### 2. Diffraction and the Reciprocal Lattice

#### 2.1 Scattering of a plane wave by a crystal

If we take a "lump of stuff", and we look at an atom at  $\underline{r_1}$  within the "lump of stuff". Have an incoming wave with wave-vector  $\underline{k_r}$ . (its' magnitude is the wave number, and the vector shows the direction of the wave).

$$\Phi_I = a_1 e^{i\left(\underline{k}_{\underline{r}} \cdot \underline{r} - \omega t\right)}$$

NB: this is now 3D. c.f.  $e^{i(kx-\omega t)}$  for 1D.

Have an out-coming wave from the lump of stuff, as a result of the incoming wave, now with wave-vector  $\underline{k}_{f}$ , which heads into a detector at  $\underline{R}_{d}$ .

$$\Phi_f = a_I e^{(\underline{k}_I \cdot \underline{r} - \omega_I)} b_1 \frac{e^{i\underline{k}_f \cdot (\underline{R}_d - \underline{r}_1)}}{|\underline{R}_d - \underline{r}_1|}.$$

Where  $b_1$  is the scattering length of atom 1. For a number of atoms, j:

$$\Phi_{f} = \sum_{j} a_{I} e^{i\left(\underline{k}_{I} \cdot \underline{r}_{j} - \omega t\right)} b_{j} \frac{e^{i\underline{k}_{f} \cdot \left(\underline{R}_{d} - \underline{r}_{j}\right)}}{\left|\underline{R}_{d} - \underline{r}_{j}\right|}$$

NB; the  $|\underline{R}_d - \underline{r}_j|^{-1}$  denotes that the flux will decay with distance. For a detector at a large distance  $R_d$  away, take the origin at the sample  $|\underline{R}_d - \underline{r}_j| \approx |\underline{R}_d| \quad \forall j$  (for all j), so:

$$\Phi_f = a_I \frac{e^{i\left(\underline{k}_f \cdot \underline{R}_d - \omega t\right)}}{\left|\underline{R}_d\right|} \sum_j b_j e^{i\left(\underline{k}_I - \underline{k}_f\right) \cdot \underline{r}_j}$$

This is a wave traveling in the direction of  $\underline{k}_{f}$  whose amplitude is determined by the summation over all atoms j.

Let  $Q = \underline{k}_I - \underline{k}_f$ , called the wavevector transfer.



 $\hbar Q$  is the momentum transfer, i.e. the change of momentum. (Remember: In QM, k is just the momentum (over h-bar).  $p = \hbar k$ .)

For each atom, the position  $\underline{r}_j$  is the position of the associated lattice point,  $\underline{R}_\ell$ , plus its' position vector within the basis,  $\underline{r}_{bj}$ .

$$\underline{r}_{j} = \underline{R}_{\ell} + \underline{r}_{bj}$$

So we can split the summation into two parts, one over the lattice points, and the other over the atoms in the basis.

$$\Phi_{f} = a_{I} \frac{e^{i\left(\underline{k}_{f} \cdot \underline{R}_{d} - \omega t\right)}}{\left|\underline{R}_{d}\right|} \sum_{lattice} e^{\underline{Q} \cdot \underline{R}_{\ell}} \sum_{basis} b_{j} e^{i\underline{Q} \cdot \underline{r}_{bj}}$$

### 2.2 Sum over Lattice Points

Any of the lattice position vectors may be written as an integer sum over the lattice vectors  $\underline{a}$ ,  $\underline{b}$  and  $\underline{c}$ , so the lattice sum is:

$$\sum_{lattice} e^{i\underline{Q}\cdot(n_1\underline{a}+n_2\underline{b}+n_3\underline{c})}$$

Constructive interference is when they all add. This occurs when

$$\underline{\underline{Q}} \cdot \underline{\underline{a}} = 2\pi m_1$$
  
$$\underline{\underline{Q}} \cdot \underline{\underline{b}} = 2\pi m_2$$
  
$$\underline{\underline{Q}} \cdot \underline{\underline{c}} = 2\pi m_3$$

where  $m_1, m_2, m_3$  are integers, i.e. the exponential is an integer amount of  $2\pi$ , hence is 1.

