Solution sketch TFY 4220 August 2017.

1a) Extinct reflections are those that have (close to) zero intensity because of destructive interference. The unitcell structure factor is given by:

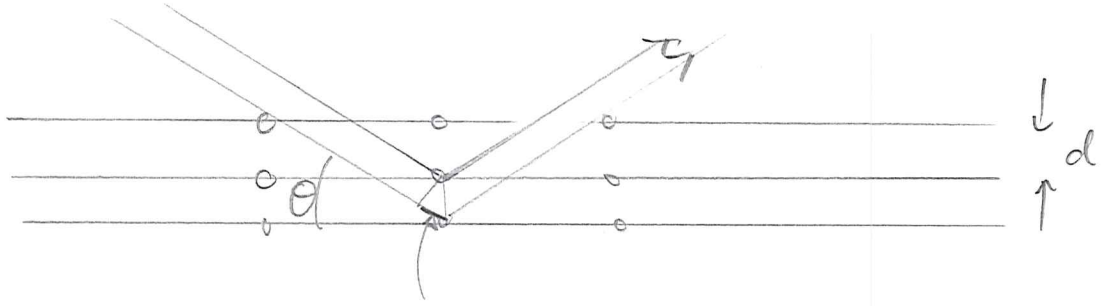
$$F_{hkl}(Q) = \sum_j f_j(Q)\, e^{2\pi i (hx_j + ky_j + lz_j)}$$

If $F_{hkl} \simeq 0$, the intensity $I_{hkl} \propto |F_{hkl}|^2 \simeq 0$, and the reflection hkl is "extinct".

		all odd	even, ≠4n	F≠0
Si:	100			
	110			
	111	v		v
	200			
	210			
	211			
	220		v	v
	221			
	222			
	300			
	310			
	311	v		v
	312			
	313			

Lowest non-zero reflections: 111, 220, 311

1b)



$\Delta = d \sin\theta$

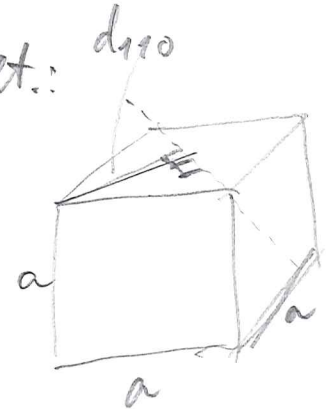
Assume specular reflection from lattice planes. Pathlength difference should correspond to a multiple of the wavelength for constructive interference:

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

220:

$$d_{220} = \frac{a}{\sqrt{h^2+k^2+l^2}} = \frac{a}{2\sqrt{2}}$$

alt.:



$$d_{110} = \frac{\sqrt{2}a}{2} = \frac{a}{\sqrt{2}}$$

$$d_{220} = \frac{1}{2}d_{110} = \frac{a}{2\sqrt{2}}$$

$$\theta = \arcsin\left(\frac{n\lambda}{2d}\right) = \arcsin\left(\frac{1.5418\,\text{Å}}{2\cdot\frac{a}{2\sqrt{2}}}\right)$$

$$= \arcsin\left(\frac{1.5418\,\text{Å}\cdot\sqrt{2}}{5.4309\,\text{Å}}\right)$$

$$\theta = 23.67° \qquad 2\theta = 47.3°$$

1c) Only reflections with the same lattice spacing as 220 will be seen. The {220} family consists of

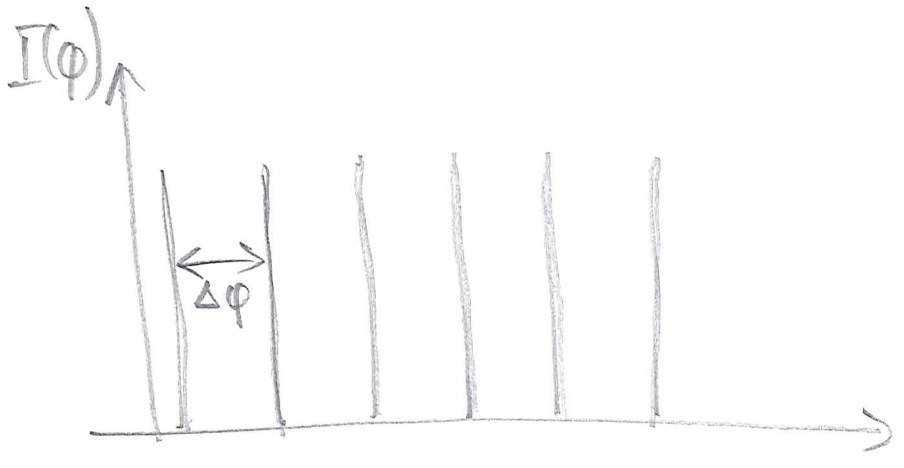
220	$\bar{2}\bar{2}0$	$2\bar{2}0$	$\bar{2}20$
202	$\bar{2}0\bar{2}$	$20\bar{2}$	$\bar{2}02$
022	$0\bar{2}\bar{2}$	$02\bar{2}$	$0\bar{2}2$

- in total 12 reflections.

