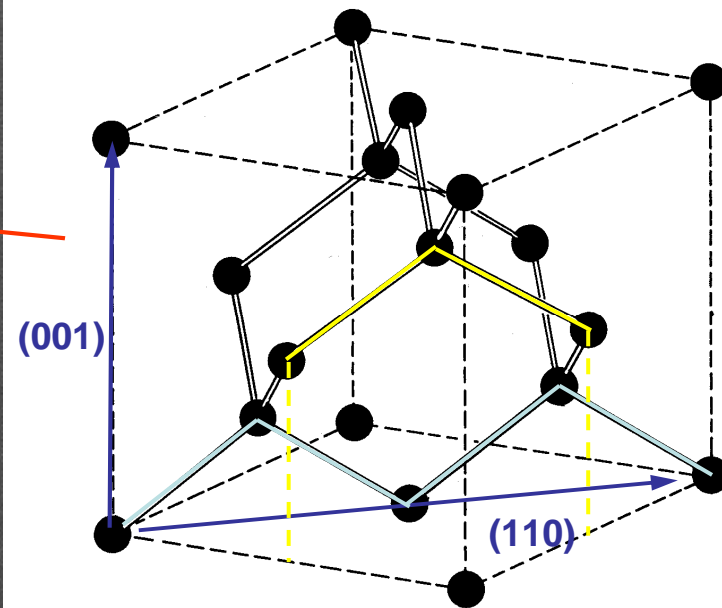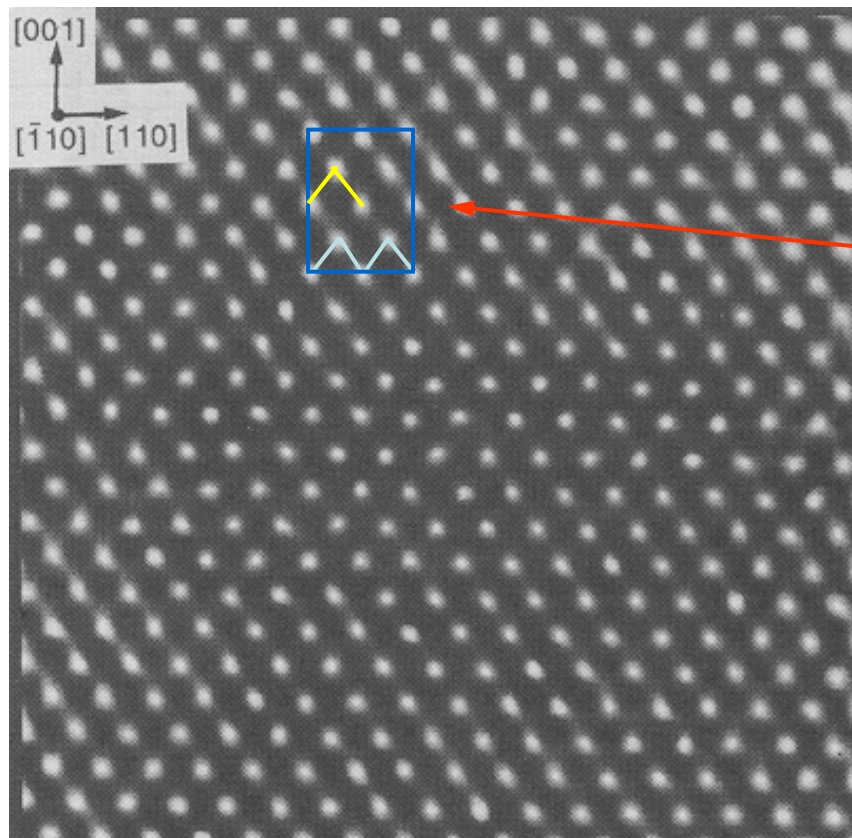# Crystal Directions, Wave Propagation and Miller Indices

D. K. Ferry, D. Vasileska and G. Klimeck

Crystal Directions; Wave Propagation

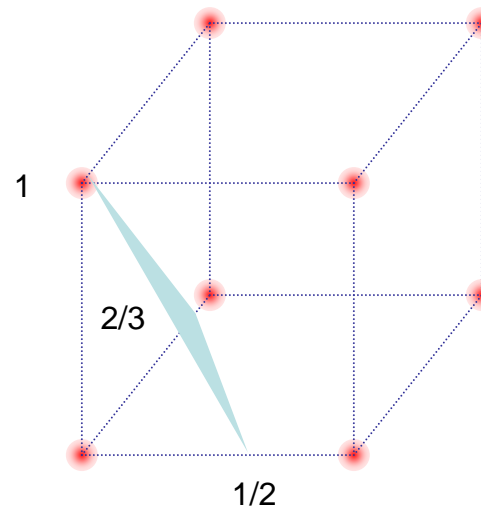**Electron beam generated pattern in TEM**

Crystal Directions

We have referred to various directions in the crystal as (100), (110), and (111). **What do these mean?**

How are these directions determined?

Consider a cube-

and a plane-

The plane has intercepts: $x = 0.5a$, $y = 0.667a$, $z = a$.

Crystal Directions

We want the NORMAL to the surface. So we take these intercepts (in units of *a*), and invert them:

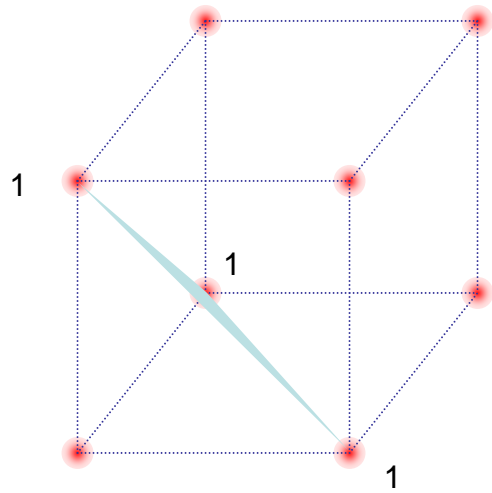$$\left(\frac{1}{2},\frac{2}{3},1\right) \Rightarrow \left(2,\frac{3}{2},1\right)$$

Then we take the lowest common set of integers:

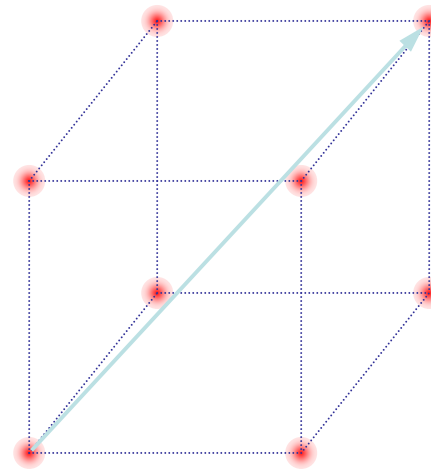$$\left(\frac{1}{2},\frac{2}{3},1\right) \Rightarrow \left(2,\frac{3}{2},1\right) \Rightarrow (4,3,2)$$

These are the MILLER INDICES of the plane.

The NORMAL to the plane is the (4,3,2) direction, which is normally written just (432). (A negative number is indicated by a bar over the top of the number.)

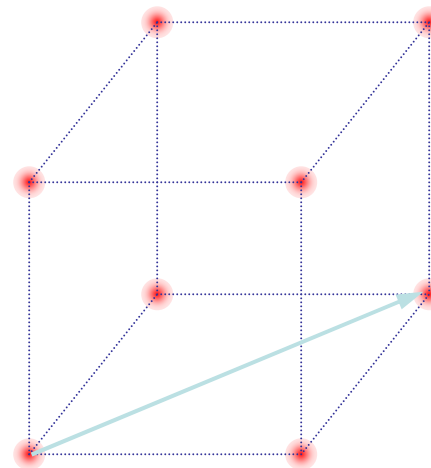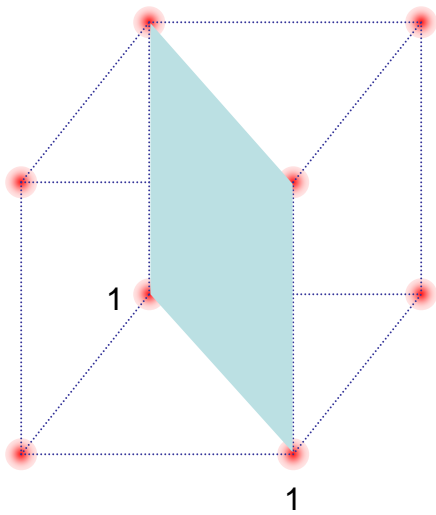# Crystal Directions

(111)

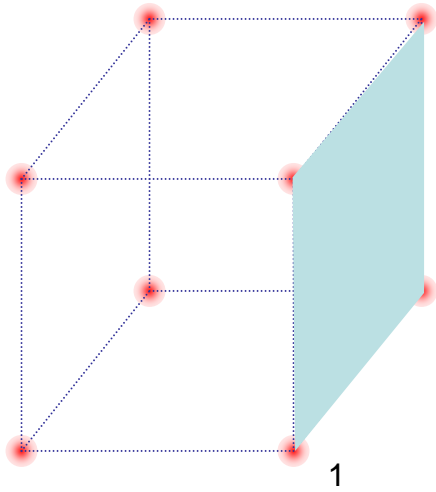**(110)**
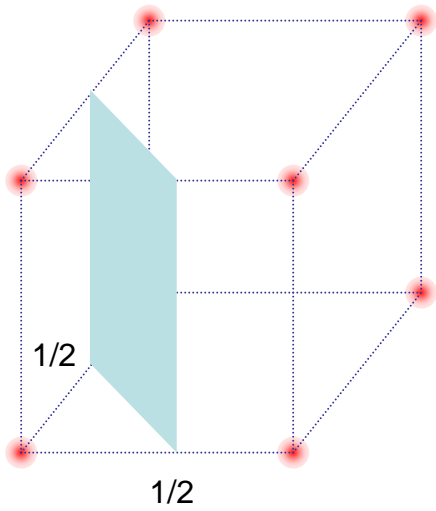
Crystal Directions

