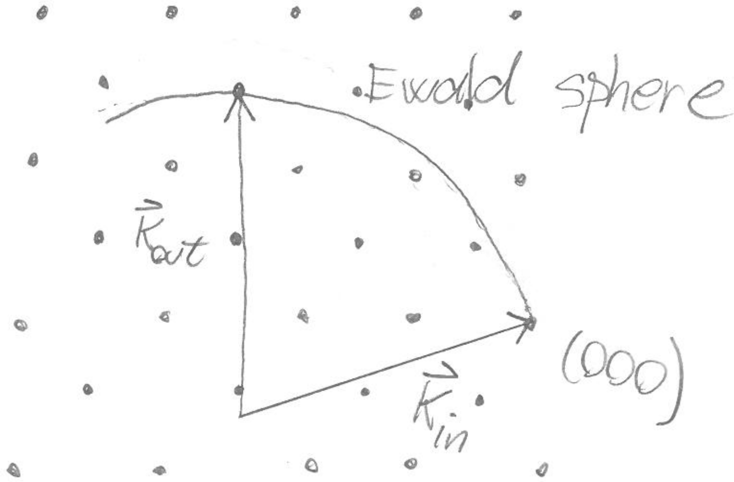
① a) The Ewald construction is made the following way (in 2D):

1) Draw the reciprocal lattice of the crystal

2) Draw $\vec{k}_{in}$ such that it ends at the (000) reciprocal lattice point. The relative orientation between $\vec{k}_{in}$ and the lattice must match the experiment.

3) Draw a circle/sphere with radius $|\vec{k}_{in}|$ centered at the start point of $\vec{k}_{in}$. This is the Ewald sphere.

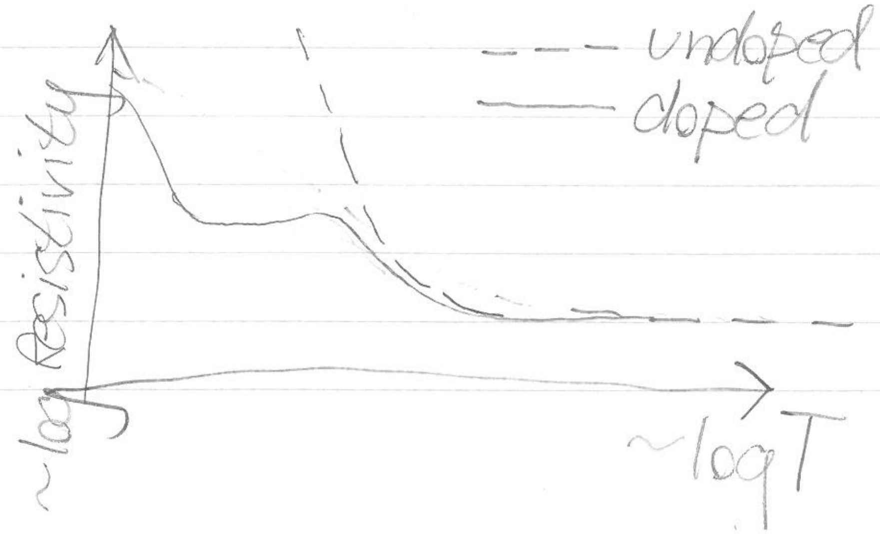


Where recip. lattice points fall on the Ewald sphere, we observe diffraction, with the direction of the outgoing wave being on a line from the start of $|\vec{k}_{in}|$ to the point.

b) Increasing T generally decreases mobility, thus increasing resistivity. However, in semiconductors, the concentration of charge carriers changes dramatically as function of T, and this effect dominates over changes in mobility when it comes to influence on the resistivity. As charge carrier concentration increases with T, the resistivity of semiconductors decreases with increasing T.

I doped semiconductors, the carrier concentration increases in two phases: First, at low T, the majority of the dopant carriers are excited, and when this has happened, the number of carriers is relatively constant until T becomes high enough to excite intrinsic carriers in large numbers.

