

Allowed reflections: cubic

sc: any h, k, ℓ

bcc: $h + k + \ell = \text{even}$

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: $\mathbf{g}_{hkl} = h\mathbf{b}_1 + k\mathbf{b}_2 + \ell\mathbf{b}_3$

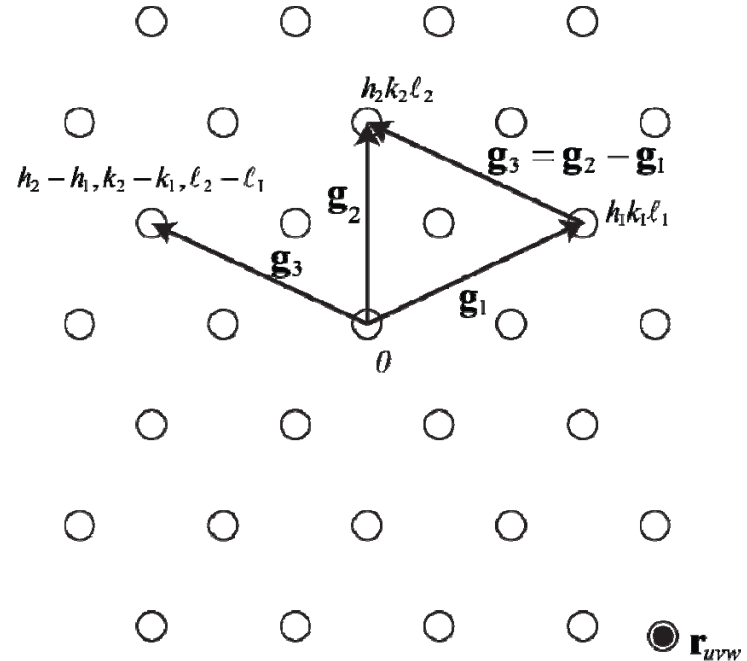
For all RLVs within the ZOLZ: $\mathbf{g}_{hkl} \cdot \mathbf{r}_{uvw} = hu + kv + \ell w = 0$

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:

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

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

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

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

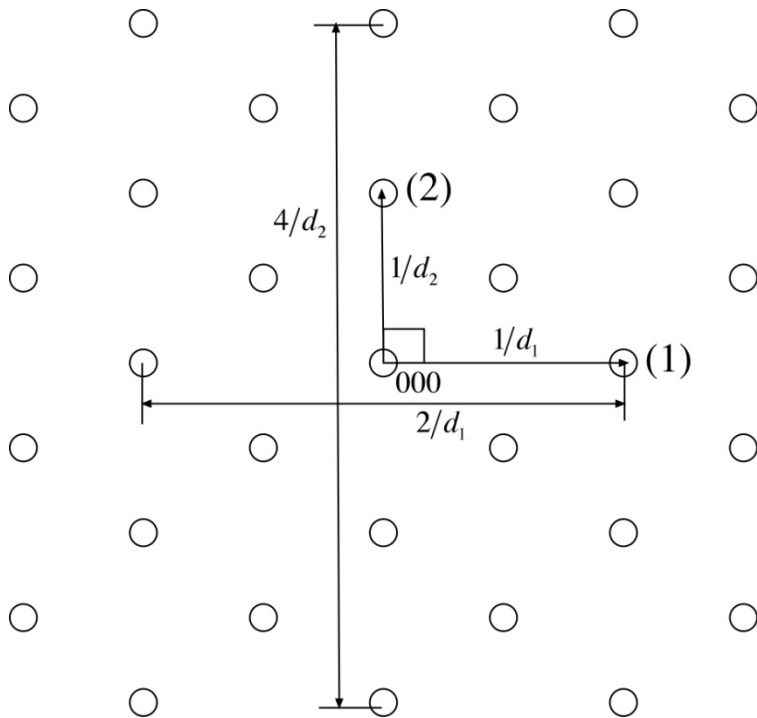
$$\mathbf{g}_1 \times \mathbf{g}_2 = \frac{1}{V} \begin{vmatrix} \mathbf{a}_1 & \mathbf{a}_2 & \mathbf{a}_3 \\ h_1 & k_1 & \ell_1 \\ h_2 & k_2 & \ell_2 \end{vmatrix}$$

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

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

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

$$d_1 = 0.208 \text{ nm}$$

$$d_2 = 0.293 \text{ nm}$$

$$\left(\frac{d_2}{d_1}\right)^2 = 1.98 \approx \frac{h_1^2 + k_1^2 + l_1^2}{h_2^2 + k_2^2 + l_2^2} = \frac{2}{1} = \frac{4}{2} = \frac{6}{3} = \frac{8}{4} = \frac{2^2 + 2^2 + 0^2}{2^2 + 0^2 + 0^2}$$