Of these, only those that are perpendicular to 111 will be seen. Because the system is cubic, we notice that we can use the dot product directly. Only reflections that contain both 2 and $\bar{2}$ will give a dot product of zero, e.g.

$$\langle 111 \rangle \cdot \langle 20\bar{2} \rangle = 0.$$

Thus, the $2\bar{2}0$ $20\bar{2}$ $02\bar{2}$ $\bar{2}20$ $\bar{2}02$ and $0\bar{2}2$ reflections will be seen. Consistently with 3-fold symmetry, we get



where $\Delta\varphi = 60°$ between all refl.
(arbitrary zero of the φ-axis).

1d) Bloch's theorem states that the wavefunction ψ that satisfies the Schrödinger equation with a periodic potential is of the form:

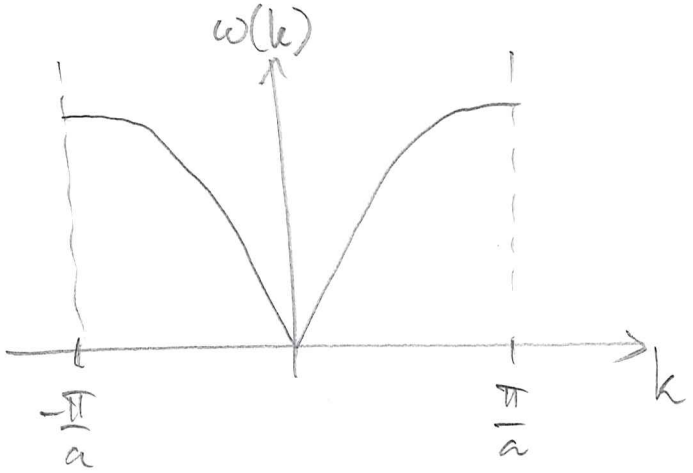
$$\psi_k(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} u_k(\vec{r}).$$

This is the mathematical expression for a plane wave modulated by a function u_k which has the periodicity of the lattice.

For large samples, periodic boundary conditions are used, $\psi_k(x) = \psi_k(x+L)$ in 1D.
For nanoscale samples, the detailed behaviour at the interfaces is important and more realistic descriptions must be used.

Problem 2

a)



All physics is contained in the 1st BZ because of the periodicity of the crystal.

There is no optical branch in the 1D mon-atomic case because this oscillation mode corresponds to having several (≥ 2) atoms in the same unit cell having "opposite" amplitudes:

2b) With a finite number of atoms N, there will be N oscillation modes. Assuming periodic boundary conditions

$$\psi(x+L) = \psi(x), \quad L = Na.$$

$$e^{ik(x+Na)} = e^{ikx}$$

$$e^{ikNa} = 1$$

$$kNa = 2\pi m, \quad m \in \mathbb{Z}.$$

$$k = \frac{2\pi m}{Na} = \frac{2\pi m}{L}$$

Smallest possible (non-zero) k:

$$k_{min} = \frac{2\pi}{L} = \frac{2\pi}{L} = 6.3 \cdot 10^{-6}\,nm^{-1}$$

$$= 6.3 \cdot 10^{3}\,m^{-1}$$

$$\left(k_{max} = \frac{2\pi}{a} = 17.5\,nm^{-1}\right)$$

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

Here: $\alpha = 50\,N\,m^{-1}$

$k = 6.3 \cdot 10^{3}\,m^{-1}$

$a = 3.6\,\text{Å} = 3.6 \cdot 10^{-10}\,m$

$m = 63.5\,u = 63.5 \cdot 1.66 \cdot 10^{-27}\,kg$

$$E = \hbar\omega = \hbar\sqrt{\frac{4\alpha}{m}\sin^2\frac{ka}{2}} = 5.19 \cdot 10^{-27}\,J$$

$$= 3.2 \cdot 10^{-8}\,eV$$

Som ventet er dette en svært liten energi.

