

Exc: 6

Structure S_{hkl}

NaCl

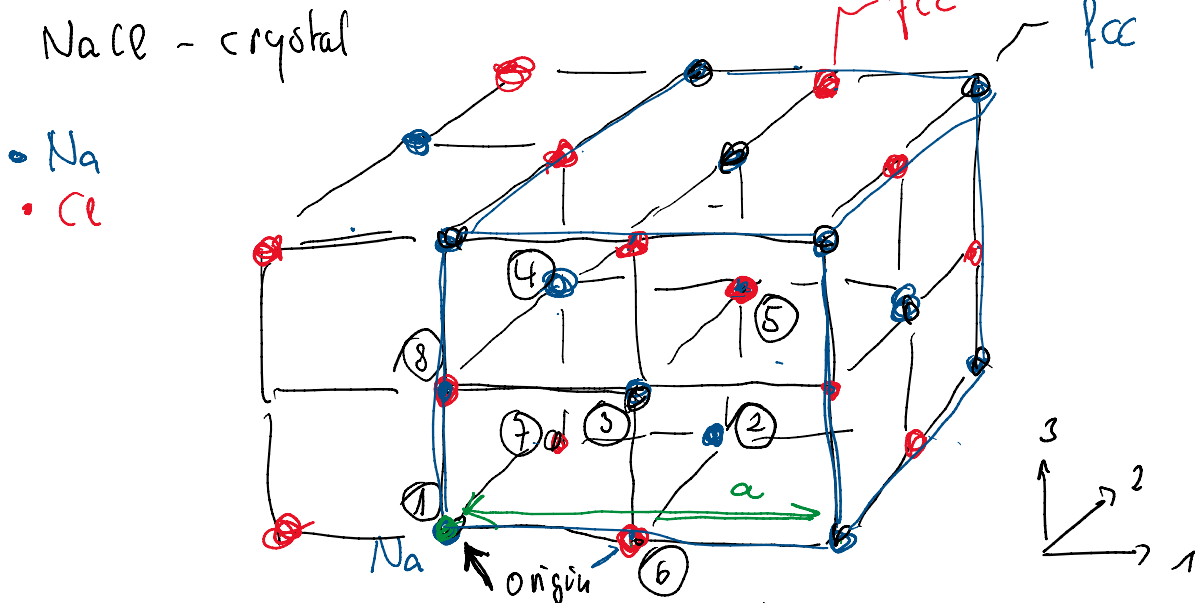
$$S_{hkl} = \sum_j e^{i \vec{G}_{hkl} \cdot \vec{r}_j} \cdot f_j$$

\sum_j : basis atoms in one unit cell
 $e^{i \vec{G}_{hkl} \cdot \vec{r}_j}$: place of atom j
 interference of diffracted waves
 f_j : atomic structure factor scattering "form"
 electron distribution

$$\vec{G}_{hkl} = h \vec{b}_1 + k \vec{b}_2 + l \vec{b}_3$$

Miller indices

Bragg: scattering vector $\vec{\Delta k} = \vec{k} - \vec{k}_0 = \vec{G}_{hkl}$
 x-rays



2 fcc lattices \Rightarrow 8 basis atoms

$$S(hkl) = \sum_j f_j \exp\{i \vec{G}_{hkl} \cdot \vec{r}_j\}$$

$$= \sum_j f_j \exp\{i 2\pi (u_j h + v_j k + w_j l)\} \leftarrow$$

$\vec{r}_j \rightarrow \dots \rightarrow \vec{r}_j$

$$\vec{r}_j = u_j \vec{a}_1 + v_j \vec{a}_2 + w_j \vec{a}_3$$

$$\vec{G}_{hkl} = h \vec{b}_1 + k \vec{b}_2 + l \vec{b}_3$$

$$\vec{F}_j = u_j \vec{a}_1 + v_j \vec{a}_2 + w_j \vec{a}_3 \Leftarrow$$

Na (u_j, v_j, w_j)

