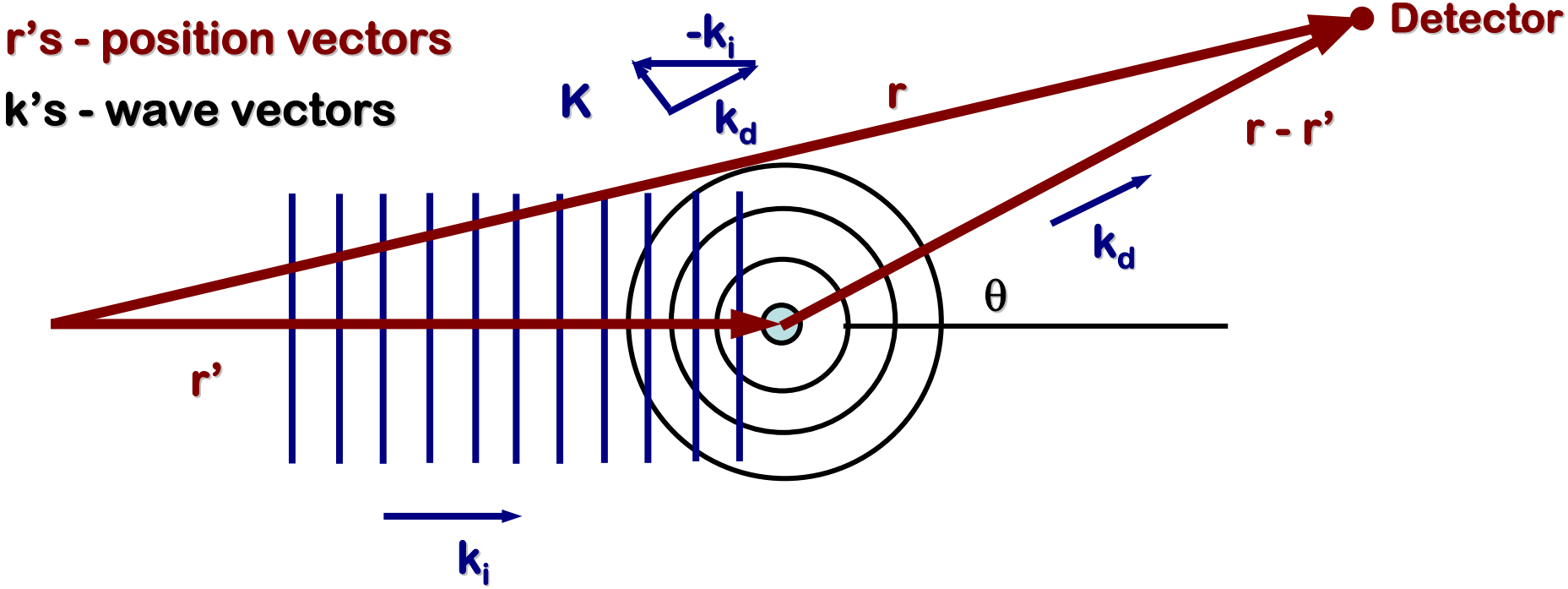
Diffraction from Crystals
“Structure Factor”

