a) What is the difference between a semiconductor and a metal? Discuss the Fermi energy when describing this difference.

If you take a look onto the conductivity of this different substances, you will recognize, that the conductivity of a semiconductor is lower than from metals, but in the same timer higher than from an insulator, at a given temperature.

One could also notice the temperature dependency from this substances. Semiconductors have a negative temperature coefficient (they tend to increase their conductivity at higher temperatures), whereas metals have a positive temperature coefficient (their conductivity is decreased at higher temperatures).

Electrons always try to occupy the lowest available energy state in an atom. The available and allowed energy states in an atom are called bands. The band with the highest energy state where we can find electrons is called valence band and is also responsible for the atomic bonds of atoms. The next available bands with higher energy states where no electron can be found at low temperatures are called conductions bands. The energy difference between the valence-, and the conduction band is called bandgap. Another important definitions are the Fermi energy and the Fermi energy level. The Fermi energy $E_f$ (also chemical potential of a substance) defines the highest occupied quantum state of electrons, where all energy states below are occupied and all above are empty. The Fermi energy can be located at the bandgap, or at an allowed energy state for electrons. The Fermi level is a hypothetical level of potential energy for an electron inside a crystalline solid and is labelled $E$ for our purpose. For temperatures at absolute zero, the Fermi energy and the Fermi energy level are the same.

The probability if a state is occupied can be calculated from: $f(E) = \frac{1}{e^{\frac{E-E_f}{k_B T}}+1}$

- $1$ if $0 < E < E_f$
- $0,5$ if $E = E_f$
- $0$ if $E_f < E$

Energy Levels below the Fermi energy don't contribute to the current flow, whereas energy levels above the Fermi energy do contribute to the current flow. Depending on the actual position of the Fermi energy we can describe substances as:

- metals: The Fermi energy is located at bands where the energy level are smeared out, which happens to be at the conduction band.
- insulators: The Fermi energy is located at the bandgap. All energy states below $E_f$ are occupied and all above are empty. The bandgap is compared to the one from semiconductors big. Therefore an electron needs more energy to get from an occupied state at the valence band into a free state at the conduction band.
- semiconductors: The Fermi energy is again located at the bandgap, but the bandgap itself is much smaller than the one compared to insulators. Electrons can be excited into the higher energy bands with much lower energy input. This energy input can be for instance either light or heat.

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1 http://en.wikipedia.org/wiki/Fermi_energy
2 http://en.wikipedia.org/wiki/Fermi_level
b) Why are the allowed electron energies divided into bands? What would happen if you injected an electron with a forbidden energy into a crystal?

First of all let's take a look onto allowed energy states in an atom. Due to the wave particle dualism you can describe the Energy from an electron with the kinetic and potential Energy

\[ E = E_{\text{kin}} + E_{\text{pot}} = -\frac{e^2}{2 \varepsilon_0 r} \]

Now due to the fact that every electron has it's own wavelength (deBroglie relations \( E = h \nu = h \frac{\lambda}{\hbar} \)) it can only orbit stable around the nucleus of the atom on orbits with multiple lengths of it's own wavelength.

Therefore we get the Bohr radius of atoms \( a_n = n^2 \left( \frac{\hbar}{2 \pi} \right)^2 \frac{4 \pi \varepsilon_0 m_0 e^2}{\hbar^2} \). If we combine both formulas we will receive \( E = -\frac{1}{2} \frac{e^2}{4 \pi \varepsilon_0 a_n} \) which gives us only discrete energy values dependant onto the actual radius at which the electron orbits around the nucleus.

Now let’s imagine we take two atoms and decrease their distance to each other at a continuous rate. We will recognize that the original energy states of the single atoms will smear out at higher energy levels in order to "energetically" move away. This will create energy bands which can't be assigned to one of the original atoms but to the whole system of atoms.

As well as in a single atom, the lowest energy states will be first occupied in the crystal. The band with the highest energy state where we can find electrons at low level temperatures (so without thermal activation of electrons) are called valence

\[ \text{http://en.wikipedia.org/wiki/Matter\_wave} \]
band and are also responsible for the atomic bonds of atoms. The next available bands with higher energy states where no electron can be found (again at low level temperatures) are called conduction bands. If an electron gets excited through light or heat and "transports" the electron from the valence band into the conduction band, it is then very easy for the electron to move around in the crystal within the conduction band.