(100)

1

(220)

1/2

1/2
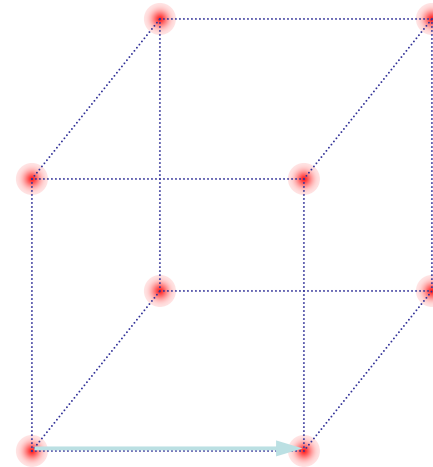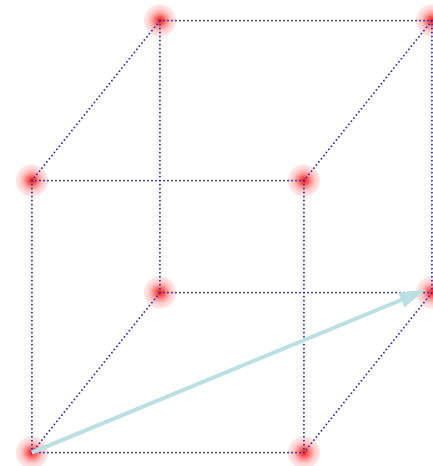
Crystal Directions

Electron beam generated pattern in TEM
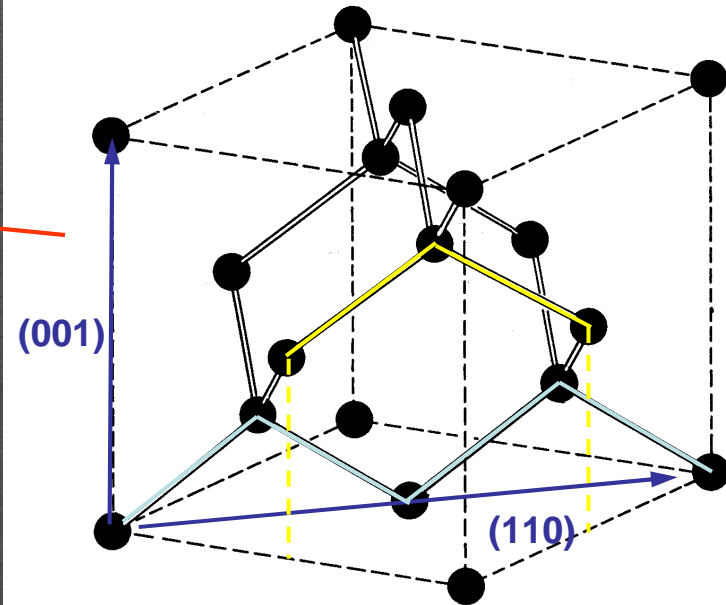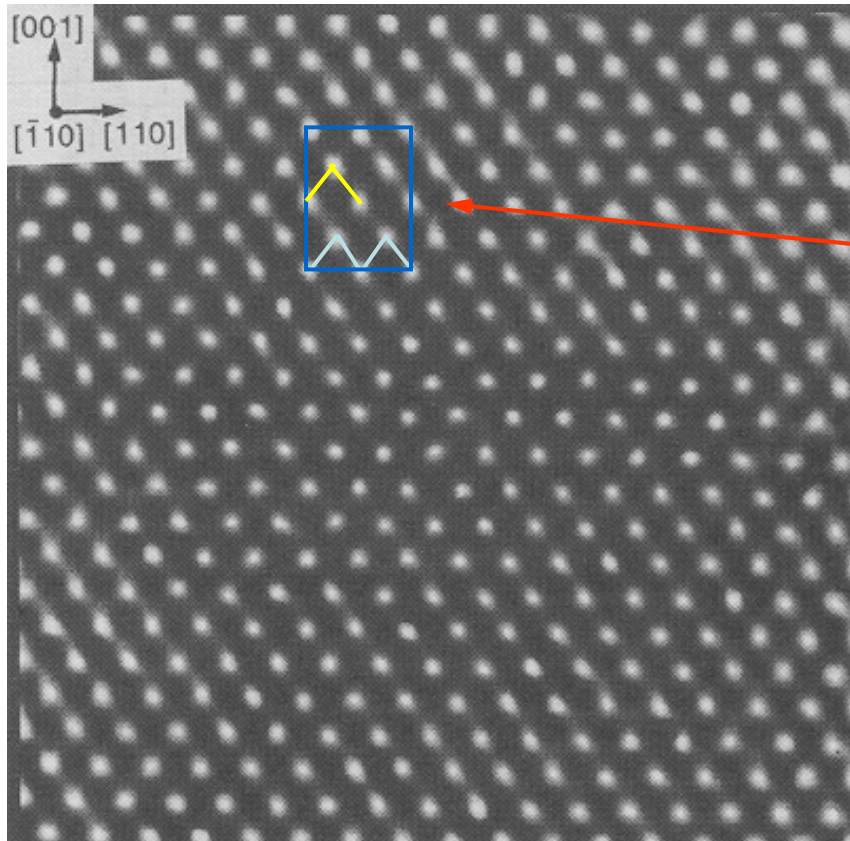
So far, we have discussed the concept of crystal directions:
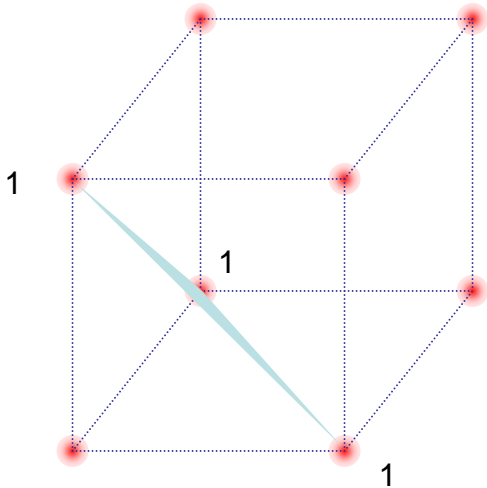
(111)
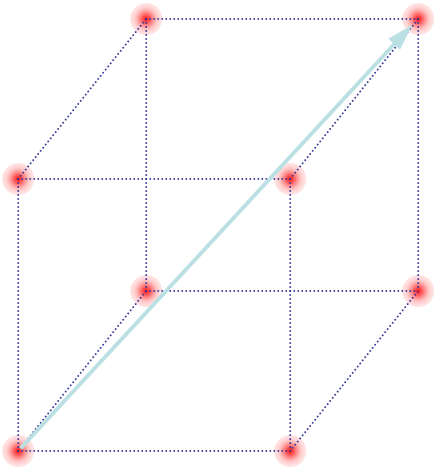
(110)
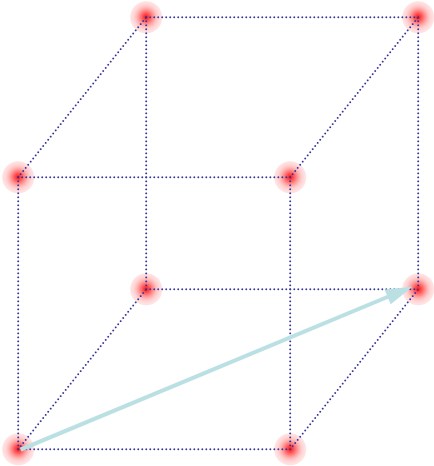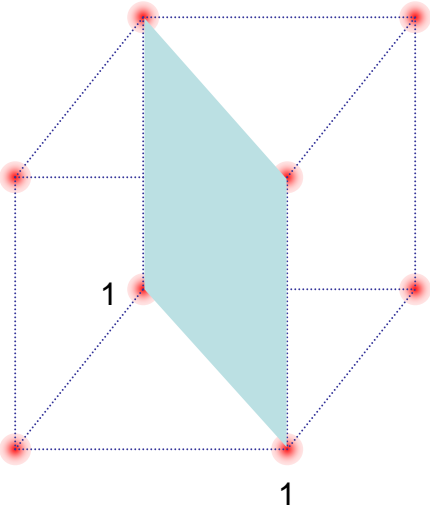
We want to say a few more things about this.
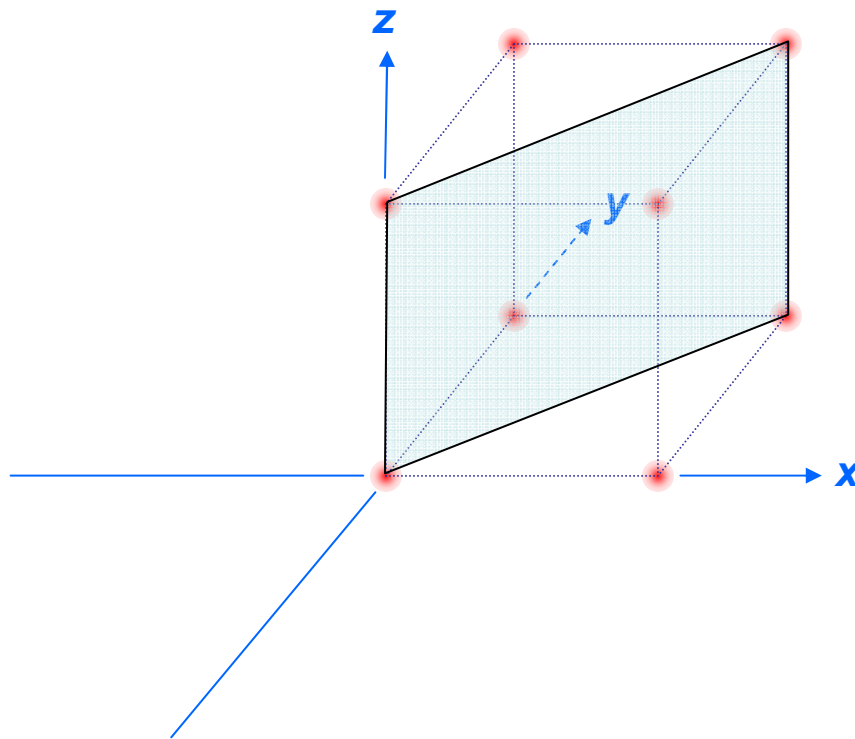
Consider this plane.