Lecture 5

Coherent elastic scattering

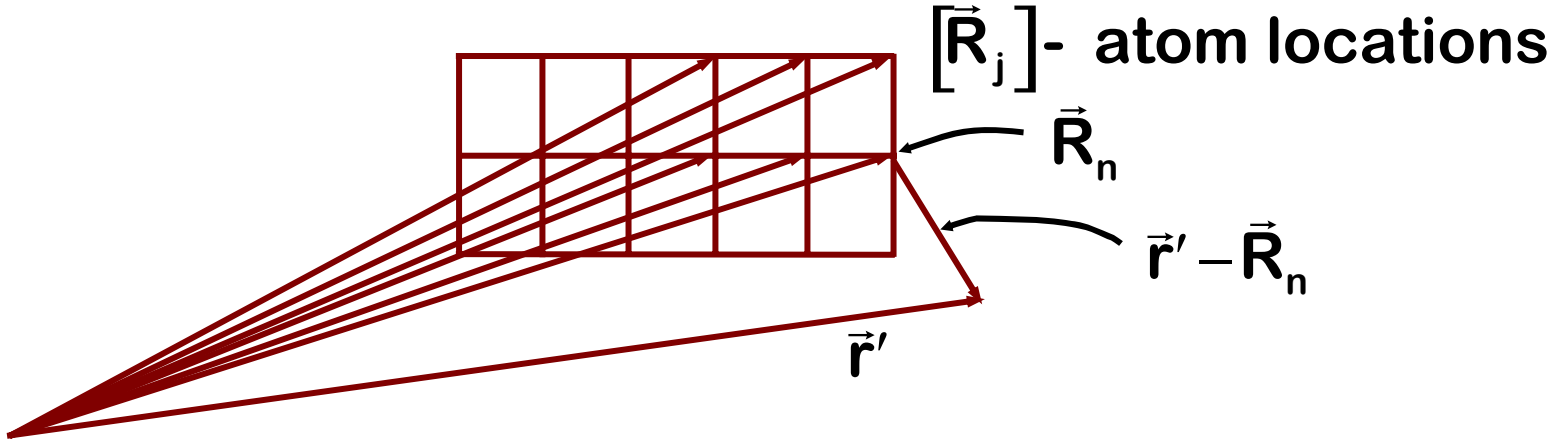


Incident plane wave: $\Psi_{\text{incident}} = \exp\left[2\pi i(\vec{k}_i \cdot \vec{r}' - \omega t)\right] = \exp\left[2\pi i(\vec{k}_i \cdot \vec{r}')\right]$

Scattered wave:

$$\Psi_{\text{scattered}} = f(\vec{k}_i, \vec{k}_d)\frac{\exp\left[2\pi i\vec{k}_d \cdot (\vec{r} - \vec{r}')\right]}{|\vec{r} - \vec{r}'|} = f(\theta)\frac{\exp\left[2\pi i\vec{k}_d \cdot (\vec{r} - \vec{r}')\right]}{|\vec{r} - \vec{r}'|}$$

Scattering from a lattice

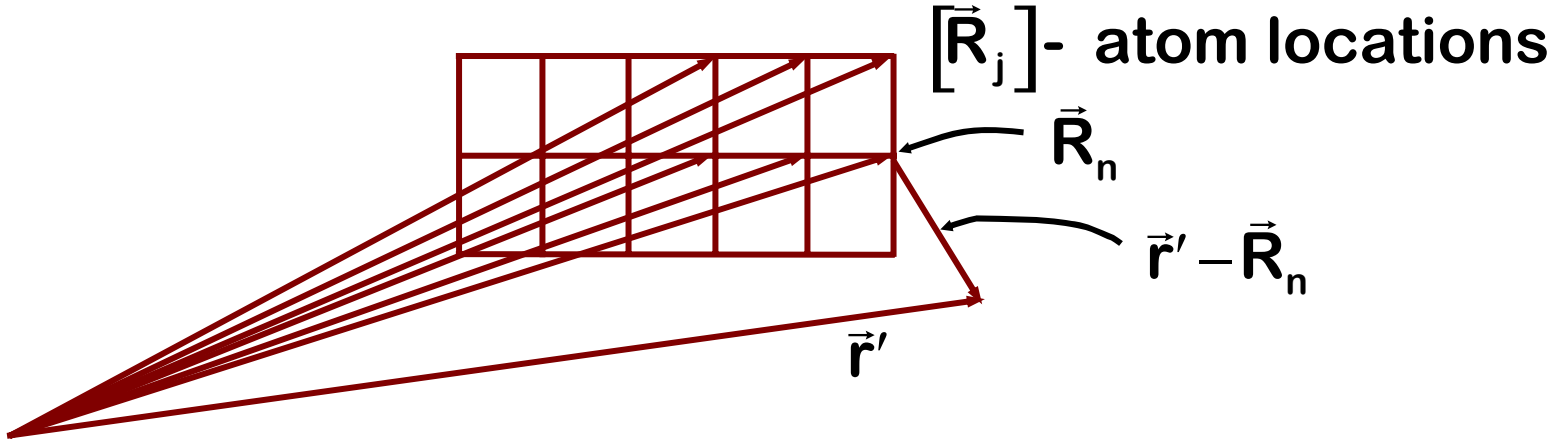


$$V_{atom}(\vec{r}') = \sum V_{at}(\vec{r}' - \vec{R}_j)$$

$$\Psi_{scattered}(\vec{K}, \vec{r}) =$$

$$\frac{-m}{2\pi\hbar^2} \frac{\exp\left[2\pi i(\vec{k}_d \cdot \vec{r})\right]}{|\vec{r}|} \int \sum V_{at}(\vec{r}' - \vec{R}_j) \exp\left[-2\pi i(\vec{K} \cdot \vec{r}')\right] d^3\vec{r}'$$