Sumarized:



c) Energy bands are caused by periodic potentials, which impose certain periodicity constraints on the electon wavefunctions.

The band gap can be determined by (infrared) spectroscopy (easy in the case of a direct gap, but possible also for an indirect gap).

See also Kittel p. 165-7 on scattering etc.

d) The effects of the periodic potential on the electrons can to a large extent be described by replacing the true electron mass m_e by the effective mass m_e^*.

The def of m_e^* is

$$m_e^* = \hbar^2 \left[\frac{d^2\mathcal{E}(k)}{dk^2}\right]^{-1}$$

where $\mathcal{E}(k)$ is the dispersion relation. In words, the effective mass is inversely proportional to the curvature of the dispersion relation.

② a) I: Body centered cubic

1 atom in the basis, at (0,0,0)

II: Face centered cubic

2 atoms in the basis, at (0,0,0) and (1/4, 1/4, 1/4) (in fractional coordinates)

III: Simple cubic

5 atoms in the basis (1 Sr, 1 Ti, 3 O) at (fractional coords)

(0,0,0) : Sr
(1/2, 1/2, 1/2) : Ti
(1/2, 1/2, 0) : O
(1/2, 0, 1/2) : O
(0, 1/2, 1/2) : O

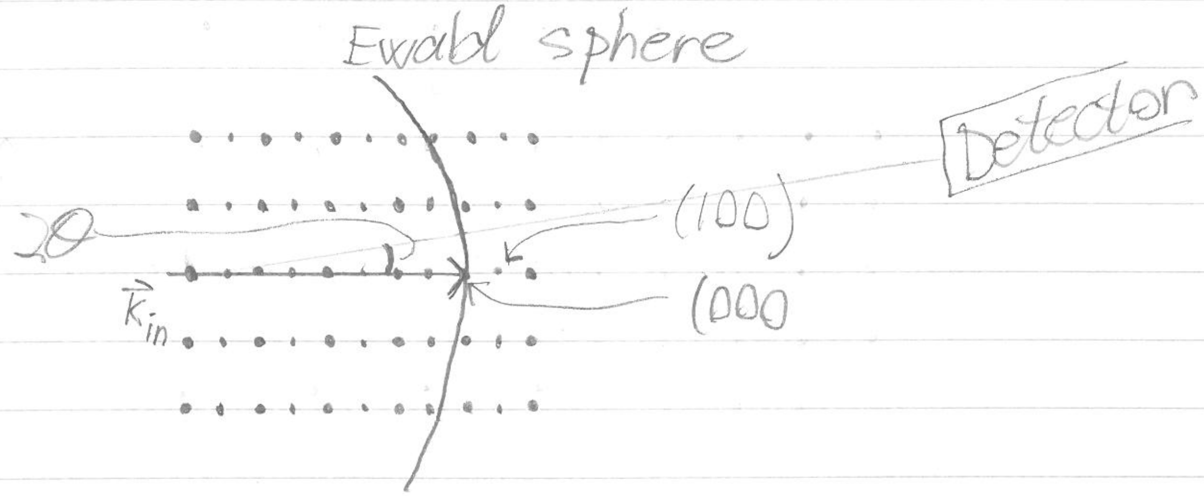
b) 1) Bragg's law, $\lambda = 2d_{hkl} \sin\theta$, gives

$2\theta = 7.36°$

with $d_{100} = 11.99$ Å and $\lambda = 1.54$ Å.