The intercepts are 0,0,∞, which leads to 1,1,0 for Miller indices.

What are the normals to the plane?

The intercepts are -1, 1, ∞, which leads to

$$\left(\overline{1}\,10\right)$$
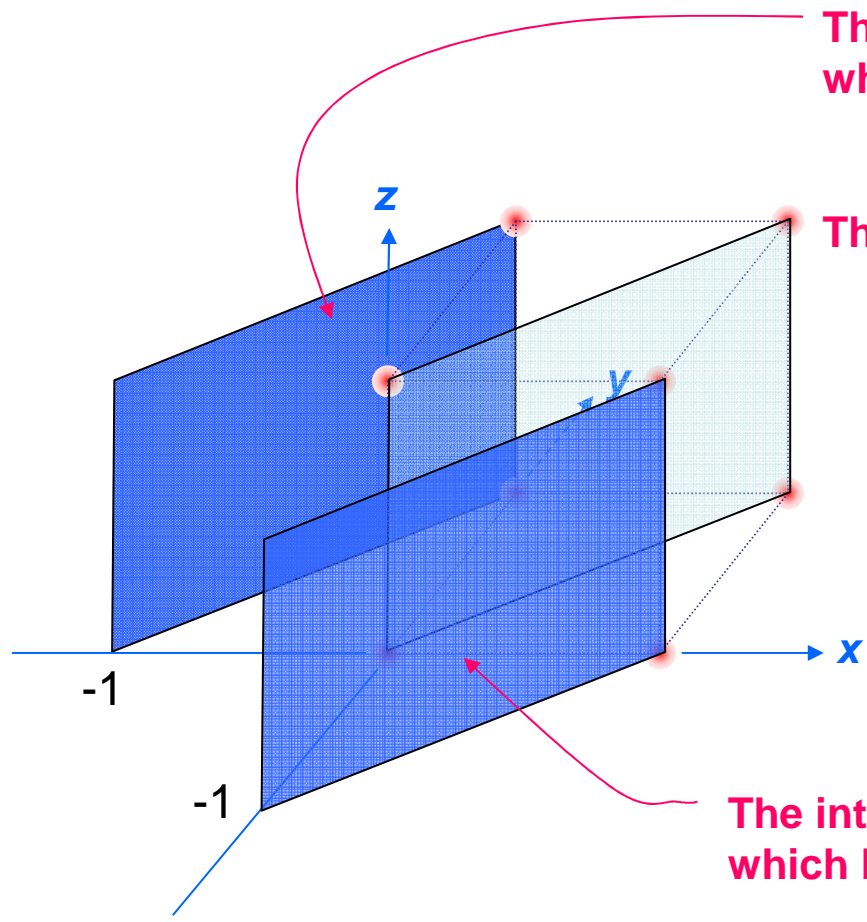
The normal direction is

$$-\hat{x}+\hat{y}\rightarrow\left[\overline{1}\,10\right]$$

The intercepts are 1, -1, ∞, which leads to

$$\left(1\,\overline{1}\,0\right)$$

The normal direction is

$$\hat{x}-\hat{y}\rightarrow\left[1\,\overline{1}\,0\right]$$

We can easily shift the planes by one lattice vector in *x* or *y*

These are two different normals to the same plane.

z $\left[\overline{1}\,10\right]$

$\left[1\,\overline{1}\,0\right]$

x

-1

-1

Directions have square brackets [...]
Planes have parentheses (...)

Now consider the following plane:

z

$[1\bar{1}0]$

$[110]$

-1

-1

x
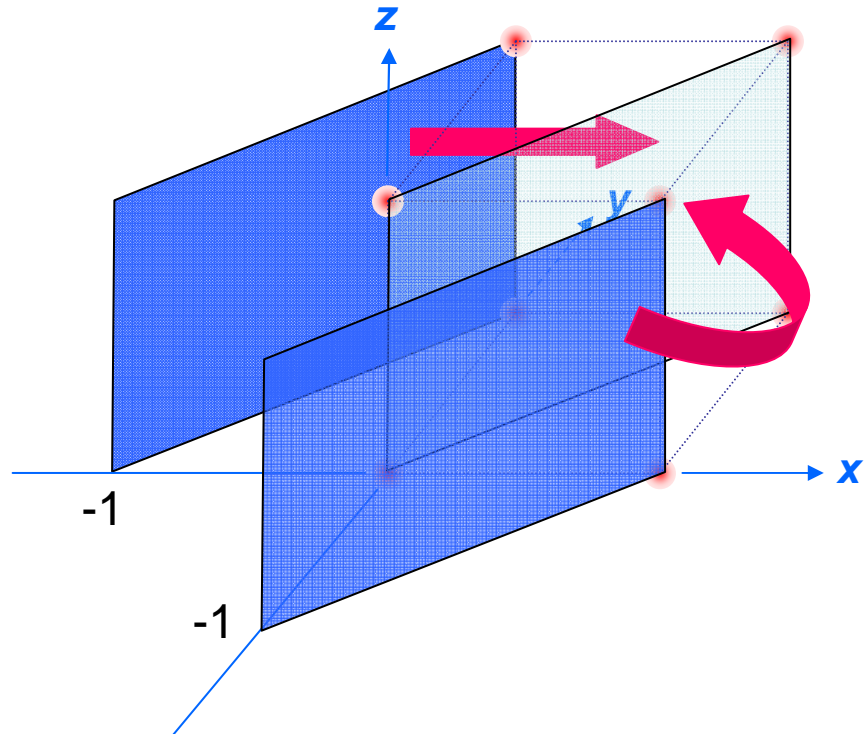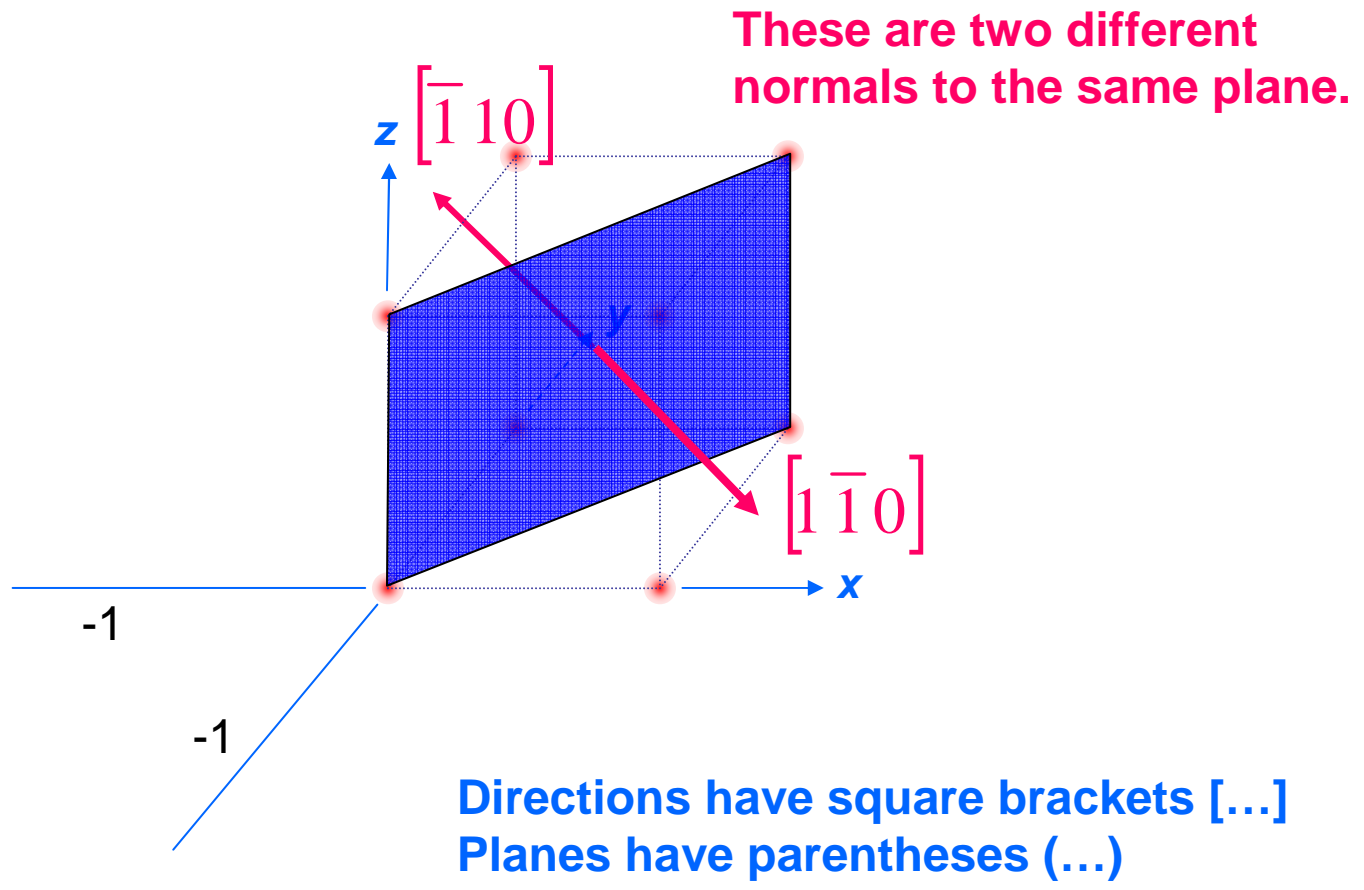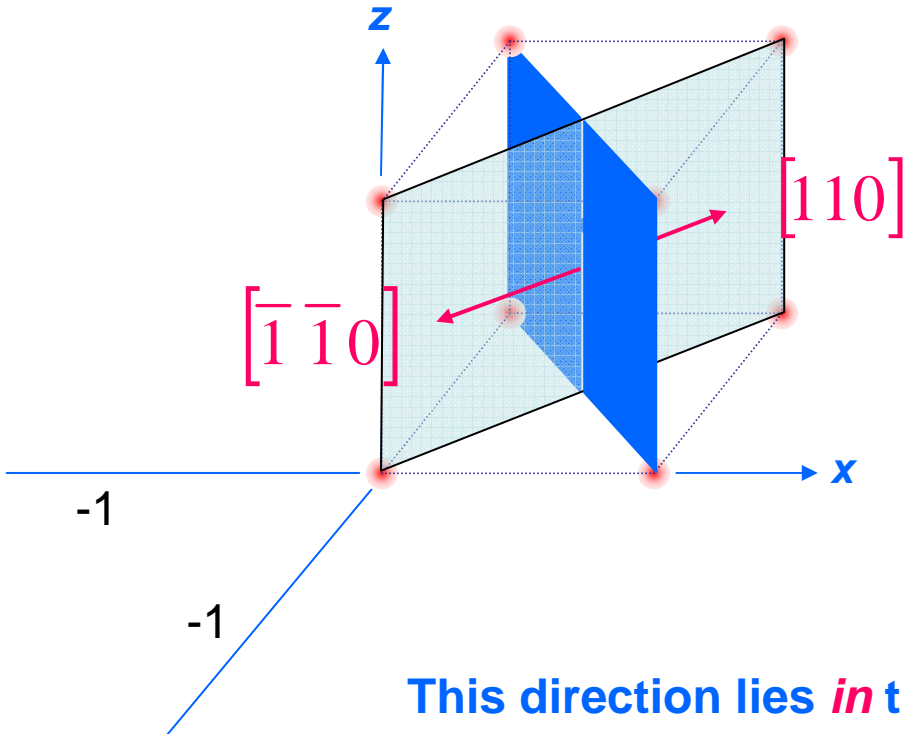
This direction lies _in_ the original plane.