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

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

6) Find zone axis

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

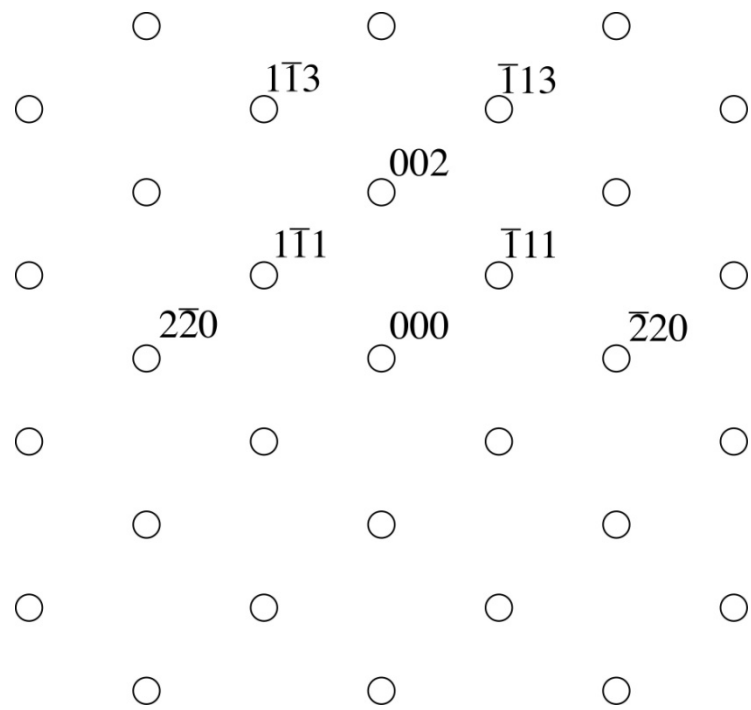
$$\longrightarrow \mathbf{B} = [\bar{1} \bar{1} 0]$$

Reconsider choice \rightarrow

Revise and index

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

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



$\mathbf{B} = [110]$

index:

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

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

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

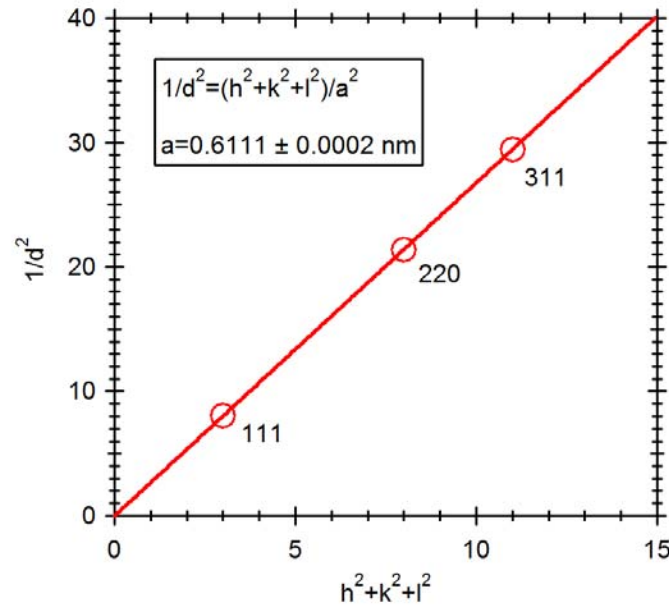
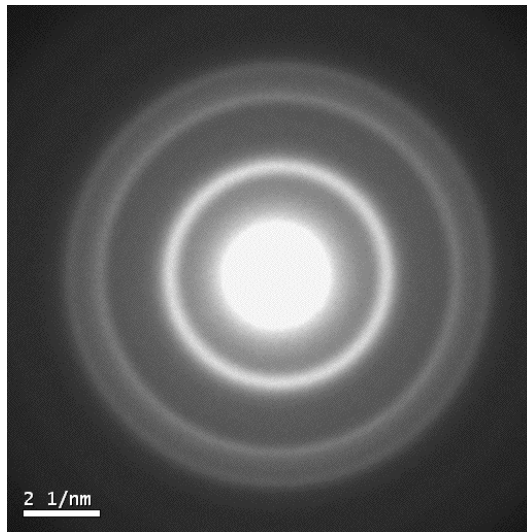
Find lattice constant:

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

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

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

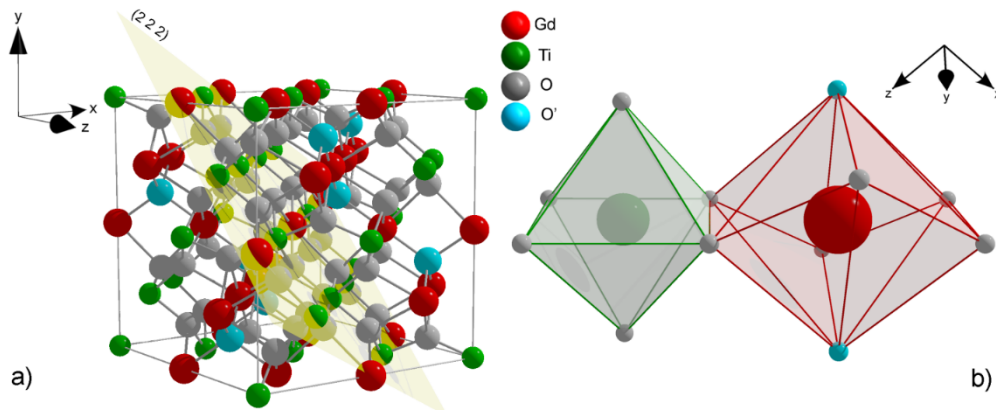
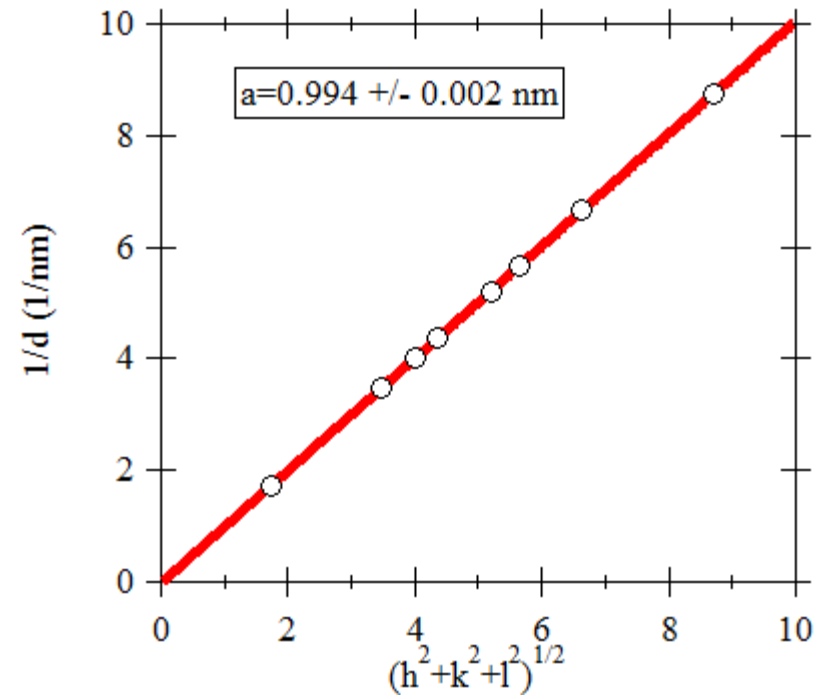
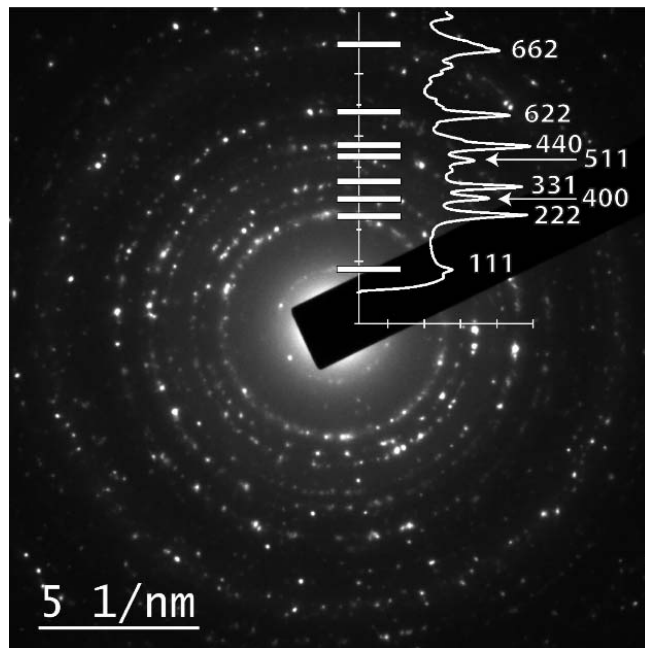
(2): 220