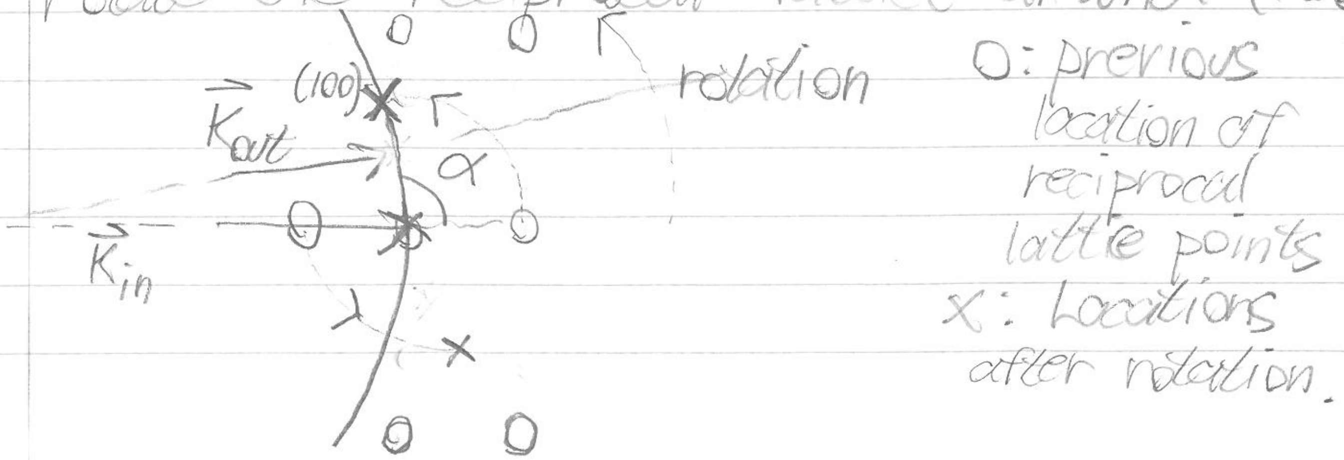
The smallest 2θ angle belongs to the largest interplane distance d_{hkl} in real space, which in our case is $d_{100} = a_1$.

b2)



Above, we have the Ewald construction for the original setup. We see that the (100) reciprocal lattice point does not fall on the Ewald sphere, hence it does not diffract.

The natural solution is to rotate the crystal, since this will also rotate the reciprocal lattice around (000)



The rotation angle α is

$$\alpha = 90^\circ + \frac{2\theta}{2}$$

(other choices are possible:

$$\alpha = \pm\left(90^\circ \pm \frac{2\theta}{2}\right)$$

(all four sign combinations)

In two of these cases, we will see diffraction at -2θ. In two of the cases, we observe the $\bar{1}00$ reflection).

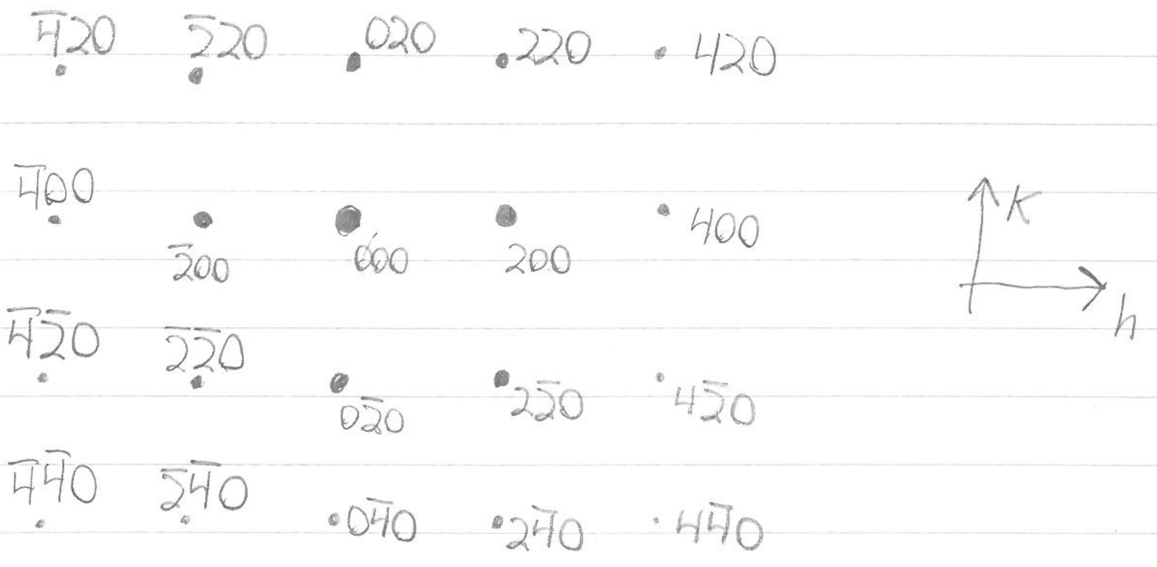
c) The TEM diffraction pattern represents a 2D slice through reciprocal space. We see fourfold symmetry, thus the zone axis has fourfold symmetry. For Al, there are three (equivalent) such axes; we will choose the zone axis [001], such that all reflections we see are of the type hk0.