If you inject an electron with a forbidden energy into the crystal (therefore an energy within the bandgap) there are two possible ways how the electron can behave. If you think of the wave particle dualism, you can think of the electron like a wave $E = h\nu = \frac{hc}{\lambda}$. So if the wave hits the first layer of atoms of the crystal, some part of the incoming waves are reflected and another part is transmitted. At the next layer of the crystal the same process happens again. Now if the reflected waves add constructively the electron get’s reflected from the crystal. This is how you can make a mirror for optical systems. The second way for the electron’s behaviour is that if the electron has enough energy to break a bond or exchange energy like a particle in the crystal it can stay in the crystal. It has to scatter in such a way that it exchanges energy like a particle so it can go into an allowed energy level and be accepted in the crystal. Electrons move like waves but exchange energy and momentum like particles. Most of electrons wouldn’t get the opportunity to exchange energy before they are reflected out.

c) What determines the density of phonons in a semiconductor? What effect do phonons have on the electrical conductivity?

When you think of an vibrating atom which is located in a solid and regular lattice material, one atom can’t vibrate without affecting the nearby atoms due to their atomic bond, so atoms can’t vibrate independently. The vibrations appear in periodic modes which propagate through the whole material. Phonons are now quantized particles of this vibration which can either appear acoustically (sound) or optically (light) and their energy is related to their frequency $E = h\nu$ at which they travel through the material. Are the atoms moving in phase, we can observe an acoustic mode. If they are moving out of phase, we observe an optical mode. Optical modes can only be observed if Phonons interact with Photons and vice versa, while the base of the atoms has to be polarized (otherwise there will be no interaction).

**Akustische Mode**

**Optische Mode**

5: optical and acoustic transversal waves (Wikipedia, 2013)

Due to the fact that Phonons are simply bosons (which means that two particles can be in the same place at the same time) the mean number of Phonons in a state is given by the Bose-Einstein formula: $\langle N \rangle_{BE} = \frac{1}{e^{\frac{\hbar\nu k}{kT}} - 1}$. Additionally Phonons have three possible polarization states and the given Formula must be multiplied by the factor 3: $\bar{N}(E) = \frac{3}{e^{\frac{\hbar\nu k}{kT}} - 1}$.

Now, the density of states can be calculated due to the solutions of Peter Debye and Albert Einstein. For our purpose we will have a look onto the model of Debye. The density of states can be calculated out of $g(\omega)d\omega = g(k)dk$ where $\omega$ represents the angular frequency $\omega = 2\pi f$ and $k = \frac{2\pi}{\lambda}$ the wave vector. Now we can rearrange the given formula in two ways, but let’s take the representation with the angular vector: $g(\omega) = \frac{g(k)dk}{d\omega}$ where $g(k) = \frac{1}{L}$ (which is applied in a k-room).

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**Notes:**

iv http://lamp.tu-graz.ac.at/~hadley/psd/lectures12/oct9/slide7.html
v http://lamp.tu-graz.ac.at/~hadley/ss1/phonons/phonons.php
vii http://lamp.tu-graz.ac.at/~hadley/ss1/phonons/phonontable.html
and $k = \frac{\omega}{v_k}$. As it is shown in VII: we receive two possible solutions: 

$$ g(\omega) = \begin{cases} \frac{3\omega^2}{2\pi^2c^2}, & \text{for } \omega < \omega_D = (6n\pi^2c^2)^{1/3} \\ 0, & \text{for } \omega > \omega_D \end{cases} $$

or

$$ g(k) = \frac{3k^2}{2\pi^2}. $$

Now let’s answer the question of how phonons affect electrical conductivity. In general, electrical resistivity is temperature dependant and for simple metal resistors we can calculate the resistivity from $R(\vartheta) = R(\vartheta_0)(1 + \alpha(\vartheta - \vartheta_0) + \beta(\vartheta - \vartheta_0)^2)$. Depending onto the structure of the material we use for the conduction, the temperature coefficient of the material can be either positive (metal structures) or negative (semiconducting structures). With a positive temperature coefficient the resistance of the material will increase linear while the temperature of the material is increasing (therefore the atom lattice vibrations) and with a negative temperature coefficient vice versa. This effect happens, due to the scattering of the free moving electrons with the atom lattice. Now phonons represent a quantized amount of the atom lattice vibration of the material (temperature). If the temperature for a metal structure material is reduced adequately, let’s say to nearly absolute zero, the phonons will be "frozen" because there will be no vibrations of the atom lattice. The resistivity also reaches a constant value, which is called the residual resistivity. For semiconducting materials, electrons will be excited into the conduction band if the temperature of the material is increased due to the thermal energy. Here the excited electrons in the conduction band and the generated holes in the valence band can move freely.

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**list of references**