2c) 1: Transverse acoustic phonons (note that the branch splits at K; there are always two TA bands).
Acoustic: $\omega \xrightarrow[k \to 0]{} 0$.

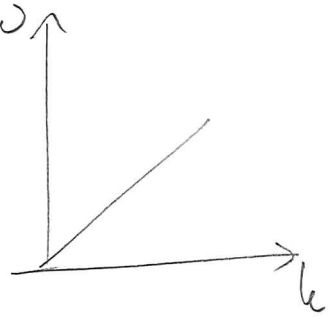
2: Longitudinal acoustic, LA.

3: Longitudinal optical, LO.

4: Transverse optical, TO. (Split at K).

Evidently, Si can have optical phonons!
This is because there are more than one (two!) atoms per primitive cell, and they have different local environments from a symmetry point of view
⇒ they can form different oscillation modes.

2d) Debye model: $\omega = v_g k$.



Must have

$$\int_0^{\omega_D} D(\omega)\,d\omega = \int_0^{k} D_k(k')\,dk'$$

$$\int_0^{k} \left(\frac{L}{2\pi}\right)^3 4\pi k'^2\,dk' = N(k)$$

$$\left(\frac{L}{2\pi}\right)^3 4\pi \frac{1}{3}k^3 = N(k)$$

$$\frac{V}{8\pi^2}\,4\,\frac{1}{3}k^3 = N(k)$$

$$\frac{V}{6\pi^2}k^3 = N(k)$$

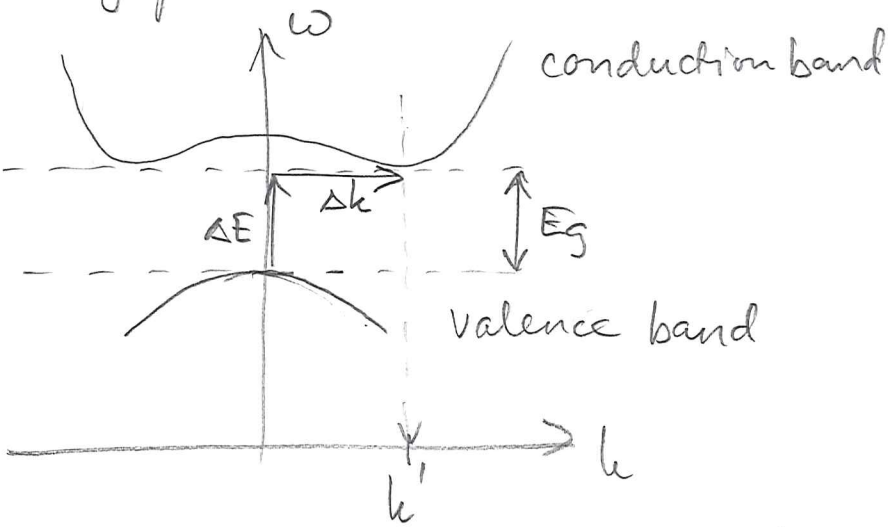
$$\frac{V}{6\pi^2}\frac{\omega^3}{v_g^3} = N(\omega)$$

$$D(\omega) = \frac{dN(\omega)}{d\omega} = \frac{\omega^2 V}{2\pi^2 v_g^3}$$

@5: We see that here, $D(\omega)$ diverges, consistently with (1) indicated in Fig. a).
For smaller ω, the Debye model is appropiate.

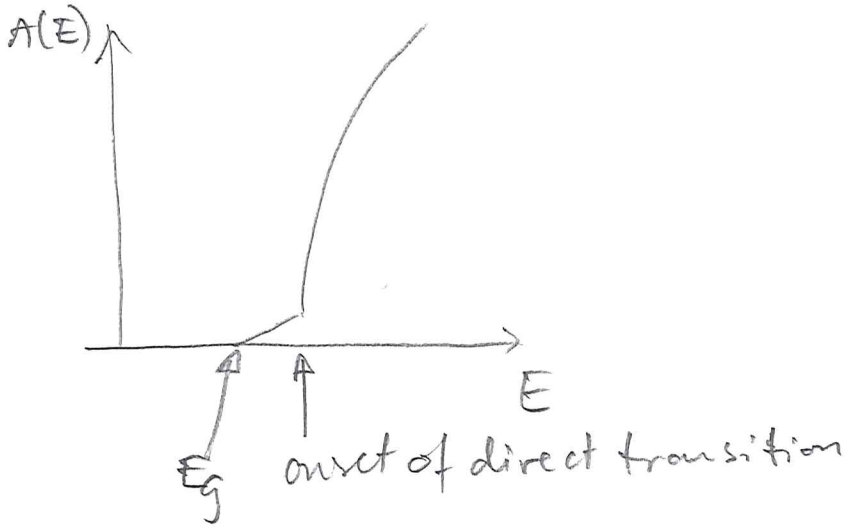
@6: Here, the optical phonons, having essentially constant $\omega(k)$ give a strong contribution to $D(\omega)$.
This can be described with the Einstein model.