$$j=1 \quad (0, 0, 0) \Leftarrow$$

$$j=2 \quad (\frac{1}{2}, \frac{1}{2}, 0)$$

$$j=3 \quad (\frac{1}{2}, 0, \frac{1}{2})$$

$$j=4 \quad (0, \frac{1}{2}, \frac{1}{2})$$

Ce

$$j=5 \quad (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$$

$$j=6 \quad (\frac{1}{2}, 0, 0)$$

$$j=7 \quad (0, \frac{1}{2}, 0)$$

$$j=8 \quad (0, 0, \frac{1}{2})$$

$$S(hkl) = f_{Na} \left(e^{\frac{1}{2}i\pi(h+k)} + e^{\frac{1}{2}i\pi(h+l)} + e^{\frac{1}{2}i\pi(k+l)} \right) + f_{Ce} \left(e^{i\pi(h+k+l)} + e^{i\pi h} + e^{i\pi k} + e^{i\pi l} \right)$$

$$= \begin{cases} 4f_{Na} + 4f_{Ce} \\ 4f_{Na} - 4f_{Ce} \\ \text{extinction} \rightarrow 0 \\ \rightarrow 0 \end{cases}$$

h, k, l all even

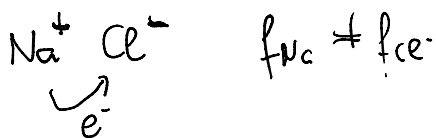
h, k, l all odd

one is odd, the other two even

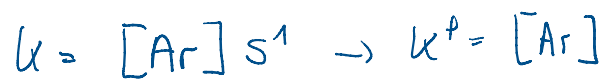
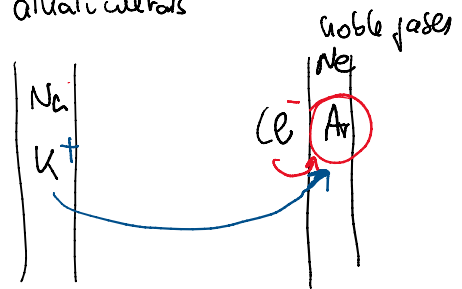
two are odd, one is even

two atoms with same structure factor f k Ce

$f_{K^+} \approx f_{Ce^-} \rightarrow$ all odd spots disappear



alkali metals



$$u = LTT \dots \rightarrow u \dots$$

$$ce^- = [Ac] \leftarrow \rightarrow$$

Exc 8: solution of 7 ^{order number charge ze}

$$f(\sin \theta) = \frac{3z}{16a^2} \cdot \left(\frac{\sin(4\pi(\sin \theta))}{4\pi(\sin \theta)^3} - \frac{\cos(4\pi \sin \theta)}{(\sin \theta)^2} \right)$$

Debye-Waller factor

$$I(T, \sin \theta) = I_0 \exp \left\{ - \frac{\Delta k^2 k_B T}{m \omega^2} \right\}$$

Scattering vector
Temperature

lithium $m = 6.94 \text{ amu} = 6.94 \frac{g}{NA}$

$$\omega = 10^{13} \text{ s}^{-1}$$

vibrational frequency $E_n = (n + \frac{1}{2}) h \omega$

$$\left. \begin{aligned} 3.45 \text{ meV} &= k_B T = k_B \cdot 4.2 \text{ K} \\ 25.8 \text{ meV} &= k_B 300 \text{ K} \end{aligned} \right\} \text{thermal energy } k_B T$$

