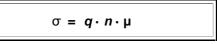
This Module comes from "Introduction to Materials Science II"; where you will find the most recent version. The <u>link</u> takes you there.

## **Required Reading**

#### **1.3.3 Ohms Law and Classical Physics**

In this subchapter we will look at the *classical* treatment of the movement of electrons inside a material in an electrical field.

In the preceding subchapter we obtained the most basic formulation of Ohms law, linking the specific conductivity to two fundamental material parameters:



For a homogeneous and isotropic material (*e.g.* polycrystalline metals or single crystal of cubic semiconductors), the *concentration* of carriers *n* and their *mobility*  $\mu$  have the same value everywhere in the material, and the specific conductivity  $\sigma$  is a *scalar*.

This is boring, however. So let's look at useful complications:

In general terms, we may have more than one kind of carrier (this is the common situation in semiconductors) and n and  $\mu$  could be functions of the temperature T, the *local* field strength  $E_{loc}$  resulting from an applied *external* voltage, the detailed structure of the material (e.g. the defects in the lattice), and so on.

- We will see that these complications are the essence of advanced electronic materials (especially semiconductors), but in order to make life easy we first will restrict ourselves to the special class of **ohmic materials**.
- We have <u>seen before</u> that this requires *n* and μ to be independent of the local field strength. However, we still may have a temperature dependence of σ; even commercial ohmic resistors, after all, do show a more or less pronounced temperature dependence their resistance increases roughly linearly with *T*.

In short, we are treating *metals*, characterized by a *constant* density of *one* kind of carriers (= electrons) in the order of **1** ...**3** electrons per atom in the metal.

### Basic Equations and the Nature of the "Frictional Force"

We consider the electrons in the metal to be "free", i.e. they can move freely in any direction - the atoms of the lattice thus *by definition* do not impede their movement

- The (local) electrical field <u>E</u> then exerts a force <u>F</u> = e · <u>Eloc</u> on any given electron and thus accelerates the electrons in the field direction (more precisely, opposite to the field direction because the field vector points from + to whereas the electron moves from to +).
- In the <u>fly swarm analogy</u>, the electrical field would correspond to a steady airflow some wind that moves the swarm about with constant drift velocity.

Now, if a single electron with the (constant) mass **m** and momentum **p** is subjected to a force **F**, the equation of motion from basic mechanics is

$$\underline{F} = \frac{\mathrm{d}\underline{p}}{\mathrm{d}t} = \frac{m \cdot \mathrm{d}\underline{v}}{\mathrm{d}t}$$

Note that **p** does not have to be zero when the field is switched on.

If this would be all, the velocity of a given electron would acquire an ever increasing component in field direction and eventually approach infinity. This is obviously not possible, so we have to bring in a mechanism that destroys an unlimited increase in  $\underline{v}$ .

In classical mechanics this is done by introducing a frictional force <u>*F*</u>fr that is proportional to the velocity.

$$\underline{F}_{fr} = -k_{fr} \cdot \underline{v}$$

with k<sub>fr</sub> being some friction constant. But this, while mathematically sufficient, is devoid of any physical meaning with regard to the moving electrons.

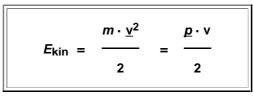
There is no "friction" on an atomic scale! Think about it! Where should a friction force come from? An electron feels only forces from two kinds of fields - electromagnetic and gravitational (neglecting strange stuff from particle physics). So we have to look for another approach.

What friction does to big classical bodies is to *dissipate* ordered kinetic energy of the moving body to the environment. Any ordered movement gets slowed down to zero (surplus) speed, and the environment gets somewhat hotter instead, i.e. *unordered* movement has increased.

This is called energy dissipation, and that is what we need: Mechanisms that take kinetic energy away from an electron and "give" it to the crystal at large. The science behind that is called (Statistical) Thermodynamics - we have encounterd it before.