Now consider the following plane:

z

y

[001]

-1

-1

x

This direction lies *in* the original plane.

z

-1

-1

x

y

$[001]$

$[111]$

$[110]$
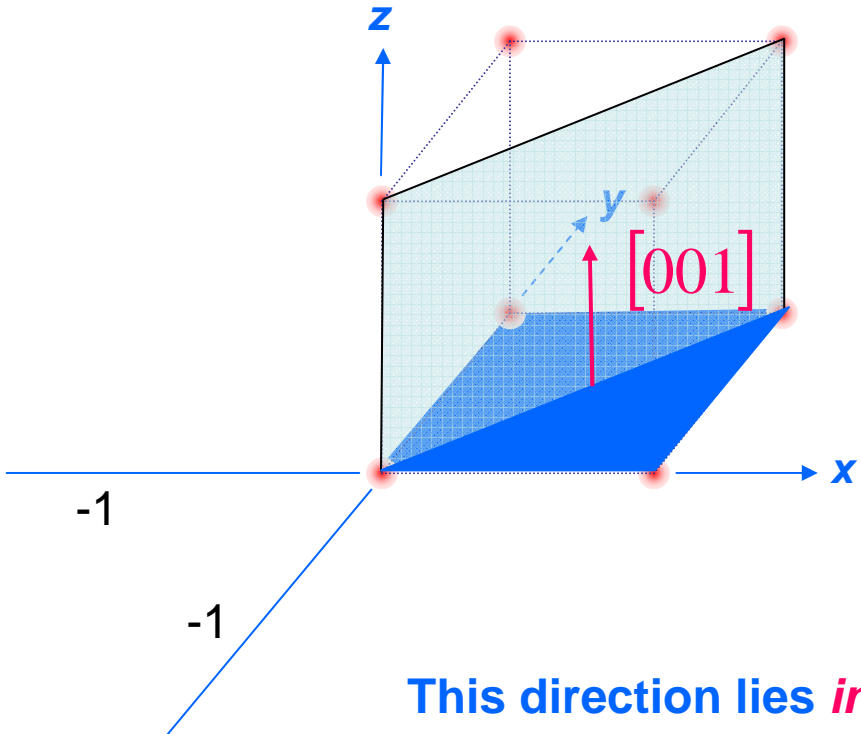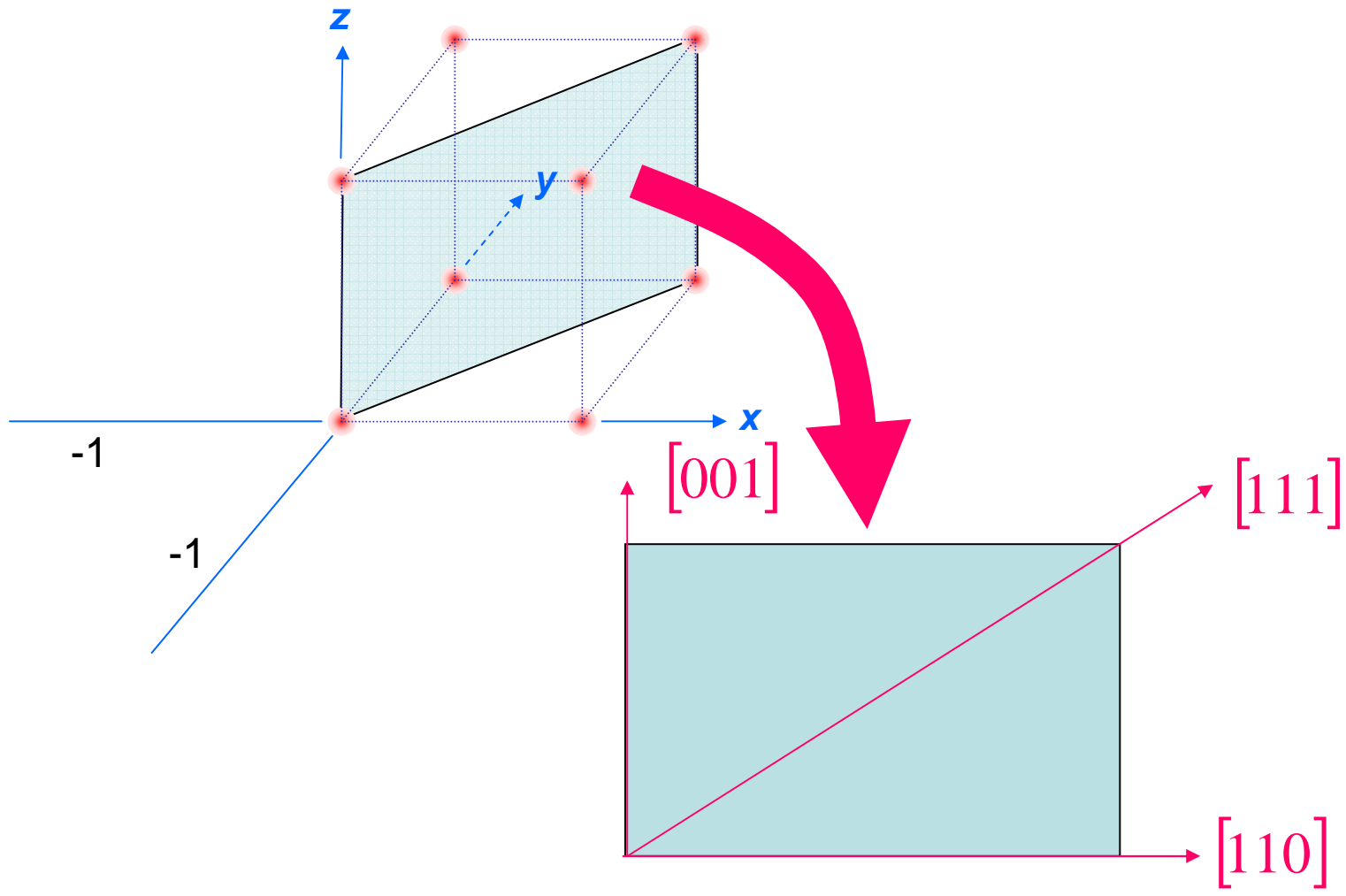
$[\bar{1}\,10]$ **points into the page**

Crystal Directions

We want the NORMAL to the surface. So we take these intercepts
(in units of *a*), and invert them:

$$\left(\frac{1}{2},\frac{2}{3},1\right) \Rightarrow \left(2,\frac{3}{2},1\right)$$

This inversion creates units of 1/cm

Then we take the lowest common set of integers:

$$\left(\frac{1}{2},\frac{2}{3},1\right) \Rightarrow \left(2,\frac{3}{2},1\right) \Rightarrow [4,3,2]$$

These "numbers" define a new VECTOR in this "reciprocal space"

These are the MILLER INDICES of the plane.

The NORMAL to the plane is the [4,3,2] direction, which is
normally written just [432]. (A negative number is indicated by a
bar over the top of the number.)

