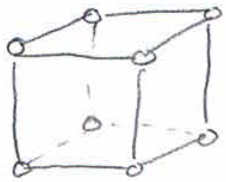
2.2



$\lambda = 1.54\,A$

$a = 2.62\,A$

cubic lattice: $d_{hkl} = \dfrac{a}{(h^2+k^2+l^2)^{1/2}}$ (eq 1.:

$n\lambda = 2d \sin\theta$

first order angle $\Rightarrow n = 1$

$\Rightarrow \theta_1 = \sin^{-1}\left(\dfrac{\lambda}{2d}\right)$

plane	d_{hkl}	θ
(1 0 0)	$d_{100} = a = 2.62\,A°$	17.09°
(1 1 0)	$d_{110} = a/\sqrt{2} = 1.85\,A°$	24.56°
(1 1 1)	$d_{111} = a/\sqrt{3} = 1.51\,A°$	30.60°
(2 0 0)	$d_{200} = a/2 = 1.31\,A°$	36°
(2 1 0)	$d_{210} = a/\sqrt{5} = 1.17\,A°$	41.08°
(2 1 1)	$d_{211} = a/\sqrt{6} = 1.07\,A°$	46.05°

2.3

a)

$$n\lambda = 2d \sin\theta$$

first order $\Rightarrow n = 1$

$$\Rightarrow d = \frac{\lambda}{2\sin\theta_1}$$

$\lambda = 1.54 \, Å$

$\theta = 19.2^\circ$

$$\Rightarrow d = \frac{1.54 \, Å}{2 \sin 19.2^\circ} \approx 2.34 \, Å$$

b) $a = \sqrt{3}\, d = 4.053 \, Å$

FCC $\Rightarrow$ 4 atoms per cell

$$N_A = \frac{(\#\text{atoms/cell})(\text{atomic weight})}{\rho \, (V \text{ of the cell})} =$$

$$= \frac{4 \cdot 27}{2.7 \, g/cm \cdot (4.053 \cdot 10^{-8} cm)^3} =$$

$$= 6.01 \cdot 10^{23}$$

2.5

Let's shift origin by $-\vec{R}$

$$\Rightarrow \vec{r}_1{}' = \vec{r}_1 - \vec{R}$$

$$\vec{r}_2{}' = \vec{r}_2 - \vec{R}$$

$$U' = f_e\left(\frac{A}{D}\right) e^{ikD}\left[e^{i\vec{S}\,\vec{r}_1{}'} + e^{i\vec{S}\,\vec{r}_2{}'}\right] =$$

$$= f_e\left(\frac{A}{D}\right) e^{ikD}\, e^{-i\vec{S}\vec{R}} \left[e^{i\vec{S}\,\vec{r}_1} + e^{i\vec{S}\,\vec{r}_2}\right] =$$

$$= f_e \frac{A'}{D} e^{ikD}\left[e^{i\vec{S}\,\vec{r}_1} + e^{i\vec{S}\,\vec{r}_2}\right]$$

where $A' = Ae^{-i\vec{S}\vec{R}}$

2.6

$$\vec{s}\,\vec{r} = s r \cos\theta$$

$$f_a = \int_0^{2\pi}\int_0^{\pi}\int_0^{r} \varrho(r)\, e^{isr\cos\theta}\, r^2 \sin\theta\, d\theta\, d\varphi =$$

$$= -2\pi \int_0^{\pi}\int_0^{r} \varrho(r)\, e^{isr\cos\theta}\, r^2\, dr\, d(\cos\theta) =$$

$$= -2\pi \int_0^{r} \varrho(r)\, r^2\, dr \left[\frac{e^{isxr}}{isr}\Bigg|_1^{-1} \right] =$$

$$= 2\pi \int_0^{r} \varrho(r)\, r^2\, dr\, \frac{2\cdot\sin(sr)}{sr} =$$

$$= \int_0^{r} 4\pi r^2\, \varrho(r)\, \frac{\sin(sr)}{sr}$$

2.8

$$F = \sum_j f_{a_j} e^{i\vec{s}\vec{\delta}_j}$$ j — sum over atom in unit cell

$$S = \sum_e e^{i\vec{s}\vec{R}_e}$$ e - sum over unitcells

$$\Rightarrow \sum_{je} = \sum_m$$ m — sum over atoms in the system

$$FS = \sum_{je} f_{a_j} e^{i\vec{s}\left(\vec{R}_e + \vec{\delta}_j\right)} =$$

$$= \sum_m f_{a_m} e^{i\vec{s}\vec{R}_m} = f_{cr}$$

2.9

$$f_a = \int_0^\infty \frac{\sin(sr)}{sr} \frac{e^{-2r/a_0}}{\pi a_0^3} \, dr \cdot 4\pi r^2 =$$

$$= \mathrm{Im}\left[\int_0^\infty \frac{4}{s a_0^3} e^{-2r/a_0 + isr} r \, dr \right] =$$

$$= \mathrm{Im}\left[\frac{4}{s a_0^3} \frac{e^{-2r/a_0 + isr}}{-\frac{2}{a_0} + is} \cdot r \Big|_0^\infty - \right.$$

$$\left. - \frac{4}{s a_0^3} \frac{1}{\left(-\frac{2}{a_0} + is\right)^2} e^{-2r/a_0 + isr} \Big|_0^\infty \right] =$$

$$= \mathrm{Im}\left[\frac{4}{s a_0^3} \frac{\frac{4}{a_0^2} + s^2 + \frac{4is}{a_0}}{\left(\frac{4}{a_0^2} + s^2\right)^2} \right] =$$