The best way to think about this, is to assume that the electron, flying along with increasing velocity, will *hit something else* along its way every now and then; it has a *collision* with something else, it will be **scattered** at something else.

This collision or scattering event will change its momentum, i.e. the magnitude and the direction of <u>v</u>, and thus also its kinetic energy *E<sub>kin</sub>*, which is always given by



In other words, we consider collisions with something else, i.e. other particles (including "pseudo" particles), where the total energy and momentum of all the particles is preserved, but the individual particle looses its "memory" with respect to its velocity before the collision, and starts with a new momentum after every collision.

What are the "partners" for collisions of an electron, or put in standard language, what are the **scattering mechanisms**? There are several possibilities:

- Other *electrons*. While this happens, it is not the important process in most cases. It also does not decrease the energy contained in the electron movement the losses of some electron are the gains of others.
- <u>Defects</u>, e.g. foreign atoms, point defects or dislocations. This is a more important scattering mechanism and moreover a mechanism where the electron can transfer its surplus energy (obtained through acceleration in the electrical field) to the lattice, which means that the material heats up
- <u>Phonons</u>, i.e. "quantized" lattice vibrations traveling through the crystal. This is the most important scattering mechanism.

Now that is a bit strange. While we (hopefully) have no problem imagining a crystal lattice with all atoms vibrating merrily, there is no immediate reason to consider these vibrations as being *localized* (whatever this means) and *particle-like*.

You are right - but nevertheless: The lattice vibrations indeed are best described by a bunch of particle-like phonons careening through the crystal.

This follows from a quantum mechanical treatment of lattice vibrations. Then it can be shown that these vibrations, which contain the thermal energy of the crystal, are quantized and show typical properties of (quantum) particles: They have a *momentum*, and an *energy* given by  $h\nu$  (h = Plancks constant,  $\nu =$  frequency of the vibration).

*Phonons* are a first example of "pseudo" particles; but there is no more "pseudo" to phonons than there is to photons.

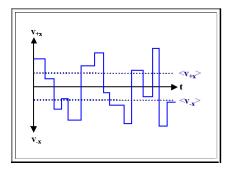
We will not go into more details here. All we need to know is that a hot crystal has more phonons and more energetic phonons than a cold crystal, and treating the interaction of an electron with the lattice vibration as a collision with a phonon gives not only correct results, it is the only way to get results at all.

At this point comes a crucial insight: It would be far from the truth to assume that only *accelerated* electrons scatter; scattering happens all the time to all the electrons moving randomly about because they all have some thermal energy. Generally, scattering is the mechanism to achieve thermal equilibrium and equidistribution of the energy of the crystal.

- If electrons are accelerated in an electrical field and thus gain energy in excess of thermal equilibrium, scattering is the way to transfer this surplus energy to the lattice which then will heat up. If the crystal is heated up from the outside, scattering is the mechanism to turn heat energy contained in lattice vibrations to kinetic energy of the electrons.
- Again: Even without an electrical field, scattering is the mechanism to transfer thermal energy from the lattice to the electrons (and back). Generally, scattering is the mechanism to achieve *thermal equilibrium* and equidistribution of the energy of the crystal.
- Our free electrons in metals behave very much like a gas in a closed container. They *careen* around with some average velocity that depends on the energy contained in the *electron gas*, which is in classical terms- a direct <u>function of the temperature</u>.

#### **Averaging over Random Scattering Events**

Lets look at some figures illustrating the scattering processes.



- Shown here is the *magnitude* of the velocity  $\underline{v}_{\pm x}$  of an electron in  $\pm x$  and -x direction *without* an external field. The electron moves with constant velocity until it is scattered, then it continues with some new velocity.
- The scattering processes, though unpredictable at single events, must lead to the averages of the velocity, which is characteristic for the material and its conditions.
- The plural in "averages" is intentional: there are different averages of the velocity
- Whereas  $\triangleleft z >= 0$ ,  $\triangleleft z >$  has a finite value; this is also true for  $\triangleleft z <= \triangleleft z = \neg z <= -x >$ . Consult the <u>"fly swarm modul"</u> if you are unsure about this.