Scattering from a lattice



$$\vec{r} \equiv \vec{r}' - \vec{R}_j \quad (\text{i.e. } \vec{r}' = r + R'_j)$$

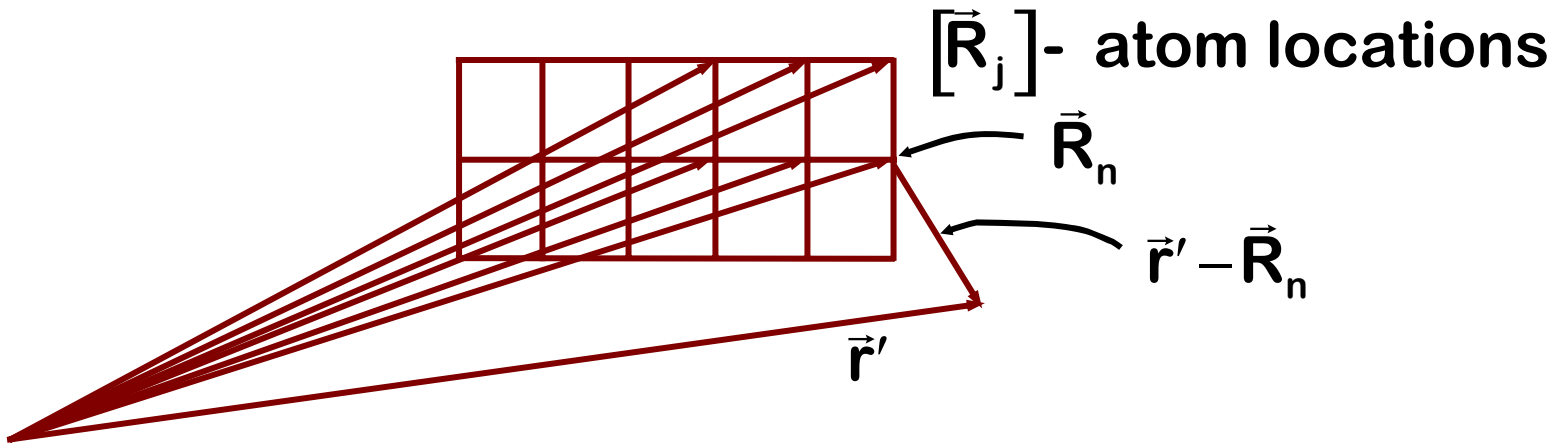
$$f_{el}(\vec{R}_j, \vec{K}) \approx f_{el}(\vec{R}_j)$$

Ignore the $1/r^2$ term to give:

$$\Psi_{scatt}(\vec{K}) = \frac{-m}{2\pi\hbar^2} \int \sum V_{at,\vec{R}_j}(r) \exp\left[-2\pi i\left(\vec{K}\cdot\left(\vec{r}+\vec{R}_j\right)\right)\right] d^3\vec{r}'$$

$$= \sum_{\vec{R}_j} \left(\frac{-m}{2\pi\hbar^2} \int V_{at,\vec{R}_j}(r) \exp\left[-2\pi i\left(\vec{K}\cdot\vec{r}\right)\right] d^3\vec{r}' \right) \exp\left[-2\pi i\left(\vec{K}\cdot\vec{R}_j\right)\right]$$

Scattering from a lattice



So scattered wave from an array of N atoms:

$$\Psi_{scatt}(\vec{K}) = \sum_{j}^{N} f_{el}(\vec{R}_j) \exp\left[-2\pi i(\vec{K}\cdot\vec{R}_j)\right]$$

Notes:

- Now have $\Psi(\vec{K})$ only, $\vec{R}_j$ are fixed. Means scattered wave depends on incident wave vector.
- This is a Fourier Transform (FT)

Diffracted intensity is proportional to the Fourier Transform of the scattering factor distribution in the material

Scattering from a lattice

In simplest form, a crystal is:

Crystal = lattice + basis + defect displacements

$$\vec{R}_j = \vec{r}_{lattice} + \vec{r}_{basis} + \vec{r}_{defects} = \vec{r}_l + \vec{r}_b + \vec{r}_d$$

For now, consider a defect free crystal:

Crystal = lattice + basis

$$\vec{R}_j = \vec{r}_{lattice} + \vec{r}_{basis} = \vec{r}_l + \vec{r}_b$$

Scattered wave:

$$\Psi_{scatt}(\vec{K}) = \sum_{r_l}\sum_{r_b} f_{el}(\vec{r}_l + \vec{r}_b)\exp\left[-2\pi i\left(\vec{K}\cdot(\vec{r}_l + \vec{r}_b)\right)\right]$$