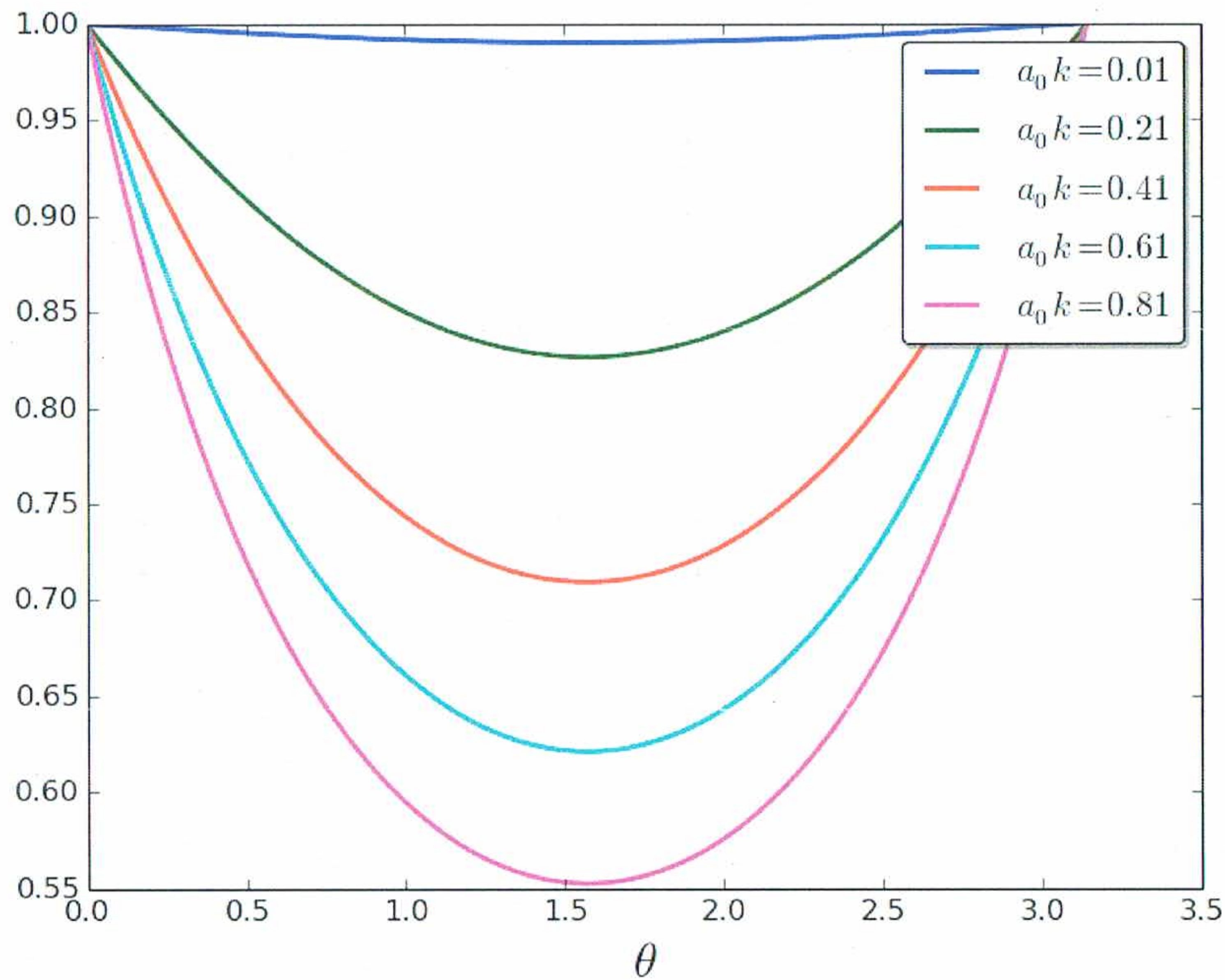
$$= \frac{16}{\left(4 + a_0^2 s^2\right)^2} \qquad s = 2k \sin\theta$$

Comments:

[1] When you have scattering on a lattice you integrate over unit cell. When it is single atom you integrate over all space

[2] $a_0 k \ll 1 \Rightarrow \lambda$ big $\Rightarrow$ does not feel an atom that much

$a_0 k \approx 1 \Rightarrow \lambda \approx a_0 \Rightarrow$ incoming wave interacts with an electron cloud a lot $\Rightarrow$ scattering


1.00
0.95
0.90
0.85
0.80
0.75
0.70
0.65
0.60
0.55
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
θ
$a_0 k = 0.01$
$a_0 k = 0.21$
$a_0 k = 0.41$
$a_0 k = 0.61$
$a_0 k = 0.81$