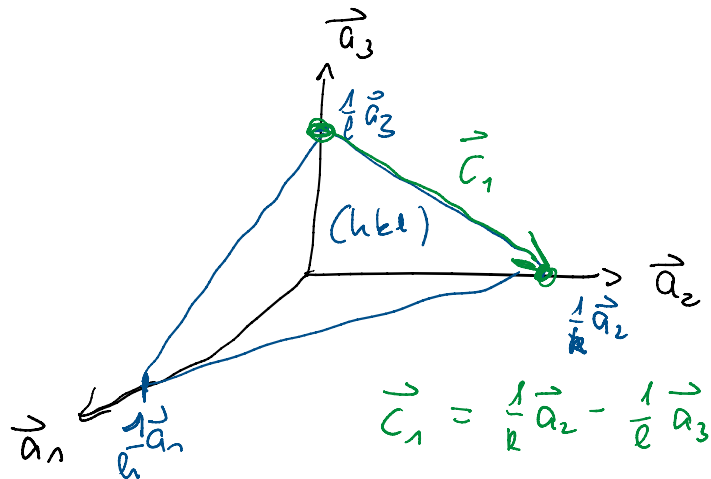
zero-point motion $\frac{1}{2} h \omega \approx 16 \text{ meV}$

$$\Delta k = 2k \cdot \sin \theta$$

Exc 9: a) $\vec{c}_{hkl} \perp (hkl)$
plane

2 vectors in the plane \vec{c}_1, \vec{c}_2
 \rightarrow show that $\vec{c}_h \perp \vec{c}_1, \vec{c}_2 \Leftrightarrow \vec{c}_h \cdot \vec{c}_1 = 0 = \vec{c}_h \cdot \vec{c}_2$

plane: (hkl)



$$\vec{c}_1 = \frac{1}{k} \vec{a}_2 - \frac{1}{l} \vec{a}_3$$

$$\vec{c}_h \cdot \vec{c}_h = 2\pi \delta$$

an \vec{e}_n

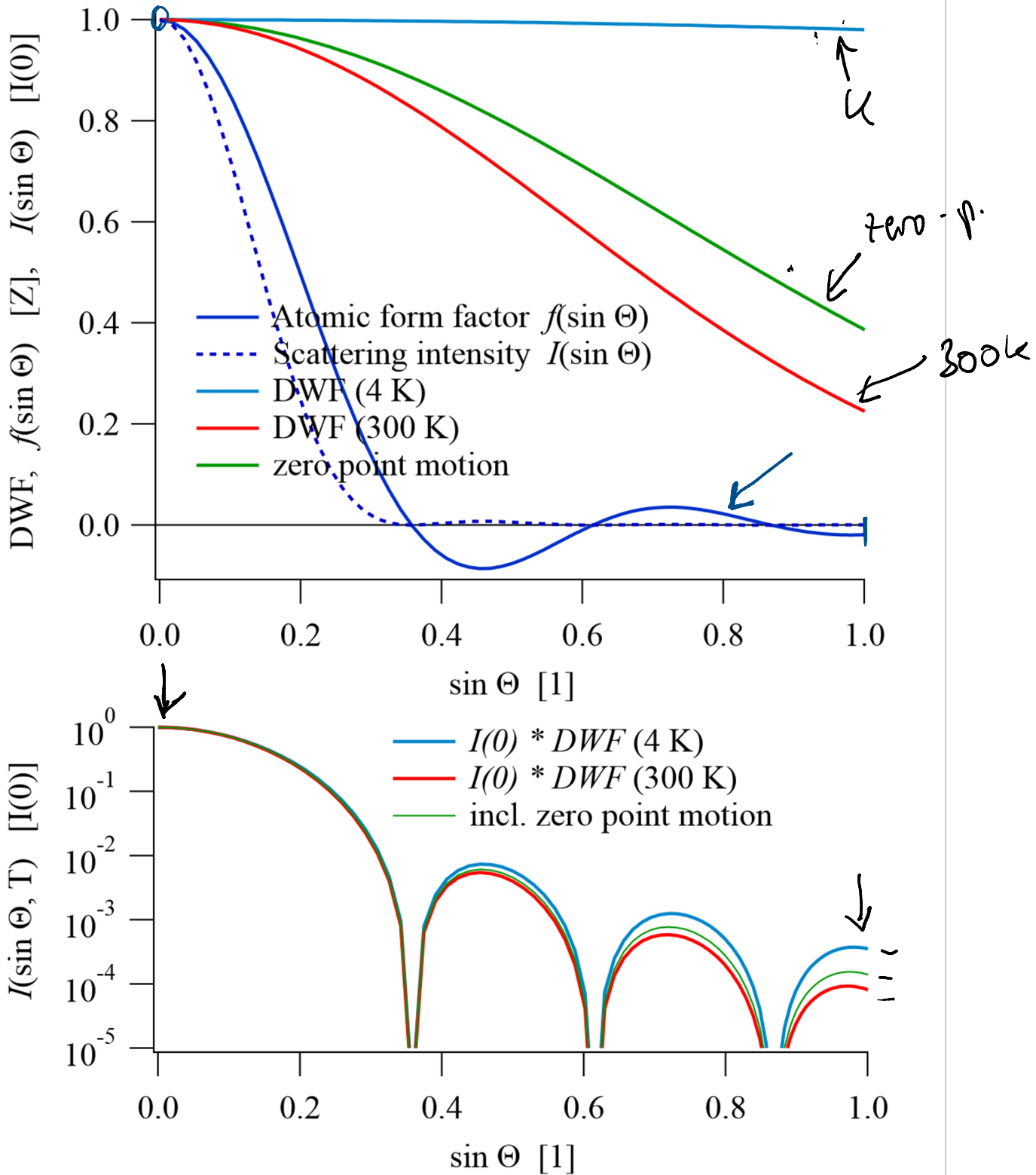
same equ: $\vec{a}_i \cdot \vec{b}_j = 2\vec{u} \delta_{ij}$