Crystal Directions

[100]

1

1/2

1/2
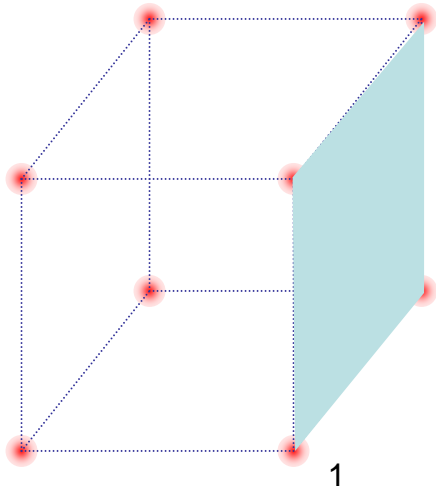
These vectors are normal to the planes, but are defined in this new space.
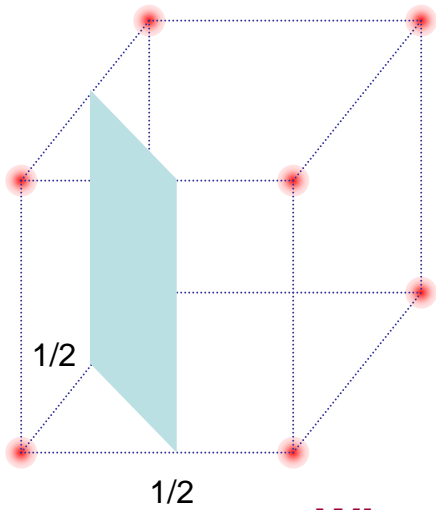
[220]
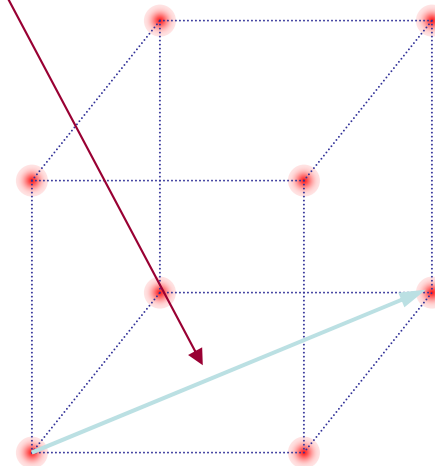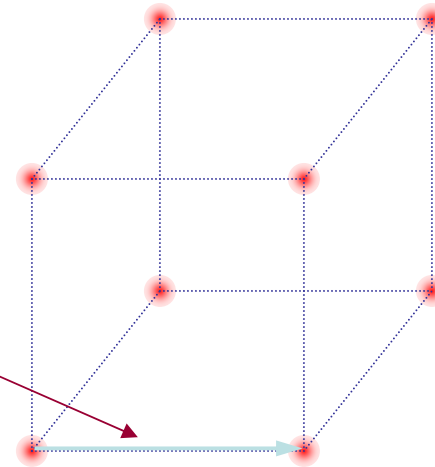
What is this new reciprocal space?

Now, let's talk a little more about waves, and how these waves will be important in our crystals.

In earlier circuit courses, we used Laplace transforms, such as

$$e^{-st}$$

If we let $s = \sigma + i\omega$, we can get the Fourier transform as ($\sigma = 0$)

$$e^{-i\omega t}$$

units = 1/*time* = $2\pi Hz$ units = *time*

Hence, frequency space is the reciprocal space for time. The units are 1/*seconds*.

In electromagnetics (EEE 340), we deal with waves (more on this next time). In this course, we deal with exponentials that vary as:

$$e^{ikx - i\omega t}$$

Spatially varying part of the exponent.

x corresponds to distance (cm)

k corresponds to 1/distance or 1/cm
This is the reciprocal space term

Fourier transformation in space and time:

distance

time

frequency
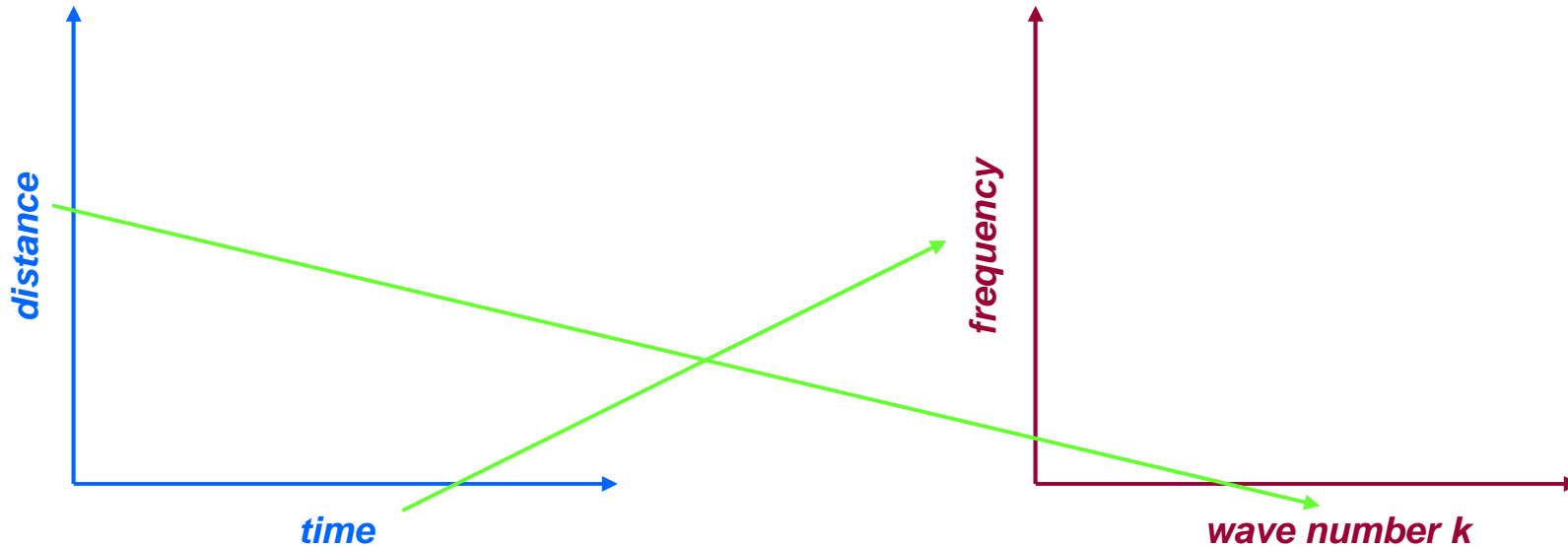
wave number k

The dimensions of space and time go into the dimensions of "wave number" (reciprocal space) and frequency (reciprocal time)
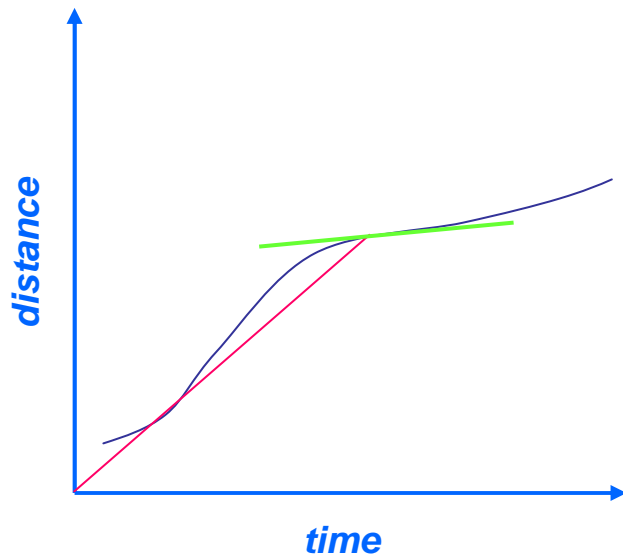
Velocity is distance per unit time, but can be defined in at least two ways:

$$v = \frac{x}{t}$$

$$v' = \frac{\partial x}{\partial t}$$

In either case, the units of velocity are *cm/s*.
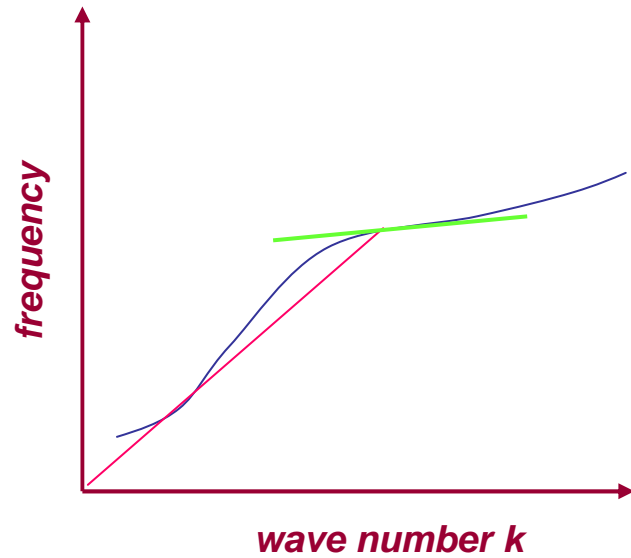
The idea of velocity must carry over to the Fourier transform space:

$$v = \frac{\omega}{k}$$ **Phase velocity**

$$v' = \frac{\partial \omega}{\partial k}$$ **Group velocity**

The units remain *cm/s*.

frequency

wave number k

What about multiple spatial dimensions?