The extiction rules in the hk0-plane of Al are (one can also derive the general rules)

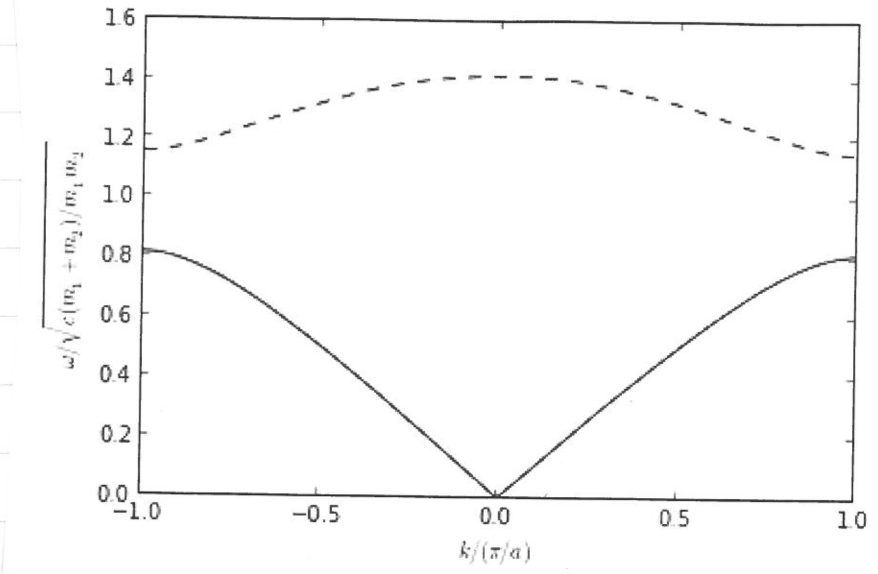
$$F_{hk0} = 1 + e^{i\pi(h+k)} + e^{i\pi h} + e^{i\pi k}$$

$$F_{hk0} = 1 + (-1)^{(h+k)} + (-1)^{h} + (-1)^{k}$$

If h and k are both even, $F_{hk0} \neq 0$, otherwise, the reflection is extinct.



③ a) 1)



The dispersion relation for $m_1/m_2 = 2$

2) For acoustic modes $\omega \to 0$ as $k \to 0$, while this is not true for optical modes. $k \to 0$ corresponds to a translation of the entire crystal for acoustic modes. $k \to \pi/a$ corresponds to standing waves for both types of mode.

Another way of distinguishing acoustical and optical modes, is that for small k, atoms in the basis vibrate in phase in acoustic modes and out of phase in optical modes.

b) 1) There are no optical modes (only a single atom in the basis); the 1BZ is twice as large.

2) Setting $M_1 = M_2 = m$:

$$\omega^2 = \frac{2C}{m}\left[1 \pm \sqrt{1-\sin^2 Kb}\right]$$

$$\omega^2 = \frac{2C}{m}\left[1 \pm \cos(Kb)\right]$$

We must choose the minus sign to ensure $\omega \to 0$ as $K \to 0$ (we need to have an acoustic mode)

$$\omega^2 = \frac{4C}{m}\sin^2\left(\frac{Kb}{2}\right)$$

$$\omega = 2\sqrt{\frac{C}{m}}\left|\sin\left(\frac{Kb}{2}\right)\right|$$

Now, the DOS is

$$D_\omega(\omega)\,d\omega = D_K(K)\,dK,$$

where $D_K(K) = \frac{L}{2\pi}$.