Exc 12:

Afg8 - DWF

Donnerstag, 12. Oktober 2023 15:59

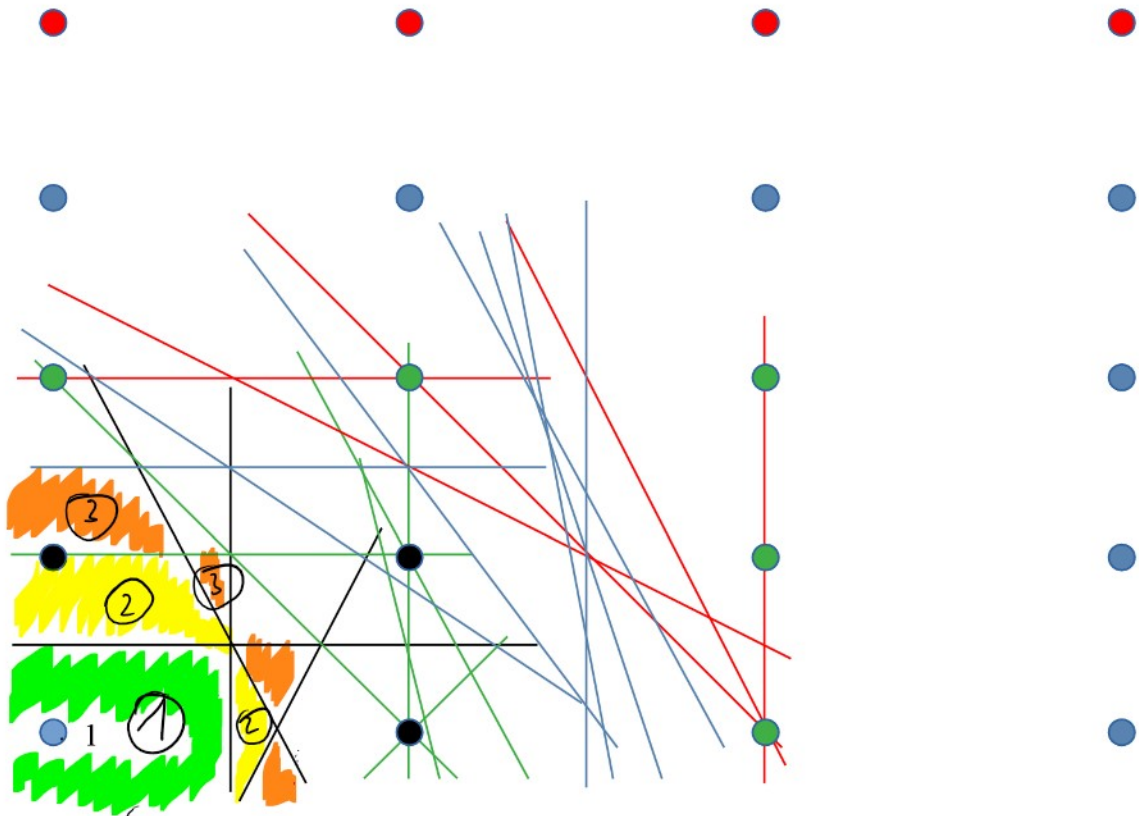
Plot zu Aufgabe 8:
Debye-Waller-Faktor und Nullpunktenergie