The Multiple Space of Concern is the Lattice

For the **FACE CENTERED CUBIC** lattice, we have to define the three lattice vectors so that they fully account for the atoms at the face centers.
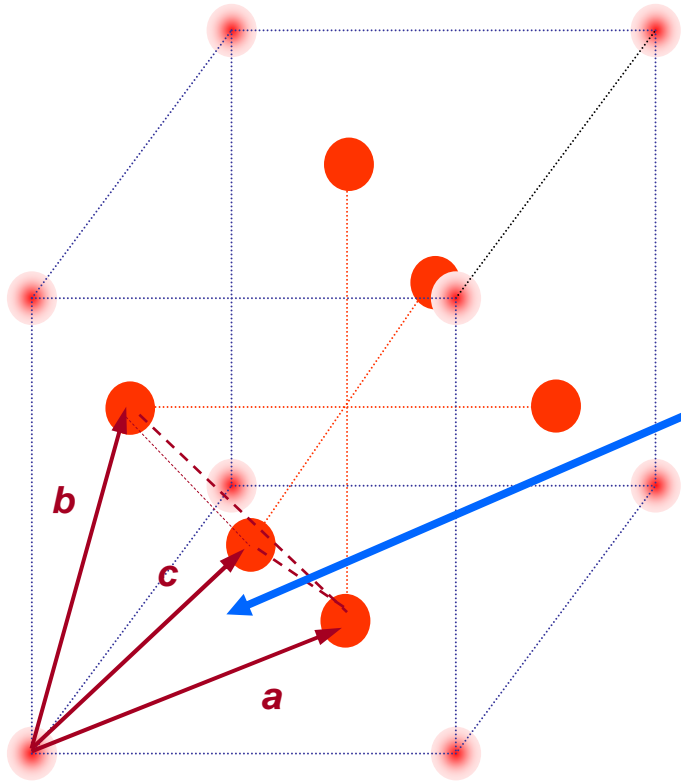
The three primitive vectors run from a corner atom to the three adjacent faces of that corner. Again, these form a tetrahedron.

There will be 3 vectors in the reciprocal space, which correspond to the three vectors *a, b, c* in real space.

These will define a unit cell in the reciprocal space!

We do not care what these vectors are at present; the important point is that our reciprocal space is periodic, just as the lattice. We will learn what the period is later.

So, why do we care about this reciprocal space?

We will learn later that the onset of quantum mechanics around 1900 led to a connection between energy and frequency, which is known as the Planck relation:

$$E = hf = \hbar\omega$$

$$\hbar = h/2\pi$$

$$h \sim 6.6 \times 10^{-34} J \cdot s$$

Hence, the *frequency* space goes into the *energy* space!

Similarly, momentum is *mv*, which is

$$mv = \frac{\partial E}{\partial v} \sim \hbar \frac{\partial \omega}{\partial v} \sim \hbar k$$

Hence, the *wave number* space goes into the *momentum* space!

Max Karl Ernst Ludwig Planck, Nobel Prize in Physics, 1918

frequency

wave number k

$E = \hbar\omega$

energy

$p = mv = \hbar k$

momentum
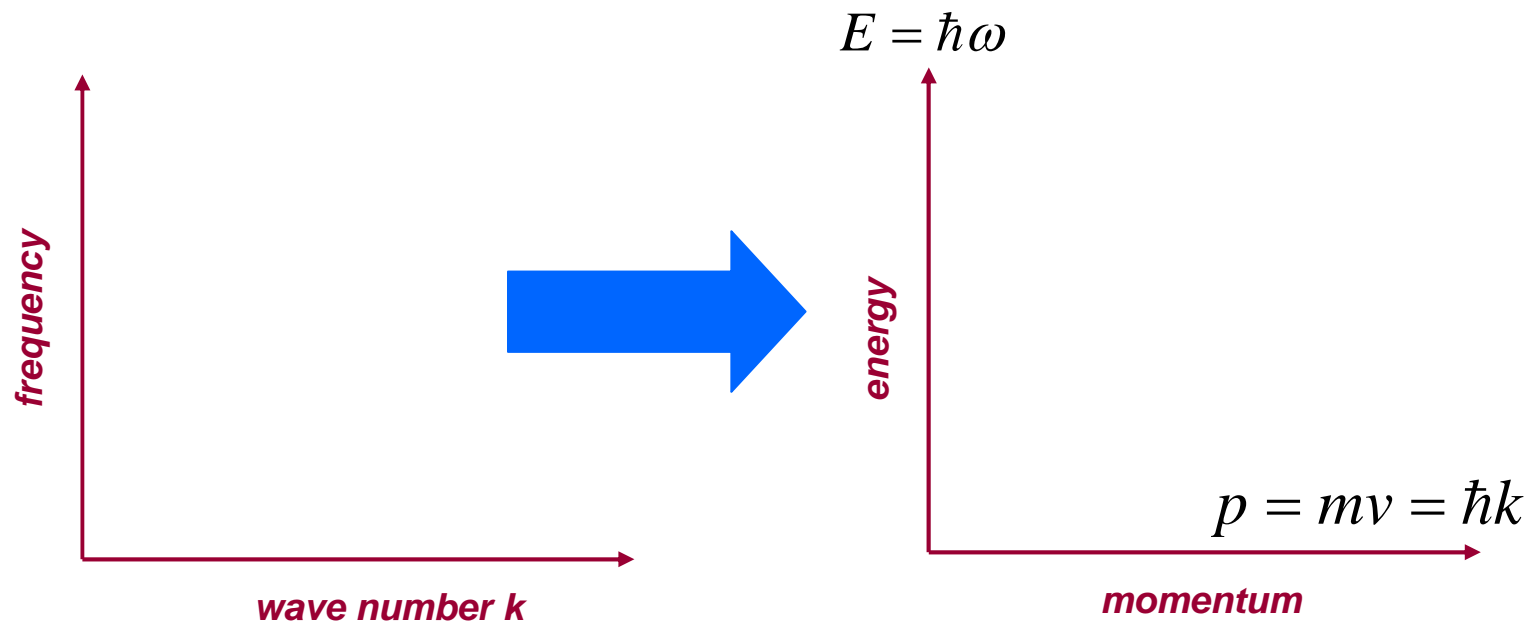
The two axes scale equally with the so-called reduced Planck's constant $\hbar$

A Brief Review of Classical Physics

• **A hundred years ago our understanding of nature relied on CLASSICAL PHYSICS**

   * **NEWTON'S laws of motion and MAXWELL'S equations**

• **An important notion in classical physics is the concept of PARTICLES and WAVES**

   * **Particles are SOLID objects such as PLANETS and ATOMS**

   * **While waves show the property of PROPAGATING through space (*would you ever think of water as particles?*)**

PARTICLES	WAVES
PLANETS	WATER
TENNIS BALLS	LIGHT
ORANGES	RADIO
BALL BEARINGS	HEAT
ATOMS	RADIATION
ELECTRONS	X-RAYS
PROTONS	

CLASSICAL PHYSICS MAKES AN IMPORTANTDISTINCTION BETWEEN PARTICLES & WAVES

In our classical world, waves and particles are distinct and separate entitites.

In electromagnetics and optics, waves have the properties:

$$f = \frac{c}{\lambda} \quad , \quad E = \frac{hc}{\lambda} = hc\left(\frac{k}{2\pi}\right) = \hbar k \cdot c$$

wavelength

Particles, on the other hand, have a different behavior:

$$E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m} = \left(\frac{\hbar k}{m}\right)\frac{\hbar k}{2} = \hbar k \frac{v}{2} \quad , \quad \omega = \frac{\hbar k^2}{2m} = \left(\frac{\hbar k}{m}\right)\frac{k}{2} = \frac{kv}{2}$$

The two velocities are different!

What is the velocity?

$$v' = \frac{\partial \omega}{\partial k} = \frac{\hbar k}{m} = particle\ velocity$$

$$v = \frac{\omega}{k} = \frac{1}{k}\frac{\hbar k^2}{2m} = \frac{\hbar k}{2m}$$
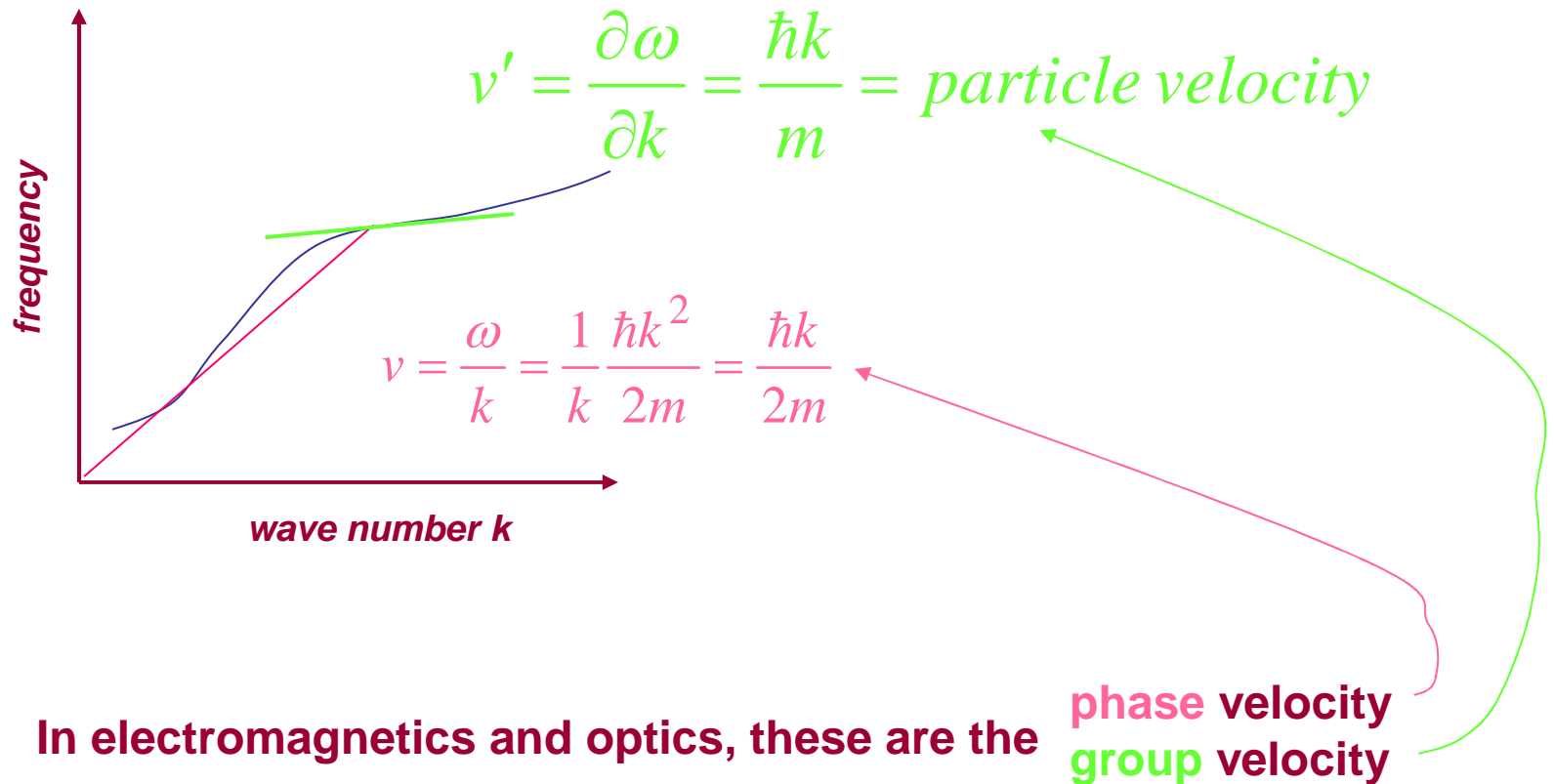
In electromagnetics and optics, these are the phase **velocity** group **velocity**

In free space, these two velocities are equal for optics, but not for particles. Particles are *dispersive*.