We know that  $\underline{b} \times \underline{c} (\equiv \underline{b} \land \underline{c})$  is orthogonal to both  $\underline{b}$  and  $\underline{c}$ . If we write

$$\underline{Q} = \frac{2\pi\underline{b} \times \underline{c}}{\underline{a} \cdot \underline{b} \times \underline{c}} m_1 + \frac{2\pi\underline{c} \times \underline{a}}{\underline{a} \cdot \underline{b} \times \underline{c}} m_2 + \frac{2\pi\underline{a} \times \underline{b}}{\underline{a} \cdot \underline{b} \times \underline{c}} m_3$$

where  $\underline{a} \cdot \underline{b} \times \underline{c}$  is the triple product. Then the constructive interference condition is satisfied for all lattice points.

If we write:

$$\underline{a}^{*} = \frac{2\pi\underline{b} \times \underline{c}}{\underline{a} \cdot \underline{b} \times \underline{c}}$$
$$\underline{b}^{*} = \frac{2\pi\underline{c} \times \underline{a}}{\underline{a} \cdot \underline{b} \times \underline{c}}$$
$$\underline{c}^{*} = \frac{2\pi\underline{a} \times \underline{b}}{\underline{a} \cdot \underline{b} \times \underline{c}}$$

then diffraction happens when

$$\underline{Q} = m_1 \underline{a}^* + m_2 \underline{b}^* + m_2 \underline{c}^*.$$

Since  $\underline{a}$ ,  $\underline{b}$  and  $\underline{c}$  are non-coplanar vectors, so are  $\underline{a}^*$ ,  $\underline{b}^*$  and  $\underline{c}^*$ . Therefore these  $\underline{Q}$  values also represent a Bravais lattice, but in the space of the wave-vectors.

Let

$$\underline{G} = h\underline{a}^* + k\underline{b}^* + \ell\underline{c}^*$$

where h, k and  $\ell$  are integers. We now have a Bravais lattice in wavevector space, or k-space. It tells us in which directions diffraction happens from a crystal. This space is sometimes called "reciprocal space" (since the dimensions of k are inverse length). The lattice is called "the reciprocal lattice". The diffraction condition is when  $Q = \underline{G}$ , where  $\underline{G}$  is any reciprocal lattice vector.

### 2.3 Reciprocal Lattice Vectors

Note that  $\underline{a}^* \cdot \underline{a} = 2\pi$ , and  $\underline{a}^* \cdot \underline{b} = \underline{a}^* \cdot \underline{c} = 0$ . So  $\underline{a}^*$  is orthogonal to  $\underline{b}$  and  $\underline{c}$ , but that does not imply that  $\underline{a}^*$  is parallel to  $\underline{a}$ , although it may be.

For 
$$\underline{R} = n_1 \underline{a} + n_2 \underline{b} + n_3 \underline{c}$$
, and  $\underline{G} = h \underline{a}^* + k \underline{b}^* + \ell \underline{c}^*$ ;  
 $\underline{G} \cdot \underline{R} = 2\pi (n_1 h + n_2 k + n_3 \ell)$ 

so that

$$e^{i\underline{G}\cdot\underline{R}}=1.$$

This is true for all of the lattice vectors  $\underline{R}_{\ell}$ .

If  $\underline{a}$ ,  $\underline{b}$  and  $\underline{c}$  are chosen as non-primitive, then this construction for the reciprocal lattice vectors is not correct, since the diffraction condition needs to be satisfied for all lattice vectors. The effect is to generate points which are not really reciprocal lattice vectors.

Example: Non-primitive lattice vectors in a bcc lattice.



Conventional, non-primitive.  $\underline{a} = a(1,0,0)$  $\underline{b} = a(0,1,0)$ 

$$\underline{c} = a(0,0,1)$$

$$\underline{a} \cdot \underline{b} \times \underline{c} = a^{3}$$

$$\underline{a}^{*} = \frac{2\pi}{a}(1,0,0)$$

$$\underline{b}^{*} = \frac{2\pi}{a}(0,1,0)$$

$$\underline{c}^{*} = \frac{2\pi}{a}(0,0,1)$$

Primitive lattice vectors: (we are looking at the centre atoms -a' looks at the one in front of the cube drawn, b' the one to the left, and c' the one below.)