3a) Indirect bandgap:



To get across the bandgap, both energy and momentum must be conserved. This can be realized by "phonon assistance".
The diagram above indicates photon excitation accounting for (most of) ΔE and a phonon accounting for (most of) Δk.

Light absorption:



We ignore the phonon energy, and find

$$E_g = \frac{hc}{\lambda}$$

$$\lambda = \frac{hc}{E_g} = 1.13 \cdot 10^{-6}\ m = \underline{1130\ nm}\ (\text{infra red}).$$

3b) $$n = \frac{1}{\sqrt{2}} \left(\frac{m_e^* k_B T}{\pi \hbar^2} \right)^{3/2} e^{-(E_g - \mu)/k_B T}$$

This expression is derived based on an almost free electron model, with the effective mass accounting for interactions with the lattice and other electrons.

The Fermi-Dirac distribution is replaced by the Maxwell-Boltzmann distribution, assuming that the chemical potential is near the center of the bandgap and that $T \sim T_{room}$. E_g - energy at bottom of conduction band.

Similarly, we get, with $1 - f(E,T)$ for holes,

$$p = \frac{1}{\sqrt{2}} \left(\frac{m_h^* k_B T}{\pi \hbar^2} \right)^{3/2} e^{-\mu/k_B T}.$$

$$np = 4 \left(\frac{k_B T}{2\pi \hbar^2} \right)^3 \left(m_e^* m_h^* \right)^{3/2} e^{-E_g/k_B T}$$

$$\therefore A = \left(\frac{k_B T}{2\pi \hbar^2} \right)^3$$

Note: np does not depend on μ.

3c) Intrinsic semiconductor: hypothetical idealized case with no impurity atoms present to dope the semicond.

$\Rightarrow n = p = n_i = p_i$

We find

$$n = p = n_i = p_i = \sqrt{np} = 2\left(\frac{k_B T}{2\pi\hbar^2}\right)^{3/2} \left(m_e^* m_h^*\right)^{3/4} e^{-E_g/2k_BT}$$

$$= 2\left(\frac{k_B T}{2\pi\hbar^2}\right)^{3/2} m_e^{3/2} e^{-E_g/2k_BT}, \quad E_g = 1.1\,eV$$

With numbers inserted:

$T = 150\,K$: $n_i = p_i = \underline{\underline{2.22 \cdot 10^6\ m^{-3}}}$

$T = 300\,K$: $n_i = p_i = \underline{\underline{1.24 \cdot 10^{16}\ m^{-3}}}$

Not surprising that the conductivity increases strongly with T!

3d) $n = p$ (equal amounts of electrons and holes).

$$\frac{1}{\sqrt{2}}\left(\frac{m_e^* k_B T}{\pi \hbar^2}\right)^{3/2} e^{-(E_g-\mu)/k_B T} = \frac{1}{\sqrt{2}}\left(\frac{m_h^* k_B T}{\pi \hbar^2}\right)^{3/2} e^{-\mu/k_B T}$$

$$\Downarrow$$

$$\left(\frac{m_e^*}{m_h^*}\right)^{3/2} = e^{-\mu/k_B T + (E_g-\mu)/k_B T}$$

$$\Downarrow$$

$$\frac{3}{2} \ln \frac{m_e^*}{m_h^*} = \frac{1}{k_B T}\left(E_g - 2\mu\right)$$

$$\Downarrow$$

$$\frac{1}{2}\left(\frac{3}{2} k_B T \ln \frac{m_h^*}{m_e^*} + E_g\right) = \mu$$

$$\underline{\mu = \frac{E_g}{2} + \frac{3}{4} k_B T \ln \frac{m_h^*}{m_e^*}}$$

q.e.d.

With $k_B T \sim 0.025\,\text{eV} \ll E_g$,
and $\ln\left(\frac{m_h^*}{m_e^*}\right)$ a small number

$$\underline{\mu \approx E_g/2}$$

The chemical potential is near the center of the bandgap, where there are no states, $D(E = E_g/2) = 0$.

Thus, there is <u>no Fermi surface</u> for semiconductors