Allowed reflections: cubic

sc: any h, k, ℓ

bcc: $h + k + \ell =$ even

fcc: h, k, ℓ all even or all odd

Note the dependence of atomic concentration on nearest-neighbor distance:

sc: $d_{\text{n-n}} = a$

$\rho = 1/a^3 = 1/d_{\text{n-n}}^3$

bcc: $d_{\text{n-n}} = \sqrt{3}a/2 = 0.87a$

$\rho = 2/a^3 = 3\sqrt{3}/8d_{\text{n-n}}^3 = 0.65/d_{\text{n-n}}^3$

fcc: $d_{\text{n-n}} = a/\sqrt{2} = 0.71a$

$\rho = 4/a^3 = \sqrt{2}/d_{\text{n-n}}^3 = 1.41/d_{\text{n-n}}^3$

h	k	ℓ	$h^2+k^2+\ell^2$	sc	bcc	fcc
1	0	0	1	√		
1	1	0	2	√	√	
1	1	1	3	√		√
2	0	0	4	√	√	√
2	1	0	5	√		
2	1	1	6	√	√	
2	2	0	8	√	√	√
2	2	1	9	√		
2	2	2	12	√	√	√
3	0	0	9	√		
3	1	0	10	√	√	
3	1	1	11	√		√
3	2	0	13	√		
3	2	1	14	√	√	
3	2	2	17	√		
3	3	0	18	√	√	
3	3	1	19	√		√
3	3	2	22	√	√	
3	3	3	27	√		√
4	0	0	16	√	√	√
4	1	0	17	√		
4	1	1	18	√	√	
4	2	0	20	√	√	√
4	2	1	21	√		
4	2	2	24	√	√	√
4	3	0	25	√		
4	3	1	26	√	√	
4	3	2	29	√		
4	3	3	34	√	√	

The Zone Axis

Direct lattice vector: $\mathbf{r}_{uvw} = u\mathbf{a}_1 + v\mathbf{a}_2 + w\mathbf{a}_3$

Reciprocal lattice vector: $\mathbf{g}_{hk\ell} = h\mathbf{b}_1 + k\mathbf{b}_2 + \ell\mathbf{b}_3$

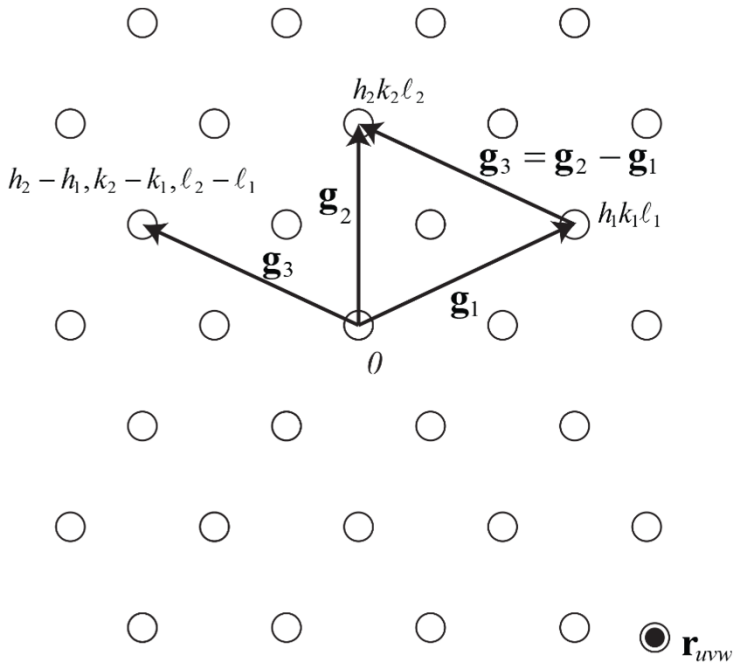
For all RLVs within the ZOLZ: $\mathbf{g}_{hk\ell} \cdot \mathbf{r}_{uvw} = hu + kv + \ell w = 0$

If $\mathbf{g}_1 \cdot \mathbf{r}_{uvw} = 0$

and $\mathbf{g}_2 \cdot \mathbf{r}_{uvw} = 0$

then $(\mathbf{g}_1 - \mathbf{g}_2) \cdot \mathbf{r}_{uvw} = 0$

This is the [*uvw*] zone axis.



Any reflection (*hkl*) in the [*uvw*] ZOLZ has: $hu + kv + \ell w = 0$

Finding the zone axis

If $\mathbf{g}_1$ and $\mathbf{g}_2$ reside in the [*uvw*] ZOLZ, then:

$$[uvw] \| \mathbf{g}_1 \times \mathbf{g}_2$$

$$\mathbf{b}_k = \frac{\mathbf{a}_i \times \mathbf{a}_j}{V} \qquad \mathbf{b}_i = \frac{\mathbf{a}_j \times \mathbf{a}_k}{V}$$

Notice that: $$(\mathbf{a}_i \times \mathbf{a}_j) \times (\mathbf{a}_j \times \mathbf{a}_k) = \left[(\mathbf{a}_i \times \mathbf{a}_j) \cdot \mathbf{a}_k \right] \mathbf{a}_j = V \mathbf{a}_j$$

So: $$\mathbf{b}_k \times \mathbf{b}_i = \frac{\mathbf{a}_j}{V}$$

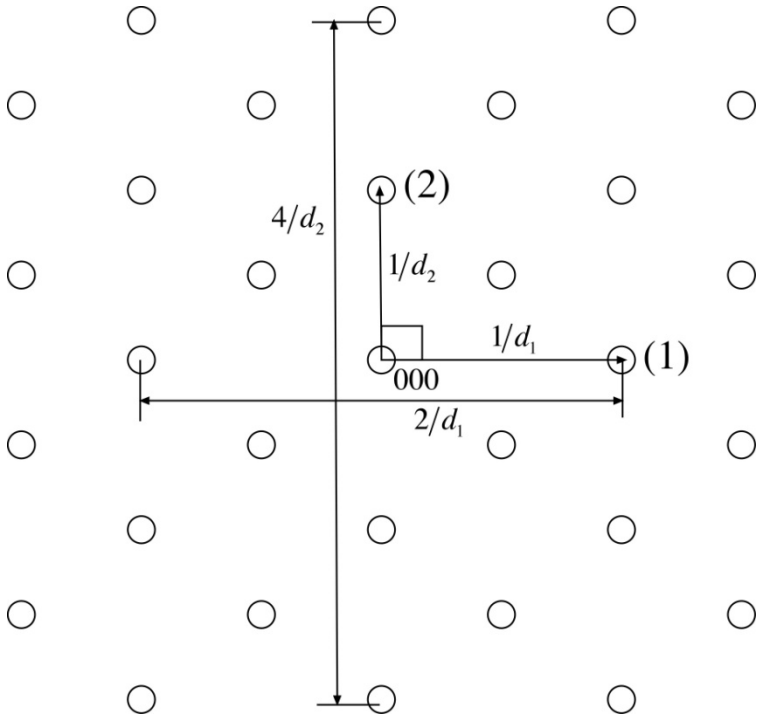
$$\mathbf{g}_1 \times \mathbf{g}_2 = \frac{1}{V} \begin{vmatrix} \mathbf{a}_1 & \mathbf{a}_2 & \mathbf{a}_3 \\ h_1 & k_1 & \ell_1 \\ h_2 & k_2 & \ell_2 \end{vmatrix}$$

The zone axis of a ZOLZ *in any crystal system* satisfies the condition:

$$[uvw] \| [k_1\ell_2 - \ell_1 k_2, \ell_1 h_2 - h_1 \ell_2, h_1 k_2 - k_1 h_2]$$

Determining Orientation

Assume we know the structure (fcc), but not the lattice constant or orientation:



Procedure:

1) measure d_1 and d_2
2) Determine $(d_2/d_1)^2$
3) Look for integer ratio, consistent with fcc
4) Determine types of reflections
5) Select indices, based on angle

$d_1 = 0.208$ nm

$d_2 = 0.293$ nm

$$\left(\frac{d_2}{d_1}\right)^2 = 1.98 \approx \frac{h_1^2+k_1^2+\ell_1^2}{h_2^2+k_2^2+\ell_2^2} = \frac{2}{1} = \frac{4}{2} = \frac{6}{3} = \frac{8}{4} = \frac{2^2+2^2+0^2}{2^2+0^2+0^2}$$

(1): {220}, (2): {200}

$$\mathbf{g}_1 \cdot \mathbf{g}_2 = 0 \Rightarrow (1): 2\bar{2}0,\ (2): 002$$

6) Find zone axis

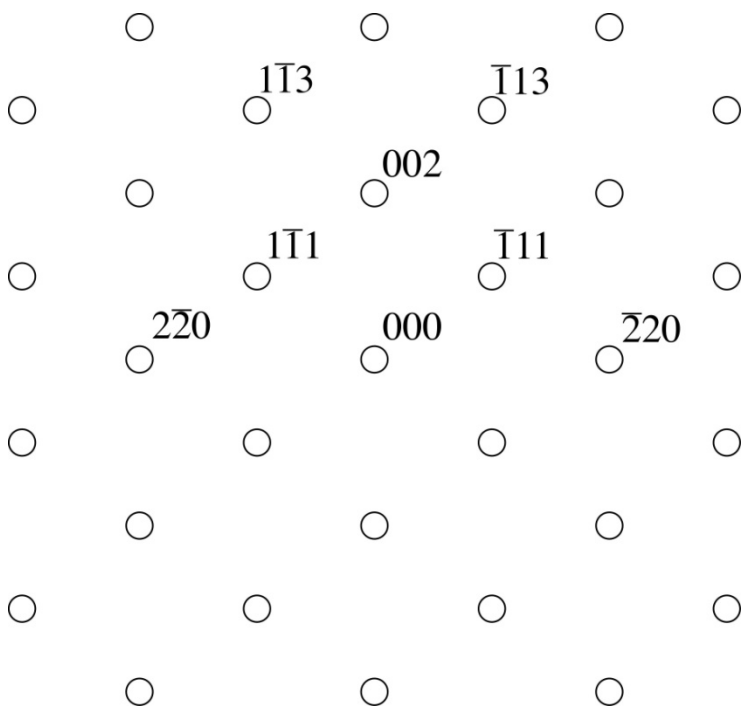
$$[uvw] = [\bar{1}\cdot 1 - 0\cdot 0, 1\cdot 0 - 1\cdot 1, 1\cdot 0 - 0\cdot 1] = [\bar{1}\,\bar{1}0] \longrightarrow \mathbf{B} = [\bar{1}\,\bar{1}0]$$

Reconsider choice→

Revise and index

change: $2\bar{2}0 \rightarrow \bar{2}20$

zone axis: $[uvw] = [1\cdot 1 - 0\cdot 0, 0\cdot 0 - 1\cdot \bar{1}, \bar{1}\cdot 0 - 0\cdot 1] = [110]$



B = [110]

index:

$$\frac{1}{2}[(002)+(\bar{2}20)] = (\bar{1}11)$$

$$(\bar{1}11)+[(002)-(000)] = (\bar{1}13)$$

$$(000)-[(2\bar{2}0)-(000)] = (\bar{2}20)$$

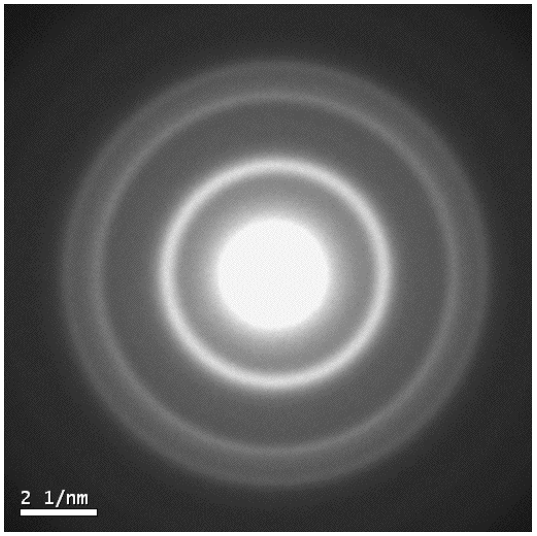
Find lattice constant:

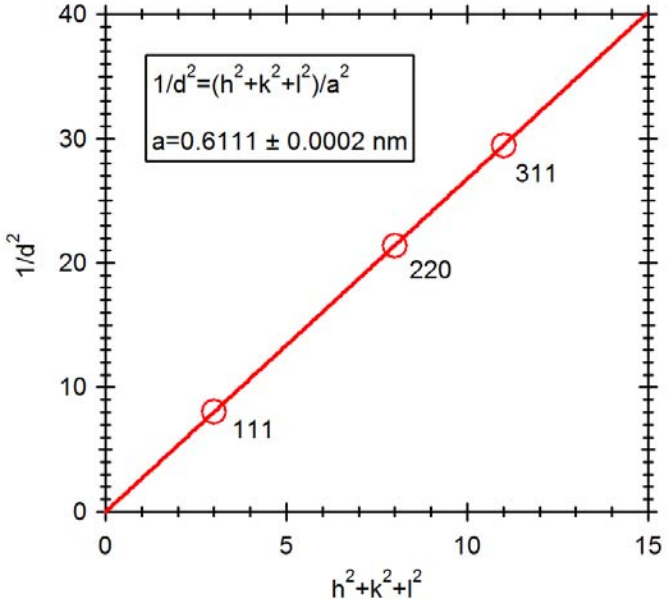
$$d_2 = d_{002} = \frac{a}{2}$$

$$a = 2d_{002} = 0.586 \text{ nm}$$

Powder pattern (I): CdSe

CdSe dots





ring	2/d (1/nm)	d (nm)
1	5.677	0.352
2	9.251	0.216
3	10.858	0.1842

Test fcc:

(1) : 111

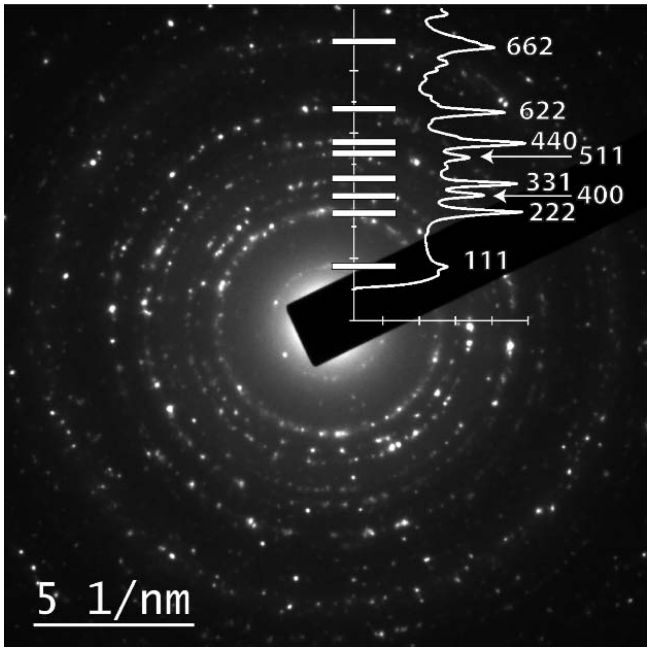
(2): 220

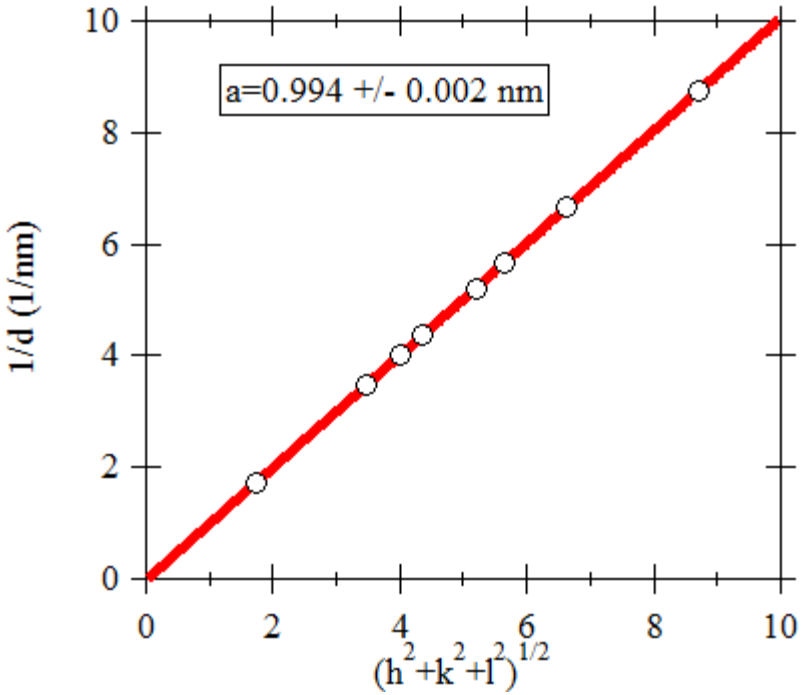
(3): 311

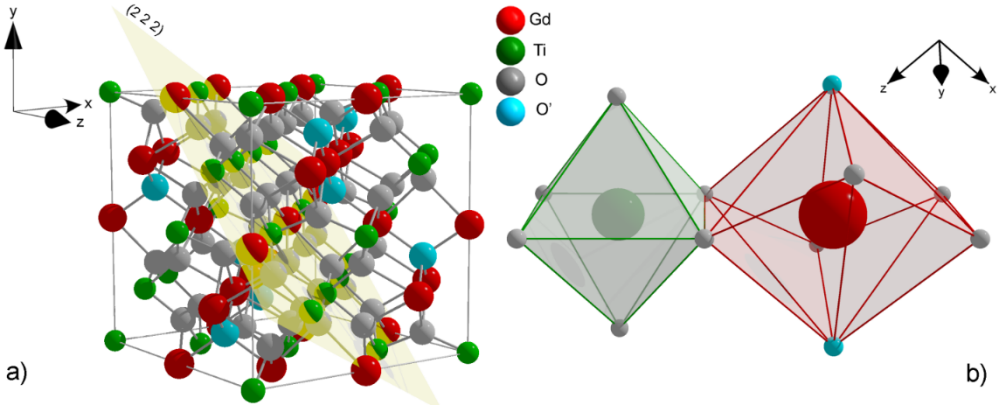
$$\left(\frac{d_2}{d_1}\right)^2 = 2.66 \approx \frac{8}{3} = \frac{2^2+2^2+0^2}{1^2+1^2+1^2}$$

$$\left(\frac{d_3}{d_1}\right)^2 = 3.66 \approx \frac{11}{3} = \frac{3^2+1^2+1^2}{1^2+1^2+1^2}$$

Powder Pattern (II): $Gd_2Ti_2O_4$

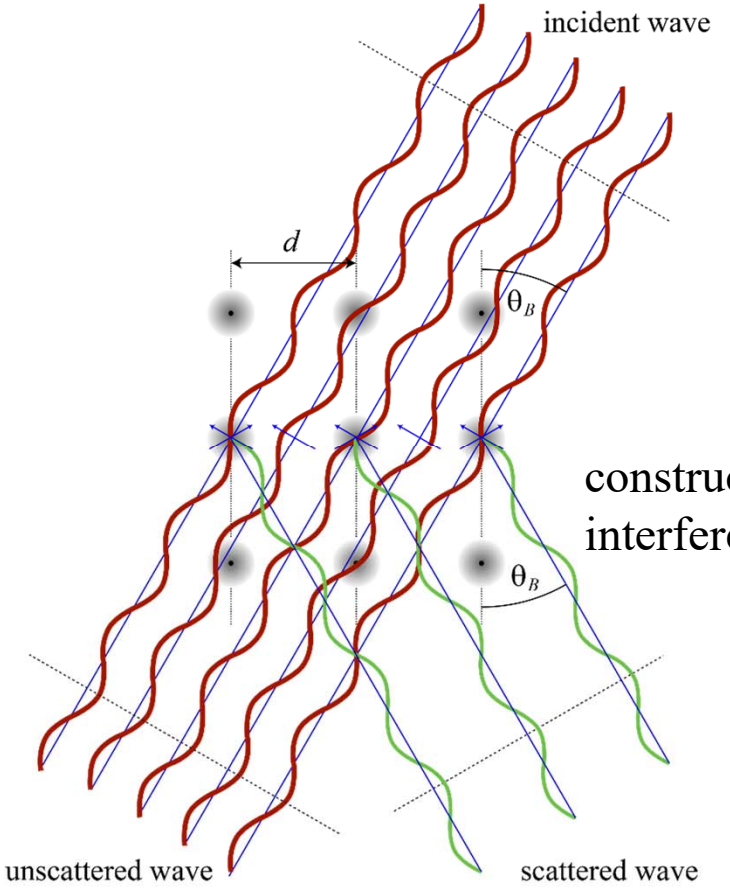






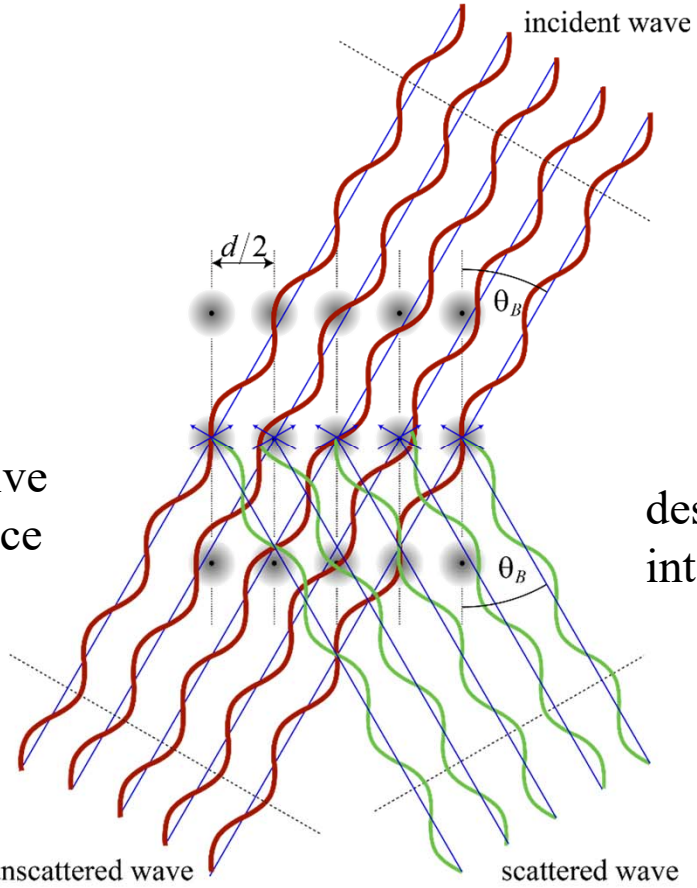
Structure factor and intensity

Inserting planes can reduce the intensities of some peaks.



constructive interference

$$F = f$$



destructive interference

$$F = f \cdot (1 + e^{\pi i}) = 0$$

Waves scattered from inserted planes are 180° out-of-phase.