$$\underline{a}' = a \left(\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}\right)$$

$$\underline{b}' = a \left(\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}\right)$$

$$\underline{c}' = a \left(-\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)$$

$$\underline{a}' \cdot \underline{b}' \times \underline{c}' = \frac{a^3}{2}$$

$$\underline{b}' \times \underline{c}' = a^2 \left(\frac{1}{2}, 0, \frac{1}{2}\right)$$

$$\underline{c}' \times \underline{a}' = a^2 \left(\frac{1}{2}, \frac{1}{2}, 0\right)$$

$$\underline{a}' \times \underline{b}' = a^2 \left(0, \frac{1}{2}, \frac{1}{2}\right)$$

$$\underline{a}^{*'} = \frac{2\pi}{a} (1, 0, 1)$$

$$\underline{b}^{*'} = \frac{2\pi}{a} (0, 1, 1)$$

We can be confident that any integer sum of the primitive reciprocal lattice vectors is a reciprocal lattice vector

e.g. 
$$2\underline{a}^{*'} = \frac{2\pi}{a}(2,0,2)$$
.  $m_1 = 2$ ,  $m_2 = 0$ ,  $m_3 = 2$ .  
 $\underline{a}^{*'} + \underline{c}^{*'} = \frac{2\pi}{a}(1,1,2)$ 

However, there are vectors which can be constructed from the conventional (nonprimitive) reciprocal lattice vectors which cannot be constructed from the primitive e.g.:

$$\underline{a}^* = \frac{2\pi}{a} (1,0,0)$$
$$\underline{a}^* + \underline{b}^* + \underline{c}^* = \frac{2\pi}{a} (1,1,1)$$

All reciprocal lattice points have to satisfy  $m_1 + m_2 + m_3 = 2n$ , where n is an integer. i.e. it must be even. All others  $(m_1 + m_2 + m_3 = 2n + 1)$  are not reciprocal lattice points.

"When using non-primitive lattice vectors, beware!"

These phantom points are referred to as *systematic absences*. They are not really absences at all, but an artifact of the choice of a non-primitive set of lattice vectors.

# 2.4 Magnitude of $\underline{G}_{hk\ell}$ in cubic system

If  

$$\underline{a} = a(1,0,0)$$
  
 $b = a(0,1,0)$   
 $c = a(0,0,1)$   
then:  
 $\underline{a}^* = \frac{2\pi}{a}(1,0,0)$   
 $\underline{b}^* = \frac{2\pi}{a}(0,1,0)$   
 $\underline{c}^* = \frac{2\pi}{a}(0,0,1)$   
 $\underline{G}_{hk\ell} = h\underline{a}^* + k\underline{b}^* + \ell\underline{c}^*$   
 $= \frac{2\pi}{a}(h,k,\ell)$   
 $|\underline{G}_{hk\ell}| = \frac{2\pi}{a}(h^2 + k^2 + \ell^2)^{\frac{1}{2}}$ 

### 2.5 Lattice Planes & Indices

Consider lattice points as belonging to planes, separated by a distance d.



Now consider these planes as the wavefronts of some wave, characterized by a wavevector  $\underline{k}$ , perpendicular to the wavefronts.  $|\underline{k}| = \frac{2\pi}{d}$ .

$$\underline{k} = \frac{2\pi}{a} (1,0,0) \text{ or } \underline{k} = \underline{a}^*$$



The wavevectors of the waves whose wavefronts are lattice planes, are the position vectors in reciprocal space of reciprocal lattice points.

Do all reciprocal lattice points represent lattice planes? What does (2,0,0) represent?



Real space separation  $=\frac{a}{2}$ .

These represent spatial harmonics. They refer to the same planes. Similarly (6,6,0) is a harmonic of (1,1,0), etc.

# 2.5.1 Indices (1)

The convention for representing lattice planes is to take the integers  $m_1, m_2, m_3$  (coefficients of  $\underline{a}^*, \underline{b}^*, \underline{c}^*$ ). Write negative *n* as  $\overline{n}$ .

e.g. (1,1,0),  $(3,\overline{1},0)$ , (7,15,2) (note that the commas can be replaced by spaces...) In general,  $(h,k,\ell)$  (or  $(hk\ell)$ ).

If the unit cell has sides  $\underline{a}, \underline{b}, \underline{c}$ , then adjacent planes intersect the axes at (0,0,0), then

at 
$$\frac{a}{h}, \frac{b}{k}, \frac{c}{\ell}$$
.



(2,0,0) planes intersect at origin, then  $\frac{a}{2}$  on a, and not at all on *b*,*c*.

Sets of lattice planes  $(hk\ell)$  related by symmetry written  $\{hk\ell\}$ . e.g. in a cubic system,  $\{2,0,0\} = (2,0,0)(0,2,0)(0,0,2)(\overline{2},0,0)(0,\overline{2},0)(0,0,\overline{2})$ 

# 2.5.2 Indices (2)

When we are interested in real lattice planes only (not the harmonics), we use *Miller indices*, where the  $h,k,\ell$  have any common factors removed. So (1,0,0), (2,0,0), (7,0,0) are all represented by the Miller indices (1,0,0).