Basis must be same for all unit cells: $f(\vec{r}_l + \vec{r}_b) = f(\vec{r}_b)$

$$\Psi_{scatt}(\vec{K}) = \sum_{r_l}\exp\left[-2\pi i\left(\vec{K}\cdot\vec{r}_l\right)\right]\sum_{r_b} f_{el}(\vec{r}_b)\exp\left[-2\pi i\left(\vec{K}\cdot\vec{r}_b\right)\right]$$

Scattering from a lattice

Repeating:

$$\Psi_{scatt}(\vec{K}) = \sum_{\vec{r}_l} \exp\left[-2\pi i(\vec{K}\cdot\vec{r}_l)\right] \sum_{\vec{r}_b} f_{el}(r_b)\exp\left[-2\pi i(\vec{K}\cdot\vec{r}_b)\right]$$

$$\Psi_{scatt}(\vec{K}) = S(\vec{K})F(\vec{K})$$

where:

$$S(\vec{K}) = \sum_{\vec{r}_l}^{lattice} \exp\left[-2\pi i(\vec{K}\cdot\vec{r}_l)\right] \quad \text{“Shape Factor”}$$

$$F(\vec{K}) = \sum_{\vec{r}_b}^{basis} f_{el}(r_b)\exp\left[-2\pi i(\vec{K}\cdot\vec{r}_b)\right] \quad \text{“Structure Factor”}$$

$F(\vec{K})$ same for all lattice points:

$$\Psi(\vec{K}) = \sum_{\vec{r}_l}^{lattice} F(\vec{K})\exp\left[-2\pi i(\vec{K}\cdot\vec{r}_l)\right]$$

Structure Factor

Structure Factor:

- Scattering from all atoms in the unit cell

$$F(\vec{K}) = \sum_{\vec{r}_b}^{\text{basis}} f_{el}(\vec{r}_b) \exp\left[-2\pi i(\vec{K} \cdot \vec{r}_b)\right]$$

In essence, Structure Factor determines whether or not constructive interference occurs at a given reciprocal lattice point

This means our prior condition - $\vec{K} = \vec{g}$ - is a necessary condition, but is not sufficient

- There may not be intensity at a given $\vec{g}$!

Structure factor

calculation

Consider i atoms in the unit cell

$$F(\vec{K}) = \sum_i f_i \exp\left[-2\pi i\left(\vec{K}\cdot\vec{r}_i\right)\right]$$

Location of i^{th} atom (with respect to real lattice):

$$\vec{r}_i = x_i\vec{a} + y_i\vec{b} + z_i\vec{c}$$

Diffraction condition (K = g):

$$\vec{K} = h\vec{a}^* + k\vec{b}^* + l\vec{c}^*$$

Using def^n of a*, b* & c*

General from:

$$F(\vec{K}) = \sum_i f_i \exp\left[-2\pi i\left(hx_i + ky_i + lz_i\right)\right]$$

Structure Factor

simple cubic

$$F = \sum_i f_i \exp\left[-2\pi i\left(hx_i + ky_i + lz_i\right)\right]$$

One atom basis: $r = (0,0,0)$

$$F = f\left\{\exp\left[-2\pi i\left(0\cdot h + 0\cdot k + 0\cdot l\right)\right]\right\}$$

$$= f\left\{\exp\left[-2\pi i\left(0\right)\right]\right\}$$

$$= f\left\{\exp\left[0\right]\right\}$$

$$= f$$

Simple result: intensity at every reciprocal lattice point

Structure Factor

body-centered cubic

Two atom basis: $\mathbf{r} = (0,0,0)$ & $\mathbf{r} = \left(\frac{1}{2},\frac{1}{2},\frac{1}{2}\right)$

$$F = f\left\{\exp\left[-2\pi i\left(0\cdot h + 0\cdot k + 0\cdot l\right)\right] + \exp\left[-2\pi i\left(\frac{1}{2}\cdot h + \frac{1}{2}\cdot k + \frac{1}{2}\cdot l\right)\right]\right\}$$

$$= f\left\{1 + \exp\left[-\pi i\left(h + k + l\right)\right]\right\}$$

h, k & l are integers, so $h + k + l = N$ (where N is an integer)

The exponential can then take one of two values:

$$\exp\left[-\pi i\left(h + k + l\right)\right] = +1 \quad \text{if } N = \text{even}$$

$$\exp\left[-\pi i\left(h + k + l\right)\right] = -1 \quad \text{if } N = \text{odd}$$

