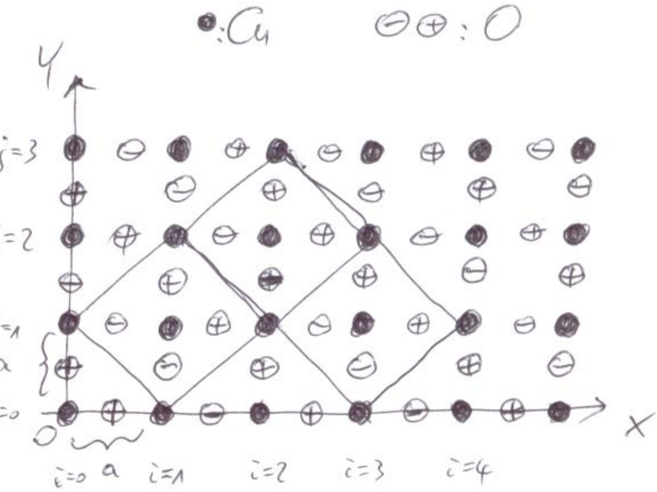
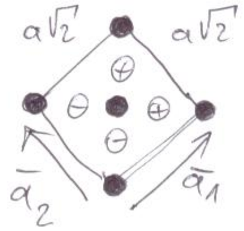
Zad 1

$$\bar r_{Cu} = ia\bar e_x + ja\bar e_y + kc\bar e_z$$

$$\bar r_{O1} = (i+\tfrac12)a\bar e_x + ja\bar e_y + (kc + \Delta z\cdot(-1)^{i+j})\bar e_z$$

$$\bar r_{O2} = ia\bar e_x + (j+\tfrac12)a\bar e_y + (kc + \Delta z(-1)^{i+j})\bar e_z$$





a) komórka prymitywna

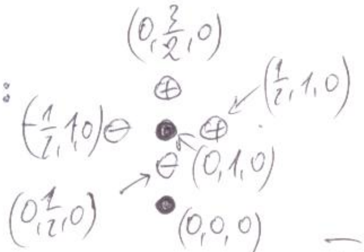
5p

jeśli z podaniem wektorów translacji prymit. i atomów bazy

w płaszczyźnie tlenowej sieć Bravais kwadratowa, w przestrzeni sieć tetragonalna: $a\sqrt2, a\sqrt2, c$

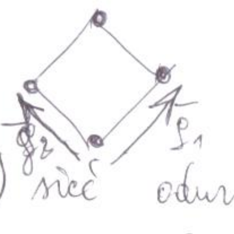
wektory translacji prymitywnych: $\bar a_1 = a[1,1,0]$
$\bar a_2 = a[-1,1,0]$
$\bar a_3 = c[0,0,1]$

atomy bazy:



$$\left.\begin{aligned} \bar b_1 &= [0,0,0] \\ \bar b_2 &= \tfrac12(\bar a_1 + \bar a_2) = a[0,1,0] \end{aligned}\right\} Cu$$

$$\left.\begin{aligned} \bar b_3 &= a\cdot[0,\tfrac12,0] - \tfrac{\Delta z}{c}\cdot c\bar e_z = \tfrac14(\bar a_1+\bar a_2) - \tfrac{\Delta z}{c}\bar a_3 \\ \bar b_4 &= a\cdot[-\tfrac12,1,0] - \dots = \bar a_2 + \tfrac14(\bar a_1 - \bar a_2) - \tfrac{\Delta z}{c}\bar a_3 \\ \bar b_5 &= a\cdot[\tfrac12,1,0] + \dots = \bar a_1 - \tfrac14(\bar a_1 - \bar a_2) + \tfrac{\Delta z}{c}\bar a_3 \\ \bar b_6 &= a[0,\tfrac32,0] + \dots = (\bar a_1 + \bar a_2)\cdot\tfrac34 + \tfrac{\Delta z}{c}\bar a_3 \end{aligned}\right\} \text{atomy tlenu}$$



b) sieć odwrotna: $\bar g_i \circ \bar a_j = 2\pi\delta_{ij}$

2p

$$\bar g_1 = \frac{2\pi}{a\sqrt2}\cdot\frac{[1,1,0]}{\sqrt2}, \quad \bar g_2 = \frac{2\pi}{a\sqrt2}\cdot\frac{[-1,1,0]}{\sqrt2}, \quad \bar g_3 = \frac{2\pi}{c}[0,0,1]$$

c) $\bar{G}_{hkl} \circ \bar{b}_1 = 0$, $\bar{G}_{hkl} = h\bar{g}_1 + k\bar{g}_2 + l\bar{g}_3 = \frac{\pi}{a}[h-k, h+k, 0] + \frac{2\pi}{c}\cdot[0,0,l]$