$$d\omega = b\sqrt{\frac{C}{m}}\cos\left(\frac{Kb}{2}\right)dK \quad \forall\ K > 0$$

and

$$d\omega = -b\sqrt{\frac{C}{m}}\cos\left(\frac{Kb}{2}\right)dK \quad \forall\ K < 0$$

$$D_\omega(\omega)\,d\omega = \frac{L}{2\pi}\left|\frac{d\omega}{dK}\right|^{-1}d\omega$$

$$= \frac{L}{2\pi b}\sqrt{\frac{m}{C}}\,\frac{1}{\cos\left(\frac{Kb}{2}\right)}\,d\omega$$

$$\frac{4C}{m} - \omega^2 = \frac{4C}{m}\left[1 - \sin^2\left(\frac{Kb}{2}\right)\right]$$

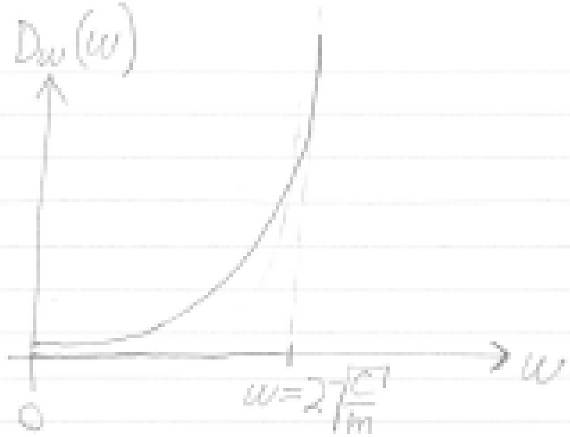
$$= \frac{4C}{m}\cos^2\left(\frac{Kb}{2}\right)$$

$$\sqrt{\frac{C}{m} - \left(\frac{\omega}{2}\right)^2} = \sqrt{\frac{C}{m}}\cos\left(\frac{Kb}{2}\right)$$

$$D_\omega(\omega)\,d\omega = \frac{L}{2\pi b}\left[\frac{C}{m} - \left(\frac{\omega}{2}\right)^2\right]^{-1/2} d\omega$$

The constants are

$C_1 = 2\pi b$ and $C_2 = \frac{C}{m}$



The material will not excite phonon states by absorbing photons directly, as there are no states of suffeiently high energy at low K (also known as optical phonons).

c) We can measure the sound velocity in ionic materials by sending in IR light and look at the resonance curve. (We did in the lattice vibration lab for SiC). It is an indirect method, as we measure the resonance between the photon in IR and the optical branch, calculate the C and then find v_g from the acoustical branch at the same energy.

Sound velocity can also be measured by time-of-flight of sound pulses or standing-wave frequency and wavelength measurements.

Typical order of magnitude is typically a few thousand m/s (3-10.000 m/s).

d) Three major observations:

1) Al has only acoustical branches, while diamond also has optical branches.
2) The shape of the acoustical branches is qualitatively similar for Al and diamond
3) The energy of all branches is higher in diamond than in Al.

From 1) we learn that Al has a monoatomic basis, while diamond has more than one atom in the basis. This agrees with fcc and diamond structures.

Observation 2) indicates similar structures, agreeing well with diamond being an fcc with a basis.

Finally, 3) indicates either higher spring constants (stronger bonds) or lower atomic mass in diamond than in Al. In this case, lower atomic mass is certainly a factor, but the increase in energy cannot be explained by this alone. The strong bonds manifest as f.ex. a higher Young's modulus.