So:

$$F = 2f \quad \text{if } N = \text{even}$$

$$F = 0 \quad \text{if } N = \text{odd}$$

Structure Factor

body-centered cubic

Allowed low order reflections are:

- 110, 200, 220, 310, 222, 321, 400, 330, 411, 420 …

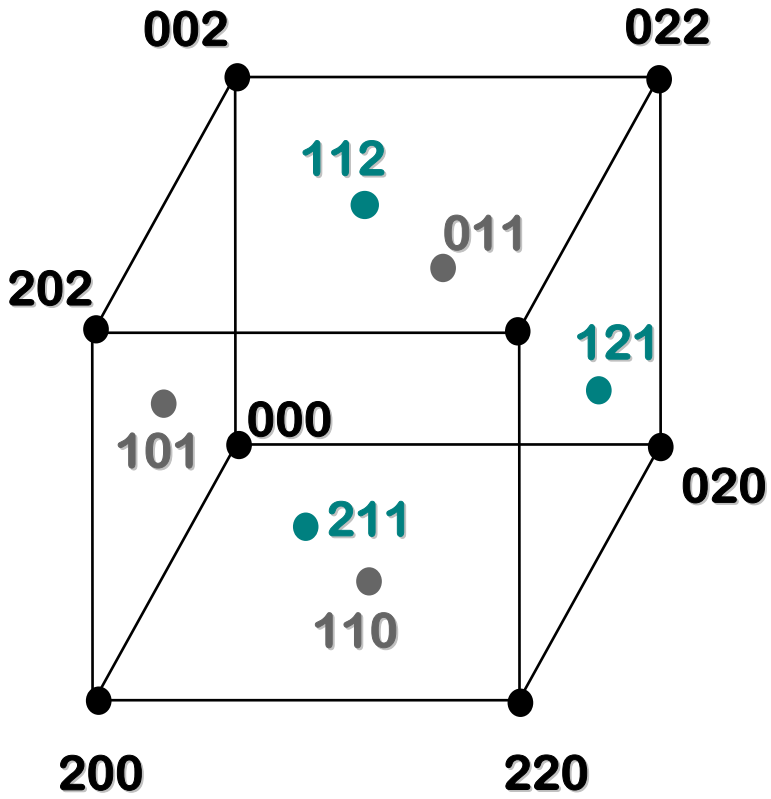
Forbidden reflections are:

- 100, 111, 210

Origin of forbidden reflections?

- Identical plane of atoms halfway between causes destructive interference

Real bcc lattice has an fcc reciprocal lattice



Structure Factor

face centered cubic

Four atom basis: $\mathbf{r} = (0,0,0)$, $\mathbf{r} = \left(\frac{1}{2},\frac{1}{2},0\right)$, $\mathbf{r} = \left(\frac{1}{2},0,\frac{1}{2}\right)$ & $\mathbf{r} = \left(0,\frac{1}{2},\frac{1}{2}\right)$

$$F = f\left\{1+\exp\left[-\pi i\left(h+k\right)\right]+\exp\left[-\pi i\left(k+l\right)\right]+\exp\left[-\pi i\left(h+l\right)\right]\right\}$$

So:

F=4f if h,k,l all even or odd

F=0 if h,k,l are mixed even or odd

Structure Factor

face centered cubic

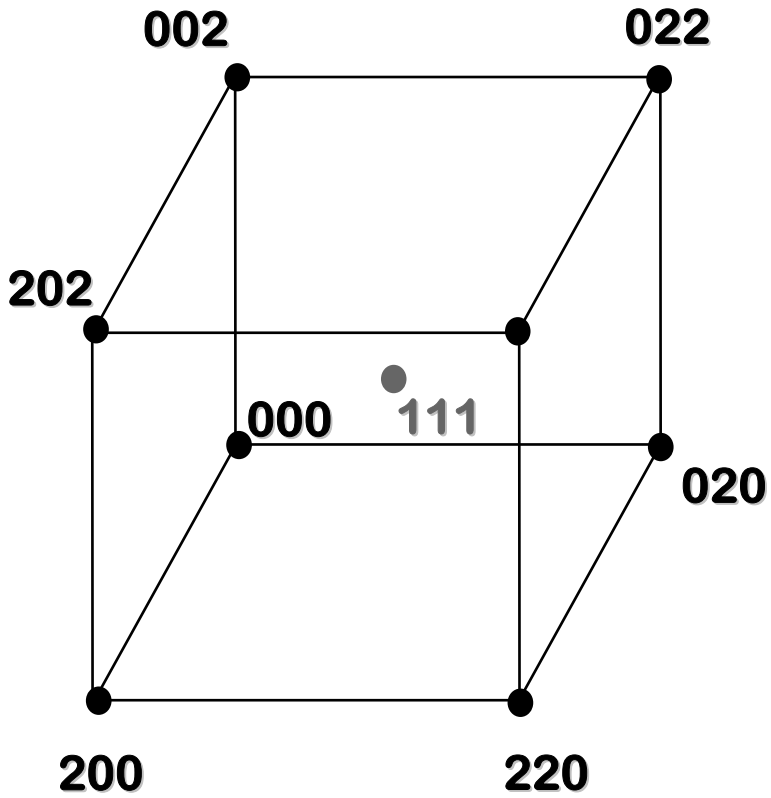
Allowed low order reflections are:

- 111, 200, 220, 311, 222, 400, 331, 310

Forbidden reflections:

- 100, 110, 210, 211

Real fcc lattice has a bcc reciprocal lattice



Structure Factor

NaCl (rock salt) structure

Na on each fcc site, but with a two atom basis:

$$r_{Na} = (0,0,0) \;\&\; r_{Cl} = \left(\frac{1}{2},\frac{1}{2},\frac{1}{2}\right)$$

$$F = \{f_{Na} + f_{Cl}\exp[-\pi i(h+k+l)]\}\times$$

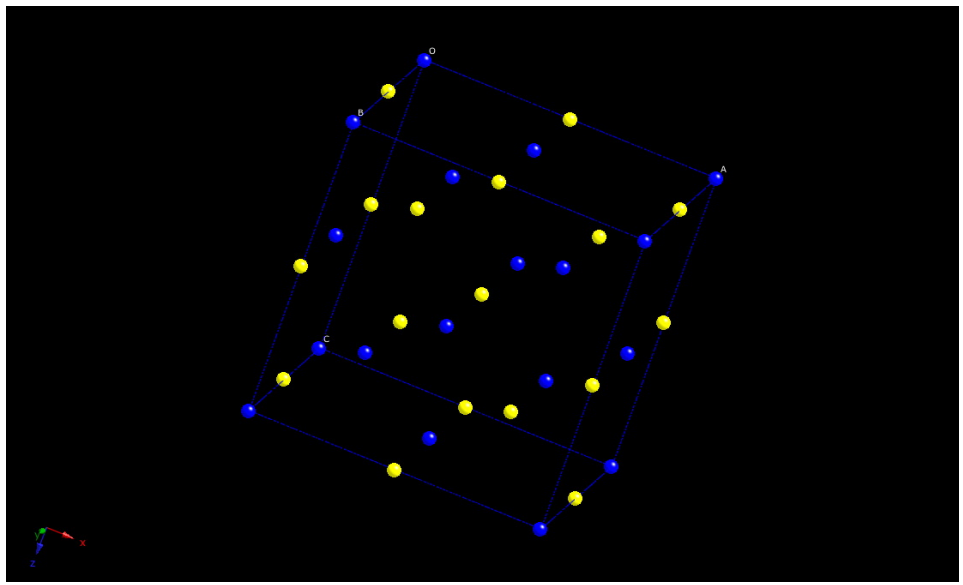
$$\{1+\exp[-\pi i(h+k)]+\exp[-\pi i(k+l)]+\exp[-\pi i(h+l)]\}$$

$F = 4(f_{Na} + f_{Cl})$ if h,k,l all even

$F = 4(f_{Na} - f_{Cl})$ if h,k,l all odd

$F = 0$ if h,k,l mixed

If h,k,l all odd have 'chemically sensitive' reflections



Structure Factor

Ni_3Al ($L1_2$) structure

Simple cubic lattice, with at four atom basis

$$r_{Al} = (0,0,0),\ r_{Ni} = \left(\frac{1}{2},\frac{1}{2},0\right),\ r_{Ni} = \left(\frac{1}{2},0,\frac{1}{2}\right) \ \&\ r_{Ni} = \left(0,\frac{1}{2},\frac{1}{2}\right)$$

$$F = f_{al} + f_{Ni}\exp\left[-\pi i(h+k)\right] + \exp\left[-\pi i(k+l)\right] + \exp\left[-\pi i(h+l)\right]$$

So :

$F=f_{Al}+3f_{Ni}$ if h,k,l all even or odd

$F=f_{Al}-f_{Ni}$ if h,k,l are mixed even or odd

Again, since simple cubic, intensity at all points.