Afg12 - FourBZs

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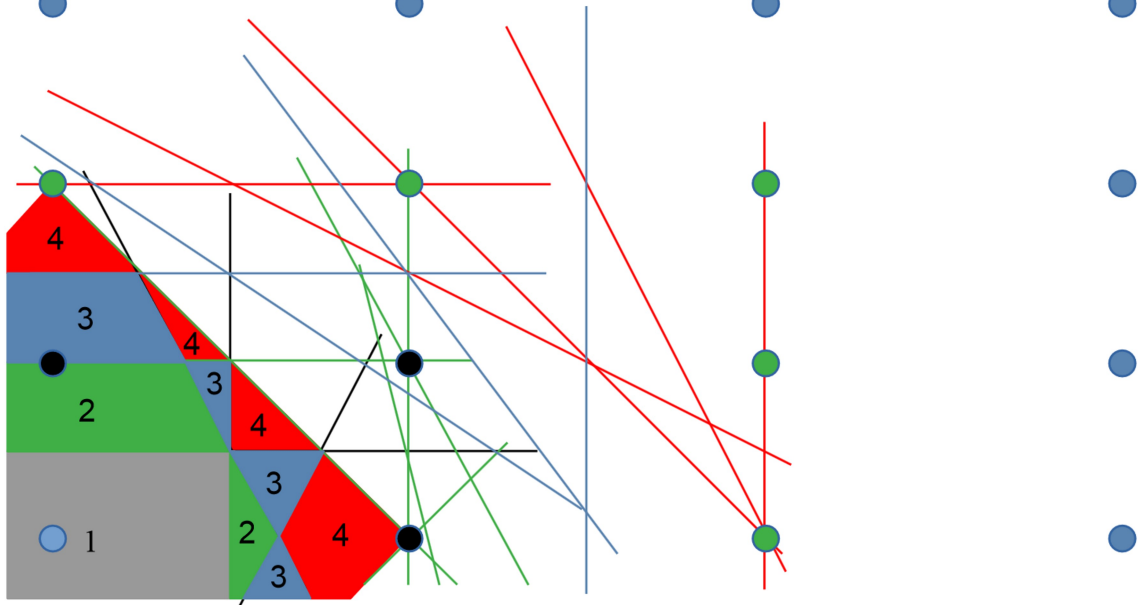
Plot zu Aufgabe 12: 4 BZen des rechteckigen Gitters



Wigner-Seitz cell $\hat{=}$ 1st Brillouin zone



Plot zu Aufgabe 12: 4 BZen des rechteckigen Gitters



every BZ surrounded by the next higher BZ
 the area (volume in 3D) of all BZs is the same.