④ a) In $\vec{k}$-space, the DOS is constant,

$$D_{\vec{k}}(\vec{k})dk_x dk_y = 2\left(\frac{L}{2\pi}\right)^2 dk_x dk_y$$

where the factor 2 accounts for spin. The dispersion relation is

$$\mathcal{E}(k) = \frac{\hbar^2 k^2}{2m},$$

hence it would be advantageous to find $D_k(k)$ on the way to $D_\mathcal{E}(\mathcal{E})$. This is easily done, as it is just a transformation to polar coordinates,

$$dk_x dk_y = k\,dk\,d\theta_k \qquad (\text{recall: } dx\,dy = r\,dr\,d\theta)$$

followed by an integration over the angle:

$$D_k(k)dk = \int_0^{2\pi} d\theta_k\, 2\left(\frac{L}{2\pi}\right)^2 k\,dk$$

$$D_k(k)dk = 4\pi k\left(\frac{L}{2\pi}\right)^2 dk$$

To arrive at $D_\mathcal{E}(\mathcal{E})d\mathcal{E}$, we must find the relation between $d\mathcal{E}$ and dk, which is done by differentiating the dispersion relation:

$$dE = \frac{\hbar^2 k}{m} dK$$

$$k dk = \frac{m dE}{\hbar^2}$$

Inserting this, we have

$$D_E(E) dE = \frac{4\pi m}{\hbar^2} \left(\frac{L}{2\pi}\right)^2 dE$$

so the constant C is

$$C = \frac{4\pi m}{\hbar^2} \left(\frac{L}{2\pi}\right)^2 = \frac{mL^2}{\pi \hbar^2}$$

b) The Fermi energy E_F for a metal is the energy of the state of highest energy that is occupied at zero temperature.

The total number of electrons $N = nL^2$ in the crystal can be calculated as

$$nL^2 = \int_0^{E_F} C dE$$

$$= E_F C$$

Inserting for C and rearranging,

$$E_F = \frac{\pi \hbar^2}{m} n$$

c) 1) The Hall effect is the appearance of a voltage across a conductor carrying a current normal to a magnetic field.

The forces on the electrons along y sum to

$$F_y = e v_x B_z - e E_y$$

where $v_x = -j_x/ne$ is the electron speed.

Requiring $F_y = 0$ yields

$$v_x B_z = E_y$$

$$-\frac{j_x B_z}{ne} = E_y$$

$$R = \frac{E_y}{j_x B_z} = -\frac{1}{ne}$$

2) The forces on electrons and holes in the y-direction are

$$F_y^h = e\left(E_y - v_x^h B_z\right)$$

$$F_y^e = -e\left(E_y - v_x^e B_z\right).$$

In the y direction, the current density must be zero in steady state conditions,

$$j_y = epv_y^h - env_y^e = 0$$

thus

$$pv_y^h = nv_y^e. \qquad (*)$$

The forces and drift velocities are related by the mobility,

$$F_y^h = \frac{ev_y^h}{\mu_h} \quad ; \quad F_y^e = -\frac{ev_y^e}{\mu_e},$$

which can be combined with the Lorenz force eqs. given previously to give

$$\frac{v_y^h}{\mu_h} = E_y - v_x^h B_z \quad ; \quad \frac{v_y^e}{\mu_e} = E_y - v_x^e B_z$$

Along the x direction, the driving force is an electric field E_x, so for both carriers, we can again use the mobility to find an expression for a drift velocity,

$$v_x^h = \mu_h E_x \quad ; \quad v_x^e = \mu_e E_x$$

which we insert for v_x to give

$$\frac{v_y^h}{\mu_h} = E_y - \mu_h E_x B_z \quad ; \quad \frac{v_y^e}{\mu_e} = E_y - \mu_e E_x B_z$$

We now use these expressions to substitute for v_y^h and v_y^e in $(*)$, yielding

$$p\mu_h\left(E_y - \mu_h E_x B_z\right) = n\mu_e\left(E_y - \mu_e E_x B_z\right) \qquad (**)$$

Considering the current density along x:

$$j_x = epv_x^h - env_x^e = eE_x\left(p\mu_h - n\mu_e\right)$$

We use this to substitute for E_x in $(**)$,

$$E_y\left(p\mu_h - n\mu_e\right) = j_x B_z \frac{p\mu_h^2 - n\mu_e^2}{e\left(p\mu_h - n\mu_e\right)}$$

$$R_H = \frac{E_y}{j_x B_z} = \frac{p\mu_h^2 - n\mu_e^2}{e(p\mu_h - n\mu_e)^2}$$