From <u>classical thermodynamics we know</u> that the (classical) electron gas in thermal equilibrium with the environment contains the energy  $E_{kin} = (1/2)kT$  per particle and degree of freedom, with k = Boltzmanns constant and T = absolute temperature. The three degrees of freedom are the velocities in x-, y- and z-direction, so we must have

$$E_{kin,x} = \frac{1}{2} \cdot m \cdot \sqrt{x} x^{2} = \frac{1}{2} \cdot kT$$
$$\sqrt{x} x^{2} = \left(\frac{kT}{m}\right) \frac{1}{2}$$

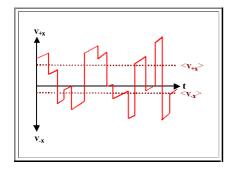
For the other directions we have exactly the same relations, of course. For the total energy we obtain

$$E_{kin} = \frac{m \cdot \langle v_{x}^{2} \rangle}{2} + \frac{m \cdot \langle v_{y}^{2} \rangle}{2} + \frac{m \cdot \langle v_{z}^{2} \rangle}{2} = \frac{m \cdot \langle v^{2} \rangle}{2} = \frac{m \cdot (v_{0})^{2}}{2} = \frac{3kT}{2}$$

- with  $v_0 = \langle v \rangle$ ,  $v_0$  is thus the average velocity of a carrier careening around in a crystal.
- At this point you should stop a moment and think about just how fast those electrons will be careening around at room temperature (300K) without plugging numbers in the equation. Got a feeling for it? Probably not. So look at the exercise question (and the solution) <u>further down!</u>.
- Now you should stop another moment and become very aware of the fact that this equation is from purely *classical* physics. It is absolutely true for *classical* particles which electrons are actually not. Electrons obey the <u>Pauli</u> <u>principle</u>, i.e. they behave about as non-classical behavior as it is possible. This should make you feel a bit uncomfortable. Maybe the equation from above is not correct for electrons then? Indeed it isn't. Why, we will see later; also how we can "repair" the situation!

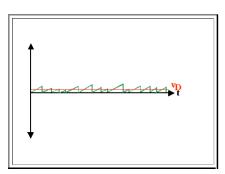
Now lets *turn on an electrical field*. It will accelerate the electrons *between* the collisions. Their velocity in field direction then increases linearly from whatever value it had right after a collision to some larger value right before the next collision.

In our diagram from above this looks like this:



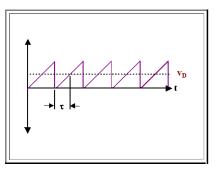
- Here we have an electrical field that accelerates electrons in in x-direction (and "brakes" in -x direction). Between collisions, the electron gains velocity in +x-direction at a constant rate (= identical slope).
- The average velocity in +x directions, <v<sub>+x</sub>>, is now larger than in -x direction, <v<sub>-x</sub>>.
- However, beware of the pitfalls of schematic drawings: For real electrons the difference is very small as we shall see shortly; the slope in the drawing is very exaggerated.

The drift velocity is contained in the difference  $\langle v_{+x} \rangle - \langle v_{-x} \rangle$ ; it is completely described by the velocity gain between collisions. For obtaining a value, we may neglect the instantaneous velocity right after a scattering event because they average to zero anyway and just plot the *velocity gain* in a simplified picture; always starting from zero after a collision.



- The picture now looks quite simple; but remember that it contains some <u>not so simple averaging</u>.
- At this point it is time to define a very meaningful *new* average quantity:
- The *mean time between collisions*, or more conventional, the mean time τ for reaching the drift velocity **v** in the simplified diagram. We also call τ the **mean scattering time** or just *scattering time* for short.

