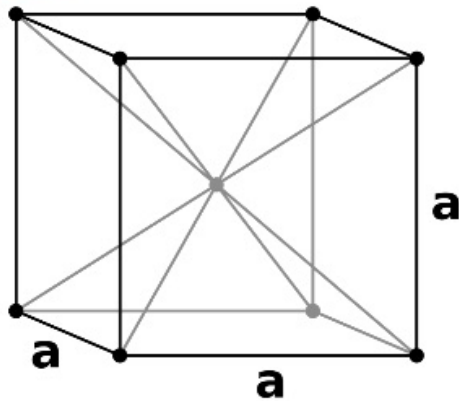


LAST NOTE: STRUCTURE FACTOR



Conventional Vectors

$$\vec{a}_1 = a \hat{x}$$

$$\vec{a}_2 = a \hat{y}$$

$$\vec{a}_3 = a \hat{z}$$

$$\text{BASIS} = (0,0,0) \left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)a$$

$$\hat{x} = (1, 0, 0)$$

$$\hat{y} = (0, 1, 0)$$

$$\hat{z} = (0, 0, 1)$$

$$\vec{q} = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3$$

$$\vec{b}_1 = \frac{2\pi}{a} \hat{x}$$

$$\vec{b}_2 = \frac{2\pi}{a} \hat{y}$$

$$\vec{b}_3 = \frac{2\pi}{a} \hat{z}$$

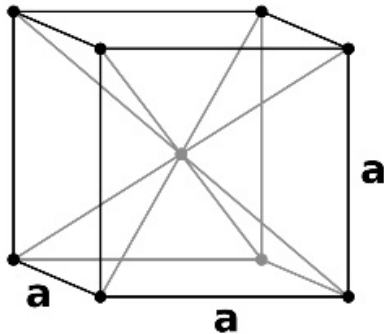
$$S = \begin{cases} 2 & \text{if } h+k+l \text{ even} \\ 0 & \text{if } h+k+l \text{ odd} \end{cases}$$

Primitive Vectors

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LAST NOTE: STRUCTURE FACTOR



Conventional Vectors

$$\vec{a}_1 = a \hat{x}$$

$$\vec{a}_2 = a \hat{y}$$

$$\vec{a}_3 = a \hat{z}$$

$$\text{BASIS} = (0,0,0) \left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)a$$

$$\vec{b}_1 = \frac{2\pi}{a} \hat{x}$$

$$\vec{b}_2 = \frac{2\pi}{a} \hat{y}$$

$$\vec{b}_3 = \frac{2\pi}{a} \hat{z}$$

$$S = \begin{cases} 2 & \text{if } h+k+l \text{ even} \\ 0 & \text{if } h+k+l \text{ odd} \end{cases}$$

Primitive Vectors

$$\vec{a}_1 = \frac{a}{2} (-\hat{x} + \hat{y} + \hat{z})$$

$$\vec{a}_2 = \frac{a}{2} (\hat{x} - \hat{y} + \hat{z})$$

$$\vec{a}_3 = \frac{a}{2} (\hat{x} + \hat{y} - \hat{z})$$

$$\text{BASIS} = (0,0,0)$$

$$\vec{b}_1 = \frac{2\pi}{a} (\hat{y} + \hat{z})$$

$$\vec{b}_2 = \frac{2\pi}{a} (\hat{x} + \hat{z})$$

$$\vec{b}_3 = \frac{2\pi}{a} (\hat{y} + \hat{x})$$

$$S = 1$$

$$\hat{x} = (1, 0, 0)$$

$$\hat{y} = (0, 1, 0)$$

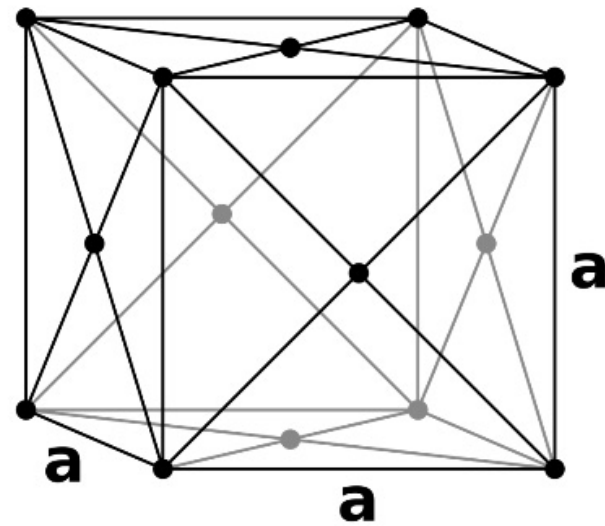
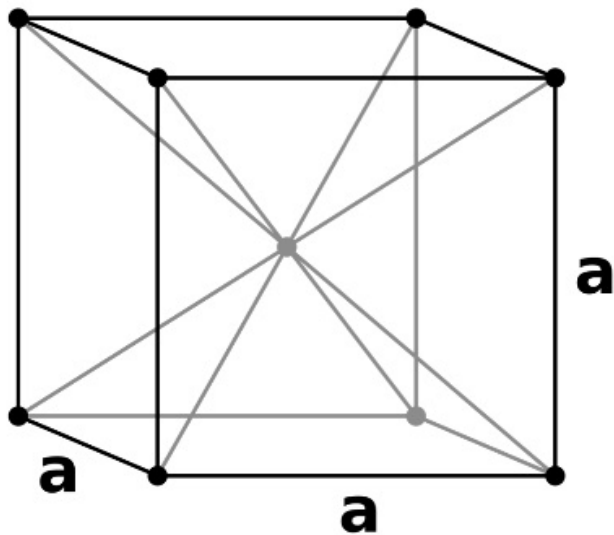
$$\hat{z} = (0, 0, 1)$$

$$\vec{r} = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3$$

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#NN = NUMBER OF NEAREST NEIGHBOURS
#NNN = NUMBER OF NEXT NN



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