(3): 311

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

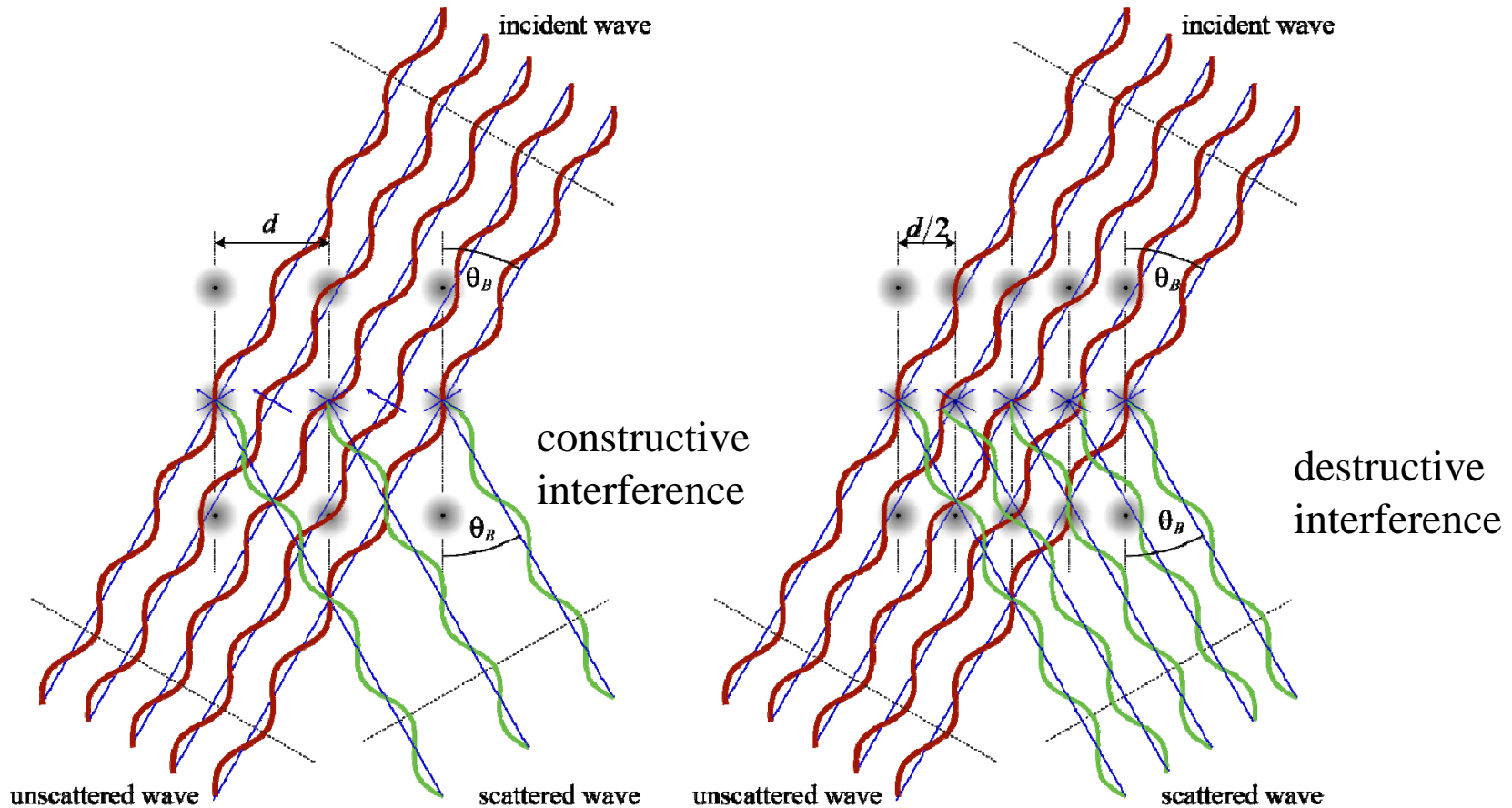
$$\left(\frac{d_3}{d_1}\right)^2 = 3.66 \approx \frac{11}{3} = \frac{3^2 + 1^2 + 1^2}{1^2 + 1^2 + 1^2}$$

Powder Pattern (II): $\text{Gd}_2\text{Ti}_2\text{O}_4$



Structure factor and intensity

Inserting planes can reduce the intensities of some peaks.



$$F = f$$

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

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