This is most easily illustrated by simplifying the scattering diagram once more: We simply use just one time - the average - for the time that elapses between scattering events and obtain:



- This is the standard diagram illustrating the scattering of electrons in a crystal usually found in text books; the definition of the scattering time τ is included
- It is highly idealized, if not to say just wrong if you compare it to the correct picture <u>above</u>. Of course, the average velocity of both pictures will give the same value, but that's like saying that the average speed v<sub>a</sub> of all real cars driving around in a city is the same as the average speed of ideal model cars all going at v<sub>a</sub> all the time.
- Note that  $\tau$  is only *half* of the average time between collisions.

So, while this diagram is not wrong, it is a highly abstract rendering of the underlying processes obtained after several averaging procedures. From this diagram only, no conclusion whatsoever can be drawn as to the average velocities of the electrons without the electrical field!

### **New Material Parameters and Classical Conductivity**

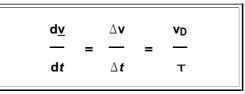
With the scattering concept, we now have two new (closely related) material parameters:

- The mean (scattering) time  $\tau$  between two collisions as defined before, and a directly related quantity:
- The **mean free path** *I* between collisions; i.e. the distance travelled by an electron (on average) before it collides with something else and changes its momentum. We have

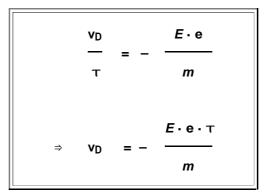
$$I = 2\tau \cdot (v_0 + v_D)$$

Note that **v**<sub>0</sub> enters the defining equation for *I*, and that we have to take twice the scattering time τ because it only refers to half the time between collisions!

After we have come to this point, we now can go on: Using  $\tau$  as a new parameter, we can rewrite Newtons equation from <u>above</u>:



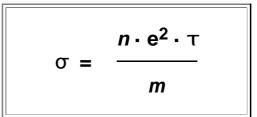
It is possible to equate the *differential* quotient with the *difference* quotient, because the velocity change is constant. From this we obtain



Inserting this equation for  $v_D$  in the old <u>definition of the current density</u>  $j = -n \cdot e \cdot v_D$  and invoking the general version of <u>Ohms law</u>,  $j = \sigma \cdot E$ , *yields* 

$$j = \frac{n \cdot e^2 \cdot \tau}{m} \cdot E := \sigma \cdot E$$

This gives us the final result



This is the *classical* formula for the conductivity of a classical "electron gas" material; i.e. metals. The conductivity contains the density n of the free electrons and their mean scattering time  $\tau$  as material parameters.

We have a good idea about *n*, but we do not yet know τ<sub>class</sub>, the mean *classical* scattering time for classical electrons. However, since we know the <u>order of magnitude</u> for the conductivity of metals, we may turn the equation around and use it to calculate the order of magnitude of τ<sub>class</sub>. If you do the exercise farther down, you will see that the result is:

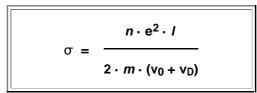
$$\tau_{\text{class}} = \frac{\sigma \cdot m}{n \cdot e^2} \approx (10^{-13} \dots 10^{-15}) \text{ sec}$$

"Obviously" (as stated in many text books), this is a value that is *far too small* and thus the classical approach must be *wrong*. But is it really too small? How can *you* tell without knowing a lot more about electrons in metals?
Let's face it: *you can't !!*. So let's look at the *mean free path I* instead. <u>We have</u>

$$I = 2 \cdot \tau \cdot (v_0 + v_D)$$
  
and  
$$(v_0)^2 = \frac{3kT}{m}$$

The last equation gives us a value  $v_0 \approx 10^4$  m/s at room temperature! Now we need  $v_D$ , and this we can estimate from the equation given <u>above</u> to  $v_D = -E \cdot \tau \cdot e/m \approx 1$  mm/sec, *if* we use the value for  $\tau$  dictated by the measured conductivities. It is much smaller than  $v_0$  and can be safely neglected in calculating *I*.