Light as a Wave Phenomenon

• **By the end of the last century light was thought of as a WAVE phenomenon**

    * **Since MANY properties of light conform to MAXWELL'S EQUATIONS**

    * **And since light exhibits many phenomena typically associated with waves**

        ⇒ **Including INTERFERENCE and DIFFRACTION**
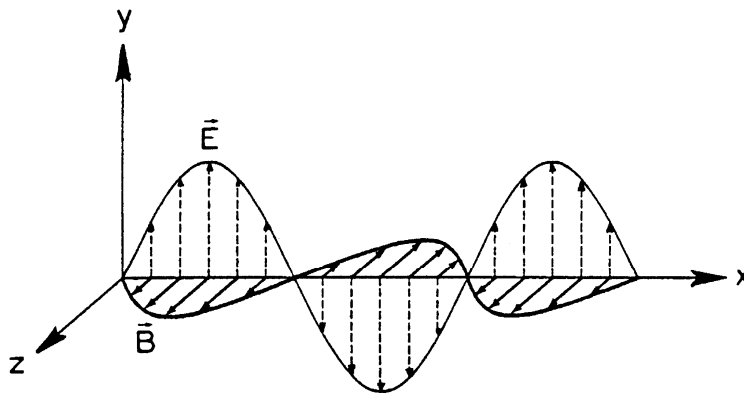
MAXWELL'S EQUATIONS

$$\nabla \times \mathbf{H} = \frac{\partial \mathbf{D}}{\partial t} + \mathbf{j}$$

$$\nabla \cdot \mathbf{B} = 0$$

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$$

$$\nabla \cdot \mathbf{D} = 0$$

CLASSICALLY LIGHT IS TREATED AS AN ELECTROMAGNETIC WAVE IN WHICH ELECTRIC AND MAGNETIC FIELD COMPONENTS OSCILLATE IN PHASE WITH EACH OTHER

[web]

Light as a Wave Phenomenon

INTERFERENCE and DIFFRACTION

INCOMING WAVE

OBSTACLE

DIFFRACTION PATTERN
FORMED ON A SCREEN

2

θ

Light as a Wave Phenomenon

INTERFERENCE and DIFFRACTION

COHERENT LIGHT SOURCE

Light is diffracted by the aperatures

Just as for X-ray diffraction, the light has constructive and destructive interference where the diffracted beams come together
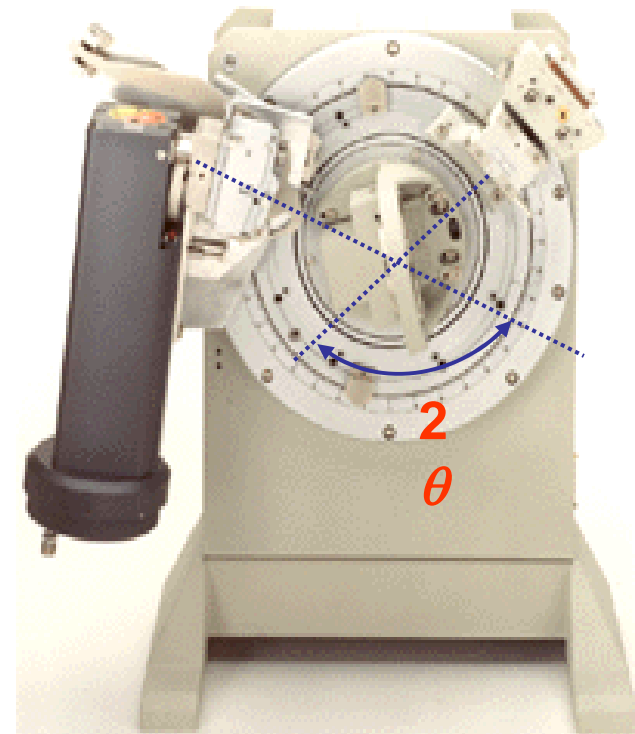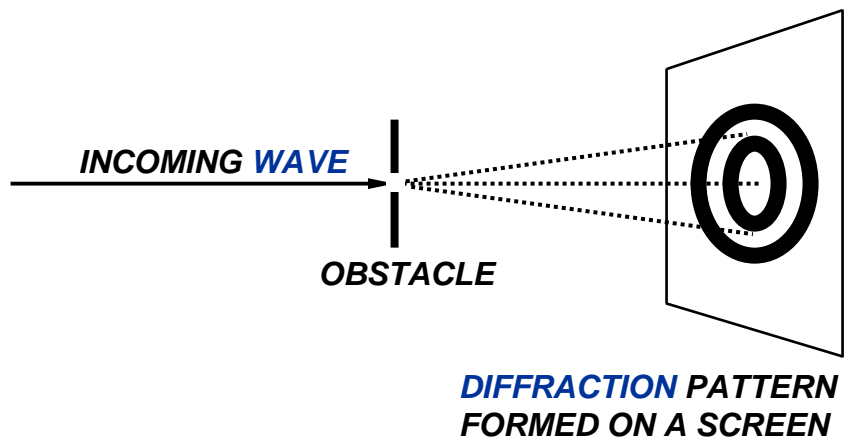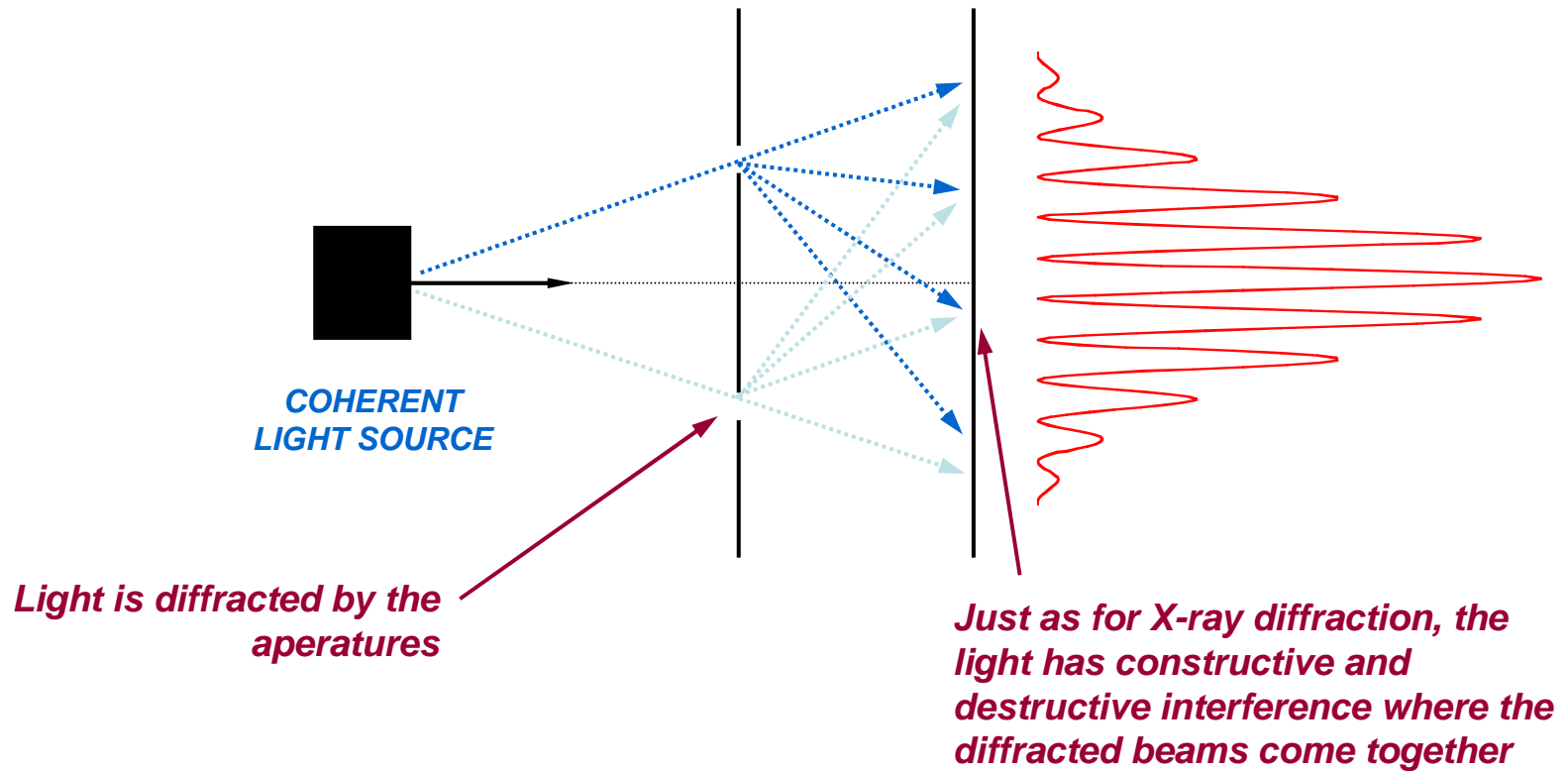
Black-Body Radiation
The Arrival of Quantum Mechanics