But each point is 'chemically sensitive'.

Chemically sensitive reflections

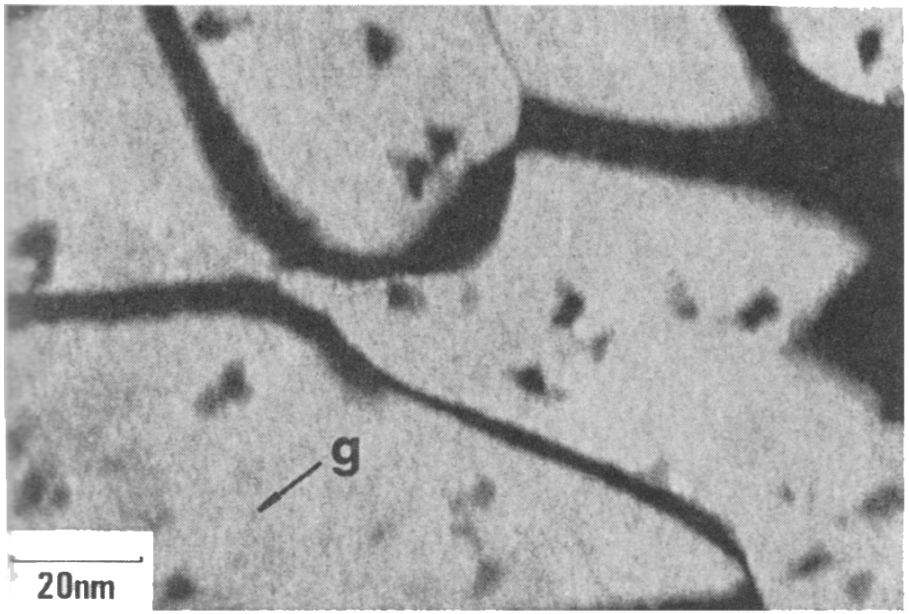


Figure 16.5. DF image from a chemically sensitive 110 reflection showing bright ordered domains in Cu_3Au. The dark areas in the bright domains are regions of local disorder induced by ion beam damage.

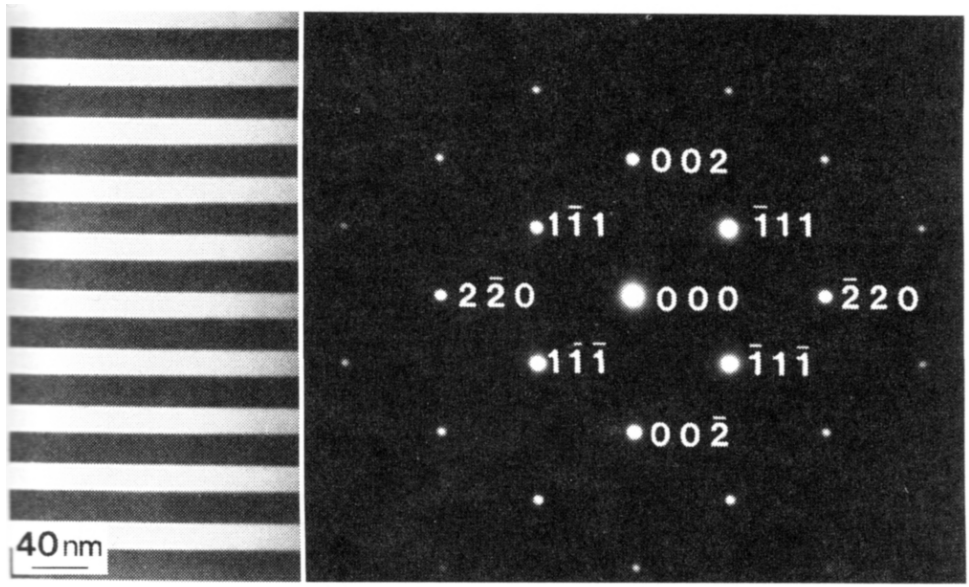


Figure 16.6. (A) DF image from a 002 superlattice reflection in GaAs. The $Al_xGa_{1-x}As$ is the lighter region because Al has replaced Ga in the GaAs (darker regions). (B) Diffraction pattern showing the less intense 002 and other superlattice reflections.