Directions in real space: For direction  $\underline{u} = u\underline{a} + v\underline{b} + w\underline{c}$ , we write [u, v, w]. Sets of directions related by symmetry  $\langle u, v, w \rangle$ . e.g. in a cubic crystal;  $\langle 1, 1, 1 \rangle = [1, 1, 1], [1, 1, 1], [1, 1, 1], [1, 1], [1, 1], [1, 1], [1, 1]]$ 

### 2.6 Bragg's Law

We have diffraction when  $\underline{Q} = \underline{G}_{hk\ell}$ . Separation of the lattice planes,  $d_{hk\ell}$ , is  $\frac{2\pi}{|G_{hk\ell}|}$ .



NB; for *n* integer,  $n\underline{G}_{hk\ell}$  has spacing  $\frac{d_{hk\ell}}{n}$ . NB2: since  $|\underline{G}_{hk\ell}| = \frac{2\pi}{a} (h^2 + k^2 + \ell^2)^{\frac{1}{2}}, d_{hk\ell} = \frac{a}{(h^2 + k^2 + \ell^2)^{\frac{1}{2}}}$ , for cubic lattices only.

### 2.7 Structure Factor

We found the diffracted wave to be

$$\Phi_F = a_I \frac{e^{i\left(\underline{k}_f \cdot \underline{R}_d \omega t\right)}}{\left|\underline{R}_d\right|} \sum_{lattice} e^{i\underline{Q} \cdot \underline{R}_\ell} \sum_{basis} b_j e^{i\underline{Q} \cdot \underline{r}_{bi}} .$$

The lattice sum tells us where diffraction (Bragg scattering) occurs in reciprocal space. This enables us to determine the properties of the lattice (symmetry and the lattice vectors themselves).

The sum over the basis (called the structure factor) determines the relative strengths of the various Bragg peaks, so this information enables us to deduce the basis.

Note that the measured intensity is proportional to the square of the structure factor.

Since Bragg scattering is restricted to reciprocal lattice points  $\underline{G}_{hk\ell}$ , we need to calculate

$$\left|\sum_{basis} b_j e^{i\underline{G}_{hk\ell}\cdot\underline{r}_{bj}}\right|^2.$$

### 2.7.1 Structure Factor for a Monatomic Structure

Where there is only one atom in the basis, we can always choose  $\underline{r}_{bi} = \underline{0}$ , so the

structure factor for all Bragg peaks is  $|b_j|^2$ , and all Bragg peaks have the same intensity.

### 2.7.2 Structure Factor for Non-Monatomic Structures

We evaluate the structure factor as a sum over each atom in the basis.

Example 1: CsCl.

Simple cubic lattice, so  $G_{hk\ell} = \frac{2\pi}{a}(h,k,\ell)$ .

Basis is  $Cs^+$  ion at (0,0,0), and  $Cl^-$  ion at a(0.5,0.5,0.5).

For X-rays, the scattering power is proportional to the number of electrons ( $Cs^+$  have 54 electrons, while  $Cl^-$  have 18). Structure factor<sup>2</sup> =  $sf^2$ 

$$sf^{2} = \left| 54 \underbrace{e^{\frac{2\pi i}{a}(h,k,\ell) \cdot a(0,0,0)}}_{1} + 18e^{\frac{2\pi i}{a}(h,k,\ell) \cdot a(0,5,0.5,0.5)} \right|^{2}$$
$$= 18^{2} \left| 3 + e^{2\pi i(h,k,\ell) \cdot (0.5,0.5,0.5)} \right|^{2}$$
$$= 18^{2} \left( 3 + e^{i\pi(h+k+\ell)} \right)^{2}$$

There are two distinct cases:  $h + k + \ell$  even, and  $h + k + \ell$  odd.  $\frac{sf^2}{18^2} = 4^2 = 16 \text{ when } h + k + \ell \text{ even.}$   $\frac{sf^2}{18^2} = 2^2 = 4 \text{ when } h + k + \ell \text{ odd.}$ 

A measurement of the Bragg scattering from a crystal of *CsCl* gives peaks which correspond to a simple cubic reciprocal lattice, with relative intensities as given. It is this intensity information which enables us to say what the basis, and hence the structure, is.

### Example 2: Silicon Si

Take a conventional *fcc* lattice, and remember that some points are systematic absences. The rule for  $h, k, \ell$  are either all even, or all odd. All other cases are systematic absences.

