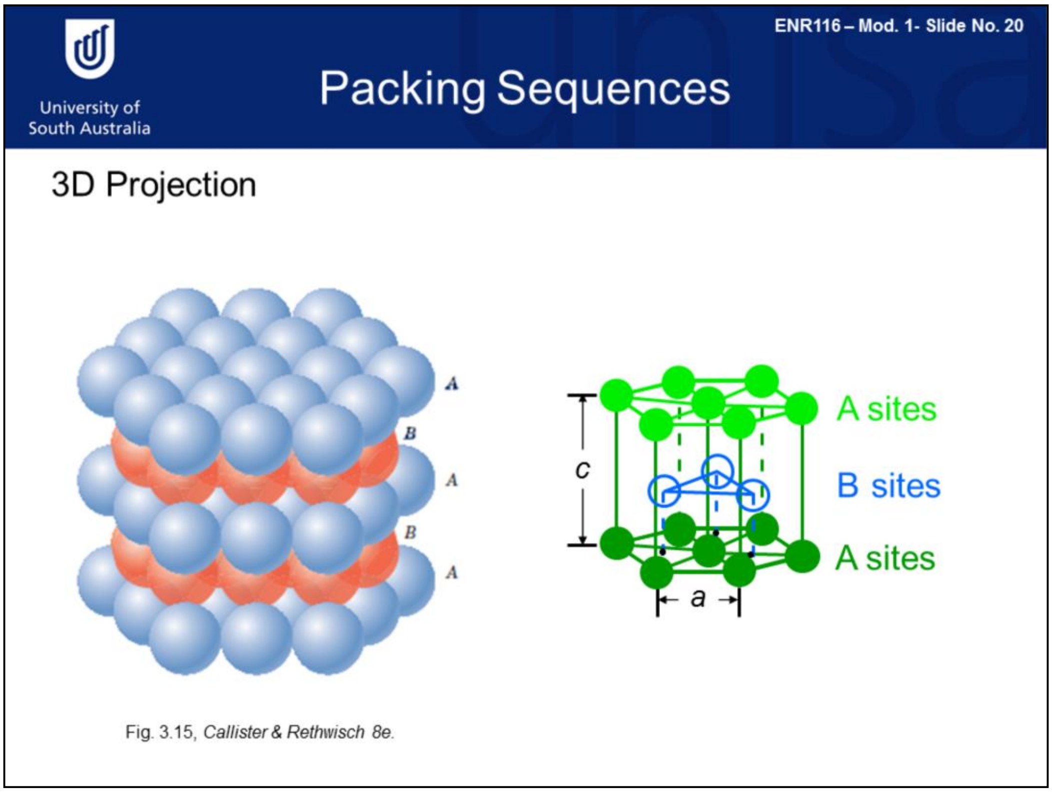
Middle layer (B)

Top layer

In the hexagonally close packed unit cell, we again have a close packed layer A, with a second layer B, sitting on top of the voids.

The difference here is that the top layer then sits directly above layer A, and therefore the stacking sequence is AB, AB etc.

Top and Bottom plane are the same



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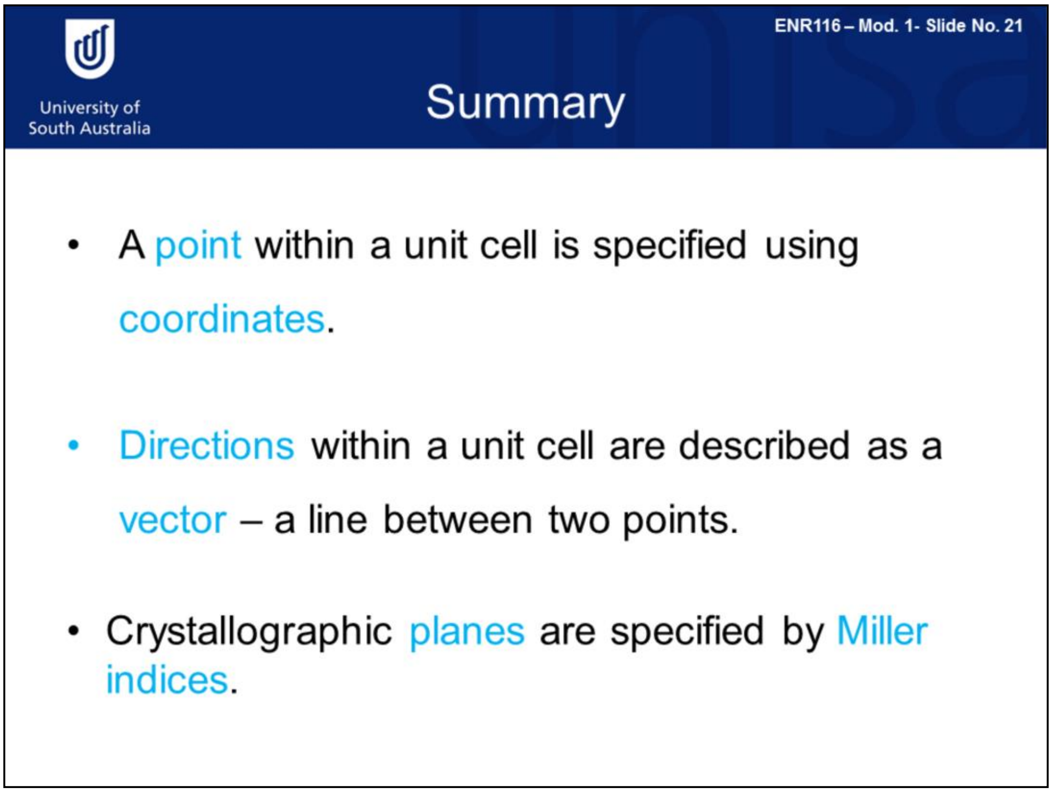
Packing Sequences

3D Projection

Fig. 3.15, *Callister & Rethwisch 8e.*

Here we can see a 3D projection of the hexagonally close packed structure, consisting of a top and bottom structure, which are the same, given as plane A, with three atoms between, given as plane B.



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Summary

- A point within a unit cell is specified using coordinates.
- Directions within a unit cell are described as a vector – a line between two points.
- Crystallographic planes are specified by Miller indices.

In summary,

A point within a unit cell is specified using coordinates.

Directions within a unit cell are described as a vector – a line between two points, and crystallographic planes are specified by Miller indices.

Points within unit cells are specified using coordinates

Directions within units are specified using vectors

Planes within unit cells are specified using Miller Indices

Thank you