Everything radiates "light" waves, whether in the visible or the infrared (heat). The intensity of this radiation is frequency dependent.
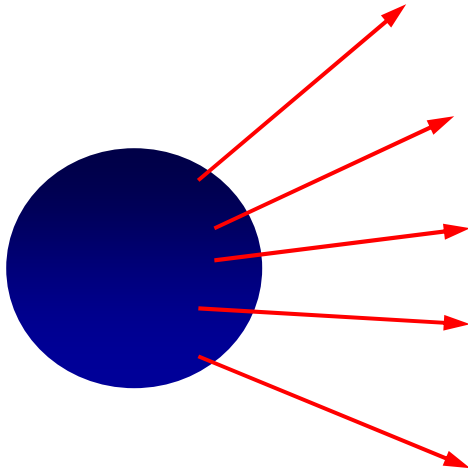
The two limiting forms were known in the mid-1800s.
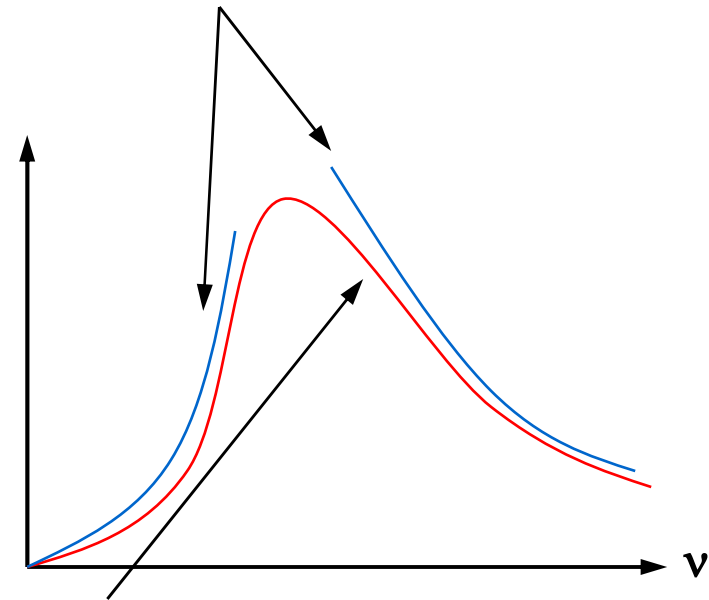
Max Planck derived this form ca. 1900. This required him to postulate

$$E = h\nu$$

$h \sim 6.6248 \times 10^{-34}$ **joule-sec**

Planck's relationship between energy and frequency requires that light be made up of small "packets" of energy. These packets have come to be known as *photons*.

That is, wave *intensity* is quantized into basic units given by the frequency and Planck's constant. If we talk about the power in a light wave (energy/time), then we must talk about so many photons/second arriving at the measurement point.

THE LIGHT WAVE HAS BECOME A SET OF PARTICLES (PHOTONS). DOES THIS CHANGE OUR UNDERSTANDING?

Miller Indices

The Miller indices **for any given plane** of atoms within a crystal are obtained by following this four-step procedure:

1. After setting up the coordinate axes along the edges of the unit cell, note where the plane to be indexed intercepts the axes. Divide each intercept value by the unit cell length along the respective coordinate axis. Record the intercept values in order *x,y,z*.

2. Invert the intercept values.

3. Using appropriate multiplier, convert the [1/intercept] set to the smallest possible set of whole numbers.

4. Enclose the whole-number set in curvilinear brackets.

Note:

- If a plane is parallel to some of the coordinate axes, then the intercept is μ , which gives Miller index =0 for that coordinate.

- If a plane to be indexed has an intercept along the negative portion of a coordinate axis, a minus sign is placed over the corresponding index number.

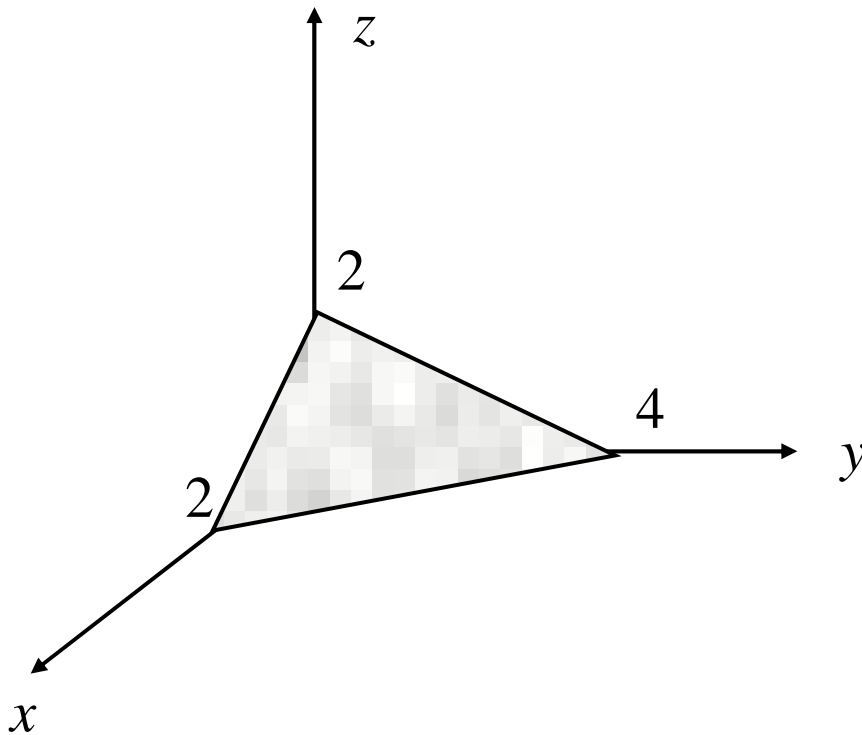## Notation:

(hkl) => Miller indices for planes

{hkl} => Miller indices for planes of equivalent symmetry

Example:

Calculate the Miller indices for the following plane:

- ➢ reciprocal of the intercepts: 1/2, 1/4, 1/2

- ➢ conversion to the smallest possible set of whole numbers: 2,1,2

- ➢ Miller indices for this plane are: (212).

The Miller indices **for direction** are established using the same procedure for finding the components of a vector:

1. Set up a vector of arbitrary length in the direction of interest.
2. Decompose the vector into its components along the principal axes.
3. Using an appropriate multiplier, convert the component values into the smallest possible whole-number set.

Notation:

[hkl]   => specific direction within crystal

<hkl>   => an equivalent set of directions

For cubic crystals, a plane and the direction normal to the plane have precisely the same indices.

Calculation of the Miller indices **using vectors** is explained through the following example:

Consider a plane defined by three points:

$$P1:(022), \quad P2:(202) \quad \text{and} \quad P3:(210).$$

Define vectors:
$$\mathbf{r} = x\mathbf{i} + y\mathbf{j} + z\mathbf{k}$$
$$\mathbf{r}_1 = 0\mathbf{i} + 2\mathbf{j} + 2\mathbf{k}$$
$$\mathbf{r}_2 = 2\mathbf{i} + 0\mathbf{j} + 2\mathbf{k}$$
$$\mathbf{r}_3 = 2\mathbf{i} + 1\mathbf{j} + 0\mathbf{k}$$

and find the differences:
$$\mathbf{r} - \mathbf{r}_1 = x\mathbf{i} + (y-2)\mathbf{j} + (z-2)\mathbf{k}$$
$$\mathbf{r}_2 - \mathbf{r}_1 = 2\mathbf{i} - 2\mathbf{j} + 0\mathbf{k}$$
$$\mathbf{r}_3 - \mathbf{r}_1 = 2\mathbf{i} - 1\mathbf{j} - 2\mathbf{k}$$

Recall that a plane is defined with the following equation:

$$(\mathbf{r} - \mathbf{r}_1) \cdot [(\mathbf{r}_2 - \mathbf{r}_1) \times (\mathbf{r}_3 - \mathbf{r}_1)] = 0$$

For vectors **a**,**b** and **c** with coordinates (A_1, A_2, A_3), (B_1, B_2, B_3) and (C_1, C_2, C_3), the above requirement is equivalent to:

$$\begin{vmatrix} A_1 & A_2 & A_3 \\ B_1 & B_2 & B_3 \\ C_1 & C_2 & C_3 \end{vmatrix} = 0$$

For our example this leads to:

$$\begin{vmatrix} x & (y-2) & (z-2) \\ 2 & -2 & 0 \\ 2 & -1 & -2 \end{vmatrix} = 0 \quad \Longrightarrow \quad 4x + 4y + 2z = 12$$

Once we have the equation for the plane, we can find the following:

➔ The intercepts of this plane are: 3,3,6

➔ 1/intercept equals to: 1/3,1/3,1/6

➔ Miller indices for the plane are (221)

Additional information:

➔ Adjacent planes (hkl) in a cubic crystal have a spacing d given by:

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

➔ The angle between planes $(h_1k_1l_1)$ and $(h_2k_2l_2)$ is given by the following expression:

$$\cos(\theta) = \frac{h_1h_2 + k_1k_2 + l_1l_2}{\sqrt{\left(h_1^2 + k_1^2 + l_1^2\right)\left(h_2^2 + k_2^2 + l_2^2\right)}}$$