The basis is 2 silicon atoms  $\underline{r}_1 = (0,0,0), \ \underline{r}_2 = a \left( \frac{1}{4}, \frac{1}{4}, \frac{1}{4} \right).$ 

$$\underline{G}_{hk\ell} = \frac{2\pi}{a} (h, k, \ell)$$

Each Silicon atom has 14 electrons.

$$sf^{2} = \left| 14e^{\frac{2\pi i}{a}(h,k,\ell) \cdot a(0,0,0)} + 14e^{\frac{2\pi i}{a}(h,k,\ell) \cdot a(0.25,0.25,0.25)} \right|^{2}$$
$$\frac{sf^{2}}{14^{2}} = \left| 1 + e^{\frac{i\pi(h+k+\ell)}{2}} \right|^{2}$$

Consider: a)  $h, k, \ell$  all odd.  $h + k + \ell$  is also odd.  $\left(\frac{sf}{14}\right)^2 = |1 + i|^2 = 2$ 

b)  $h, k, \ell$  all even.  $h + k + \ell$  is also even, and is a multiple of 4.  $h + k + \ell = 4n$  $\left(\frac{sf}{14}\right)^2 = |1+1|^2 = 4$ b)  $h, k, \ell$  all even.  $h + k + \ell$  is also even, and is not a multiple of 4.  $h + k + \ell = 4n + 2$  $\left(\frac{sf}{14}\right)^2 = |1-1|^2 = 0$ 

# 2.7.3 Accidental Absences

Note that for silicon, there are reciprocal lattice points where the structure factor is 0. These are called *accidental absences*. These arise as a result of a cancellation within the basis, and not as a result of the lattice symmetry. In silicon, (1,0,0) is

systematically absent, for example, but the (2,2,2) is accidentally absent.

Distortions of the electron cloud can result in a lack of strict cancellation of the structure factor. We have assumed in calculating the structure factor than both atoms have the same shape, in the same orientation, which is not required by the symmetry of the lattice. Careful experiments reveal some diffraction at accidental absences. This is never true for systematic absences.

# 2.8 Diffraction Experiments

Any particle can be used, provided:

- Particles interact with the crystal, but not too strongly (so they don't just interact at the surface).
- Available intense beam
- Efficient detection of scattered beam
- Wavelength less than or equal to a lattice spacing.

For most simple crystal structures, lattice spacings are around 2-5 Angstroms (1 Angstrom =  $10^{-10}$  m, or 1nm = 10 Angstrom). The ideal wavelength is  $\lambda = 0.5 \rightarrow 2$  Angstrom. The most commonly used are X-rays, electrons, and neutrons.

# 2.8.1 X-Ray Diffraction

Production of X-rays 1. X-ray tube



Cheap, easy to use. Rotating anodes, cooled by water. Can produce intense beams, particularly on the characteristic lines.

2. Synchrotron radiation

Bending radiation when highly relativistic particles (usually electrons) are accelerated in a magnetic field.

E.g.:

Daresbury Laboratory. See <u>www.srs.ac.uk</u>. ESRF, Grenoble. <u>www.esrf.fr</u>. Diamond (Rutherford-Appleton Laboratory, near Oxford) <u>www.diamond.ac.uk</u> Very intense, highly collimated, white beams. Expensive, inconvenient.

# Detection of X-rays

Originally photographic methods. Still used. Now Mostly ionization chambers, Geiger-Muller tubes, Scintillation detectors, or Solid State detectors.

# Interaction of X-rays with crystals

Incident X-ray has an oscillating  $\underline{E}$  field which accelerates all the electrons in the atom, which then radiate because they are accelerating. Emitted X-ray has the same wavelength as the incident X-ray, and is coherent with it.

We get stronger scattering from heavy elements, and it can be difficult to detect scattering from lighter elements (low Z), especially in the presence of heavier ones. Hydrogen  $(H^+)$  is especially difficult to "see" with X-rays.

Resonant scattering of X-rays if  $E_I = E_m - E_n$  in atom in crystal (i.e. the energy incoming is equal to the separation of two energy levels). This can enhance scattering power by many orders of magnitude. Needs tunable source (i.e. synchrotron).

# Form Factor

Because the electron density is diffuse (spread out), scattering is not the same as from a point scatterer. The effect is to provide some destructive interference between scattering from electrons in the same atom. This effect increases for larger scattering angles, or increasing |Q|, and it reduces the scattered intensity at higher |Q|-values.