Dark field images formed from chemically sensitive reflections produce a real space map of (highly) local chemistry

Long period superlattices

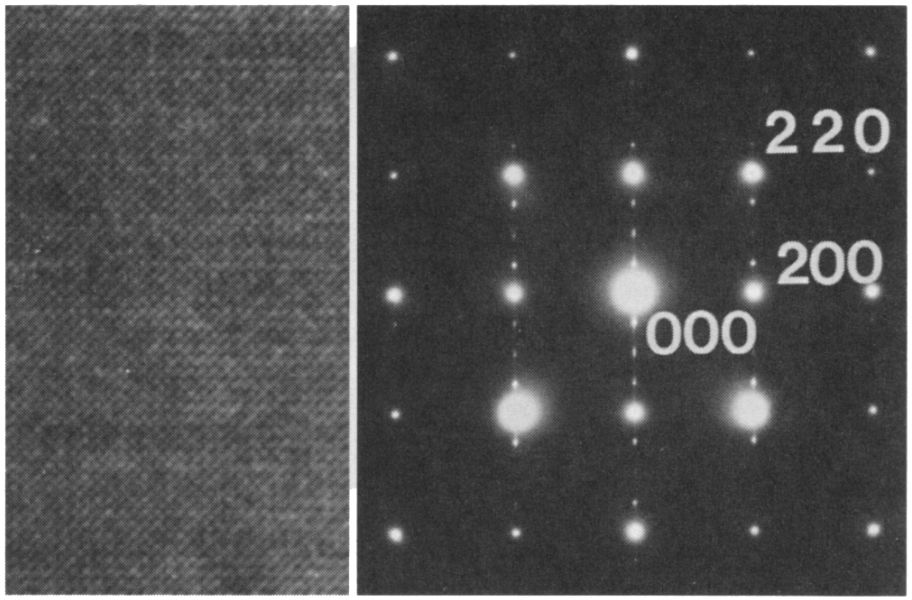


Figure 16.8. (A) Artificial GaAs/$Al_xGa_{1-x}As$ structure in which order is created by alternating four layers of GaAs and four of $(Al_xGa_{1-x})As$. (B) DP showing three superlattice spots between the fundamental reflections in the 020 direction.

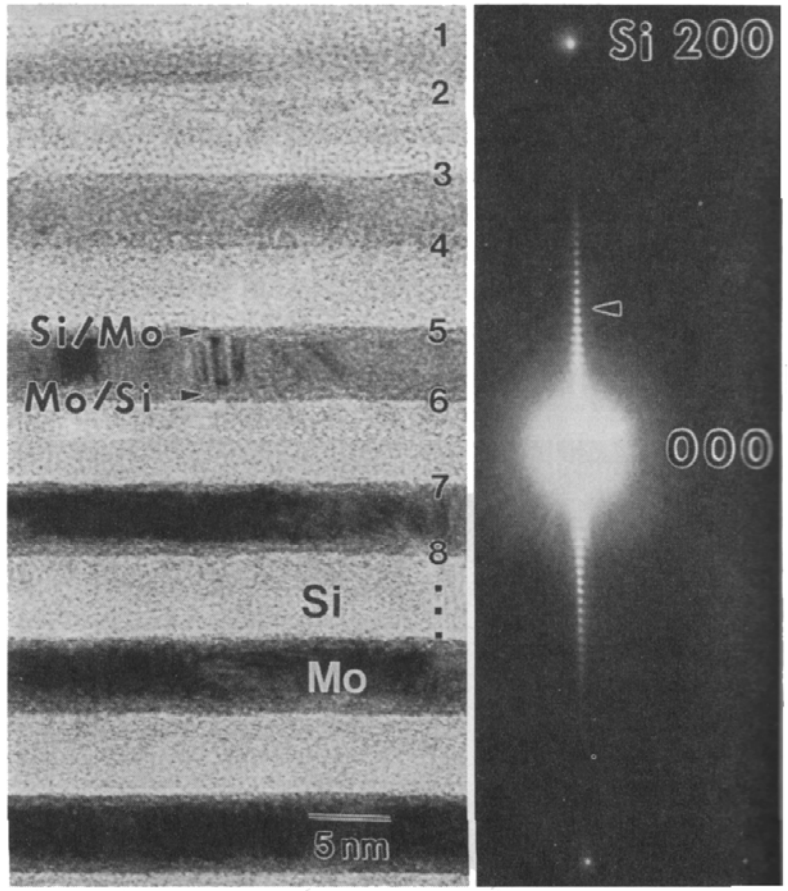


Figure 16.9. (A) Artificial superlattice of Si and Mo layers ~5 nm thick (B) Expanded DP around 000 showing many superlattice spots (arrowed). The large spacing of the superlattice in real space results in very small spacing of the superlattice reflections in the DP in reciprocal space. Compare with Figure 16.8.