3p

$$\bar{G}_{hkl} \circ \bar{b}_2 = (h\bar{g}_1 + k\bar{g}_2 + l\bar{g}_3)\cdot[0,1,0]\cdot a = \pi\cdot(h+k)$$

$$\bar{G}_{hkl} \circ \bar{b}_3 = \frac{\pi}{2}\circ(h+k) - \frac{\Delta z}{\cancel{c}}\cdot\cancel{c}\cdot l\cdot 2\pi$$

$$\bar{G}_{hkl} \circ \bar{b}_4 = \pi\cdot\left[\left(-\frac{1}{2}\right)(h-k) + (h+k)\right] - \frac{\Delta z}{\cancel{c}}\cancel{c}\, l\cdot 2\pi$$

$$\bar{G}_{hkl} \circ \bar{b}_5 = \pi\left[\left(\frac{1}{2}\right)(h-k) + (h+k)\right] + \frac{\Delta z}{\cancel{c}}\cancel{c}\, l\cdot 2\pi$$

$$\bar{G}_{hkl} \circ \bar{b}_6 = \pi\,\frac{3}{2}(h+k) + \frac{\Delta z}{\cancel{c}}\cancel{c}\, l\cdot 2\pi$$

$$\boxed{F_{hkl} = \sum_j f_j\, e^{-i\bar{G}_{hkl}\circ\bar{b}_j}}$$ ← geometryczny czynnik struktury, j numeruje atomy bazy.

$$F_{hkl} = f_{Cu}\left(1 + e^{-i\pi(h+k)}\right) + f_O\left[e^{-i\frac{\pi}{2}(h+k) + 2\pi i l\frac{\Delta z}{c}} + e^{-i\pi\left(\frac{1}{2}h + \frac{3}{2}k\right) + 2\pi i l\frac{\Delta z}{c}} + e^{-i\pi\left(\frac{3}{2}h + \frac{1}{2}k\right) - 2\pi i l\frac{\Delta z}{c}} + e^{-i\pi\frac{3}{2}(h+k) - 2\pi i l\frac{\Delta z}{c}}\right] =$$

$$= f_{Cu}\left(1 + e^{-i\pi(h+k)}\right) + f_O\cdot\left[e^{2\pi i l\frac{\Delta z}{c}}\cdot e^{-i\frac{\pi}{2}(h+k)}\cdot\left(1 + e^{-i\pi k}\right) + e^{-2\pi i l\frac{\Delta z}{c}}\cdot e^{-i\frac{3\pi}{2}(h+k)}\cdot\left(e^{i\pi k} + 1\right)\right] =$$

$$= f_{Cu}\left(1 + e^{-i\pi(h+k)}\right) + f_O\cdot e^{-i\frac{\pi}{2}(h+k)}\cdot\left(1 + e^{-i\pi k}\right)\left(e^{2\pi i l\frac{\Delta z}{c}} + e^{-2\pi i l\frac{\Delta z}{c}}\cdot e^{-i\pi(h+k)}\cdot e^{+i\pi k}\right) =$$

$$= f_{Cu}\left(1 + e^{-i\pi(h+k)}\right) + f_O\cdot e^{-i\frac{\pi}{2}(h+k)}\cdot\left(1 + e^{-i\pi k}\right)\cdot\left(e^{2\pi i l\frac{\Delta z}{c}} + e^{-2\pi i l\frac{\Delta z}{c}}\cdot e^{-i\pi h}\right)$$

dla $\Delta z \to 0$:

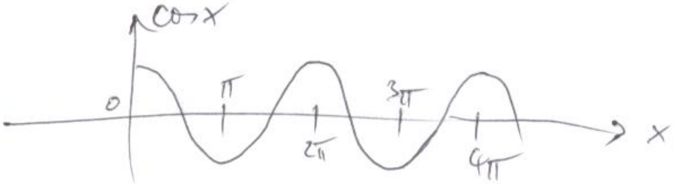
$$F_{hkl}^{(\Delta z=0)} = f_{Cu}\left(1+e^{-i\pi(h+k)}\right)+f_{O}\cdot e^{-i\frac{\pi}{2}(h+k)}\left(1+e^{-i\pi k}\right)\left(1+e^{-i\pi h}\right) *$$

$$* \quad e^{-i\pi(h+k)} = \cos\pi(h+k) - i\underbrace{\sin\pi(h+k)}_{=0}$$

$$e^{-i\pi k} = \cos\pi k - i\underbrace{\sin\pi k}_{=0}$$

$$e^{-i\pi h} = \cos\pi h - i\underbrace{\sin\pi h}_{=0}$$

$$F_{hkl}^{(\Delta z=0)} = f_{Cu}\cdot\left(1+\cos\pi(h+k)\right)+f_{O}\cdot\left(1+\cos\pi k\right)\left(1+\cos\pi h\right)\cdot\left(\cos\tfrac{\pi}{2}(h+k) - i\sin\tfrac{\pi}{2}(h+k)\right)$$



Jeśli $(h+k)$ jest nieparzyste, to $\cos\pi(h+k) = -1$

oraz $(1+\cos\pi k)\cdot(1+\cos\pi h) = 0$ – bo jedna z liczb h lub k jest nieparzysta

czyli $F_{hkl}^{(\Delta z=0)} = 0$ dla $(h+k)$ nieparzystego, czyli znikają refleksy $(h+k)$ – nieparzyste dla $\Delta z = 0$.