# **2.8.2 Neutron Diffraction**

Production of suitable neutrons We need  $\lambda \sim 1$  Angstrom  $\rightarrow$  energy:

$$E = \frac{p^2}{2m} = \frac{h^2}{2m\lambda^2} = \frac{3}{2}k_BT$$

The temperature  $T \approx 480k$ , i.e. around room temperature.

1. Thermalise neutrons from fission in the core of a thermal reactor. A tube through the biological shielding gives a white beam, characteristic temperature of  $T \sim 300k$ .



e.g. Institut Lane-Langevin, Grenoble, <u>www.ill.fr</u>.

2. Spallation

Accelerate charged particles (p, e), and aim them at a heavy metal target (Ta,

Uranium [with associated political problems], Tungsten, Mercury). Then moderate the fast neutrons which "spall" off the target.



Thermal neutrons

E.g.:

ISIS (Rutherford-Appleton Laboratory) <u>www.isis.ac.uk</u> SNS (Oak Ridge, TN) will be completed 2006. <u>www.sns.gov</u> Materials and Life Facility, MLF (J-Parc, Japan) <u>http://j-parc.jp/MatLife/en</u> to be completed in 2007.

### Interaction of neutrons with crystals

 Strong nuclear force Nuclei effectively point potentials. Scattering length *b* may be of either sign. Typically a few *fm*.

Simpler than X-ray case (no form factor). Sensitive to light atoms  $({}^{1}H, {}^{2}H)$ , so also useful in biology, polymer chemistry, etc.

2. Magnetic dipole of neutron

Interacts with magnetic (unpaired) electrons. Can measure magnetic structures directly (e.g. antiferrimagnets, ferrimagnets). Scattering lengths are similar to the 1<sup>st</sup> mechanism. But it has a form factor – depending on extent of electrons (3d, 4d, 5f).

www.ncnr.nist.gov/resources/n-lengths/

### **2.8.3 Electron Diffraction**

Electrons are very easy to produce and detect (kV give useful wavelengths). It is hard to penetrate solid material, because of the electronic charge – it interacts too strongly with the electrons in the solid. So it is mostly applicable to thin layers and surfaces.

It interacts via the Coulomb interaction (nuclei and electrons), as well as the exchange interaction with electrons. The stronger interaction makes it harder to extract quantitative information than in X-ray and neutron cases.

See Hook & Hall Chapter 12 for more information on this.

# 2.8.4 Experimental Arrangements

### 1. Single Crystal

Use a monochromatic incident beam, achieved by Bragg diffraction from a monochromator crystal.



Monochromator has spacing  $d_m$ .

White beam incoming, monochromatic beam coming out with direction  $\underline{k}_i$ .

We know that  $\lambda_I = 2d_m \sin \theta$ So

 $\left|\underline{k}_{i}\right| = \frac{\pi}{d_{m}\sin\theta}$ 

Need to establish the diffraction condition  $\underline{Q} = \underline{G}_{hk\ell}$ . Consider a plane of reciprocal lattice including the origin for a crystal with a simple cubic lattice.



The construction tells us, for any given wavelength,  $\left(\lambda = \frac{2\pi}{|\underline{k}|}\right)$  what orientation we need for the incident beam  $\underline{k}_i$  and the final beam  $\underline{k}_f$  with respect to the crystal axes (lattice vectors). In this case  $Q = \underline{G}_{110}$ .

In general, we need to calculate the relative orientations of  $\underline{a}, \underline{b}, \underline{c}$  with respect to the reciprocal lattice vectors  $\underline{a}^*, \underline{b}^*, \underline{c}^*$ .

We set this up for each  $\underline{G}_{hk\ell}$ , and measure the diffracted intensity.

### 2. Powder Diffraction

It isn't always possible to obtain a single crystal sample. We can use a powdered or polycrystalline sample. Use a monochromatic incident beam as before.



All orientations of crystallite present, may be equally distributed, or may be textured. Some small fraction of crystallites scatter with each cone. The scalar form of Bragg's law is most useful.

In cubic crystals, 
$$d_{hk\ell} = \frac{a}{\left(h^2 + k^2 + \ell^2\right)^{1/2}}$$
.

Take account of the multiplicity of equivalent planes. e.g. multiplicity of  $\{110\}$  is 6,  $\{120\}$  is 24, etc.

If planes have equal d-spacing, e.g. (333) and (511), the powder experiment cannot distinguish between them. They can be distinguished in a single crystal experiment.