We thus can rewrite the equation for the conductivity and obtain



Knowing  $\sigma$  from experiments, but not *I*, allows to determine *I*. The smallest possible mean free path  $I_{min}$  between collisions (for  $v_D = 0$ ) thus is

$$I_{\min} = \frac{2 \cdot m \cdot v_0 \cdot \sigma}{n \cdot e^2} = 2 \cdot v_0 \cdot \tau \approx (10^{-1} - 10^1) \text{ nm}$$

And this is certainly too small!.

But before we discuss these results, let's see if they are actually true by doing an exercise:



Now to the important question: Why is a mean free path in the order of the size of an atom too small?

- Well, think about the <u>scattering mechanisms</u>. The distance between lattice defects is certainly much larger, and a phonon itself is "larger", too.
- Moreover, consider what happens at temperatures below room temperatures: I would become even smaller since v<sub>0</sub> decreases somehow this makes no sense.
- It does not pay to spend more time on this. Whichever way you look at it, whatever tricky devices you introduce to make the approximations better (and physicists have tried very hard!), you will *not* be able to solve the problem: The mean free paths are never even coming close to what they need to be, and the conclusion which we will reach - maybe reluctantly, but unavoidably - must be:

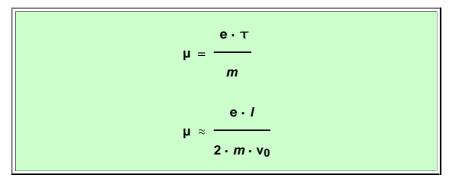


### **Scattering and Mobility**

Somewhere on the way, we have also indirectly found that the **mobility µ** as <u>defined before</u> is just another way to look at scattering mechanisms. Let's see why.

All we have to do is to compare the equation for the conductivity from above with the master equation  $\sigma = \mathbf{q} \cdot \mathbf{n} \cdot \boldsymbol{\mu}$ .

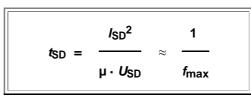
This gives us immediately



In other words:

# The *decisive* material property determining the mobility $\mu$ is the average time between scattering events or the mean free path between those events.

- The mobility µ thus is a basic material property, well-defined even without electrical fields, and just another way to express the scattering processes taken place by a number.
- In the equations above slumbers an extremely important aspect of semicoductor technology.
  - In all electronic devices carriers have to travel some distance before a signal can be produced. A MOS transistor, for example, switches currents on or off between its "Source" and "Drain" terminal depending on what voltage is applied to its "Gate". Source and drain are separated by some distance *I*<sub>SD</sub>, and the "Drain" only "feels" the "on" state after the time it takes the carriers to run the distance *I*<sub>SD</sub>.
  - How long does that take if the voltage between Source and Drain is USD?
  - Easy. If we know the mobility μ of the carriers, we now their (average) velocity v<sub>SD</sub> in the source-drain region, which by definition is v<sub>SD</sub> = μ · U<sub>SD</sub>/I<sub>SD</sub>.
  - The traveling time t<sub>SD</sub> between source and drain for obvious reasons defines roughly the maximum frequency f<sub>max</sub> the transistor can hand, we have t<sub>SD</sub> = I<sub>SD</sub> / v<sub>SD</sub> or



- The maximum frequency of a MOS transistor thus is directly proportional to the mobility of the carriers in the material it is made from (always provided there are no other limiting factors). And since we used a rather general argument, we should not be surprised that pretty much the same relation is also true for most electronic devices, not just MOS transistors.
- This is a momentous statement: We linked a prime material parameter, the material constant µ, to one of the most important parameters of electronic circuits. We would like µ to be as large as possible, of course, and now we know what to do about it!
- A simple exercise is in order to see the power of this knowlegde:

