Ohm's Law and Materials Properties

> For this basic module we simply take the **suitable module** of the Hyperscript "**Introduction to Materials Science II**" since it is the newest and updated version.
> ● The module as it existed in Sept. '01 is reprocuced below.

## Ohm's Law and Material Properties

> In this subchapter we will give an outline of how to progress from the simple version of **Ohm's "Law"**, which is a kind of "electrical" definition for a black box, to a formulation of the same law from a *materials point of view* employing (almost) first principles.
> ● In other words: The electrical engineering point of view is: If a "black box" exhibits a linear relation between the (dc) current *I* flowing through it and the voltage *U* applied to it, it is an **ohmic resistor**.
> ● In contrast, the (extreme) Materials Science point of view is: Tell me what kind of material is in the black box, and I tell you:
>   1. If it is an *ohmic* resistor, i.e. if the current relates *linearly* to the voltage for reasonable voltages and *both* polarities; and
>   2. What its (specific) resistance will be, including its temperature dependence.
>   3. And everything else of interest.

> Let's see what we have to do for this approach.

1. Step: Move to specific quantities

> First we switch from current *I* and voltage *U* to the **current density _j_** and the **field strength _E_** , which are not only independent of the (uninteresting) size and shape of the body, but, since they are *vectors*, carry much more information about the system.
> ● This is easily seen in the schematic drawing below.
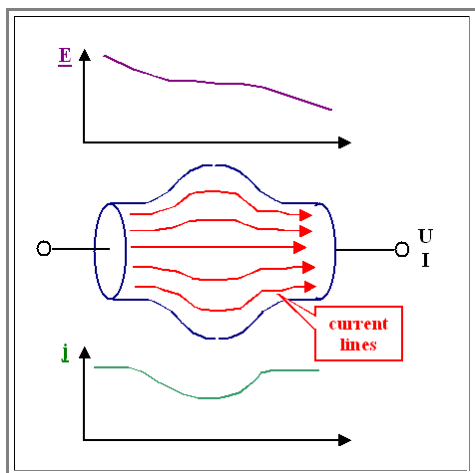
● *Current density _j_* and *field strength _E_* may depend on the coordinates, because *U* and *I* depend on the coordinates, e.g. in the way schematically shown in the picture to the left. However, for a homogeneous material with constant cross section, we may write

$$ j = \frac{I}{F} $$

● with *F*= cross sectional area. The direction of the vector *j* would be parallel to the normal vector *f* of the reference area considered, so in full splendor we must write

$$ j = \frac{I}{F} \cdot \underline{f} $$

The field strength is

$$\underline{E} = \frac{U}{d}$$

- Here, $d=$ distance between the points at which U is measured. If we want $\underline{E}$ as a vector, we have, in principle, to calculate the gradient of the potential V:

$$\underline{E} = -\nabla V$$

- For the homogeneous case $\underline{E}$ is parallel to $\underline{f}$ again which is clear without calculation.

We now write down Ohm's law with the new quantities and obtain

$$\underline{j} \cdot F = I = \frac{1}{R} \cdot U = \frac{1}{R} \cdot (E \cdot d)$$

$$j = \frac{d}{F \cdot R} \cdot E$$

The fraction $d / (F \cdot R)$ *obviously* (think about it!) has the *same numerical value* for any homogeneous cube (or ....) of a given material; it is, of course, the **specific conductance** or, for short, the **conductivity** σ:

$$\sigma = \frac{1}{\rho} = \frac{d}{F \cdot R}$$

- and ρ is the **specific resistance** or, for short, the **resistivity**.

- Of course, we will never mix up the *resistivity* ρ with the *charge density* ρ or *general densities* ρ, because we know from the context what is meant!

- The *resistivity* obtained in this way is of course identical to what you would define as specific resistance by looking at some rectangular body with cross-sectional area F and length d.

- Being *specifc* quantities, *conductivity* has the dimension $[\sigma] = \Omega^{-1}$ **cm**$^{-1}$, and the dimension of *resistivity* is $[\rho] = \Omega$**cm**. The latter is more prominent and you should at least have a feeling for representative numbers by remembering this:

$$\rho \text{ (metal)} \approx 2 \ \mu\Omega\text{cm}$$

$$\rho \text{ (semicoductor)} \approx 1 \ \Omega\text{cm}$$

$$\rho \text{ (insulator)} \approx 1 \ \text{G}\Omega\text{cm}$$

Restricting ourselves to isotropic and homogenoeus materials restricts σ and ρ to being *scalars* with the *same numerical value* everywhere, and Ohm's law now can be formulated for any material with weird shapes; we "simply" have

$$\underline{j} = \sigma \cdot \underline{E}$$

Ohm's law in this *vector form* , however, is now valid at *any point* of a body, since we do not have to make assumptions about the shape of the body.

● Take an arbitrarily shaped body with current flowing through it, cut out a little cube (with your "mathematical" knife) at the coordinates **(x,y,z)** without changing the flow of current, and you must find that the local current density and the local field strength obey equation given above *locally*.

$$\underline{j}(x,y,z) \ = \ \sigma \cdot \underline{E}(x,y,z)$$

This is a much more powerful version of Ohm's law! Especially, because we now harbor a suspicion: There is no good reason why $\underline{j}$ must always be parallel to $\underline{E}$. This means that for the most general case, conductivity is not a *scalar* quantity but a *tensor*; σ= σ_{ij}.
(There is no good way to write tensors in HTML; we use the $_{ij}$ index to indicate tensor properties.

● Ohm's law then writes

$$j_x = \sigma_{xx} \cdot E_x + \sigma_{xy} \cdot E_y + \sigma_{xz} \cdot E_z$$
$$j_y = \sigma_{yx} \cdot E_x + \sigma_{yy} \cdot E_y + \sigma_{yz} \cdot E_z$$
$$j_z = \sigma_{zx} \cdot E_x + \sigma_{zy} \cdot E_y + \sigma_{zz} \cdot E_z$$

For anisotropic inhomogeneous materials you have to take the tensor, and its components will all depend on the coordinates – that is the most general version of Ohm's law.

● Note that this is *not* so general as to be meaningless: We still have the basic property of Ohm's law: The local current density is directly proprotional to the local field strength (and not, for example, to **exp(– const. · $\underline{E}$)**.

Our goal now is to find a relation that makes possible to calculate σ_{ij} for a given material (or material composite); i.e. we are looking for

● $\sigma_{ij} = \sigma_{ij}$ **(material, temperature, pressure, defects...)**

### 2. Step: Describe σ_{ij} in Terms of the Carrier Properties

Electrical current needs *mobile* charged carriers. We therefore want to express σ_{ij} in terms of the properties of the carriers present in the material under investigation.

● To do this, we will look at an electrical current as a "mechanical" stream or current of (charged) particles and compare the result we get with Ohm's law.

First, lets define an electrical current in a wire in terms of the carriers flowing through that wire. There are three crucial points to consider

1. The external electrical current as measured in an Ampèremeter is the result of the *net* current flow through any cross section of an (uniform) wire.

● In other words, the measured current is proportional to the *difference* of the number of carriers of the same charge sign moving from the *left to right* through a given cross sectional area *minus* the number of carriers moving from the *right to the left*.

● In short: the *net* current is the difference of two *partial* currents flowing in opposite directions:
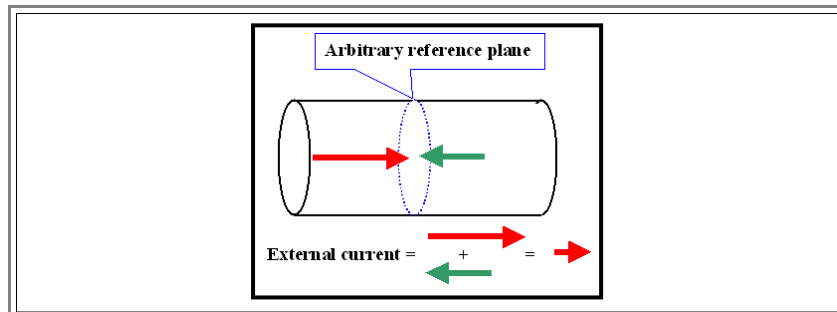

● We will encounter cases where we have to sum up **8** partial currents to arrive at the externally flowing current, so keep this in mind!

2. In summing up the individual current contributions, *make sure the signs are correct*. The rule is simple:

● The *electrical* current is (for historic reasons) defined as flowing from **+** to **–**. For a *particle* current this means:
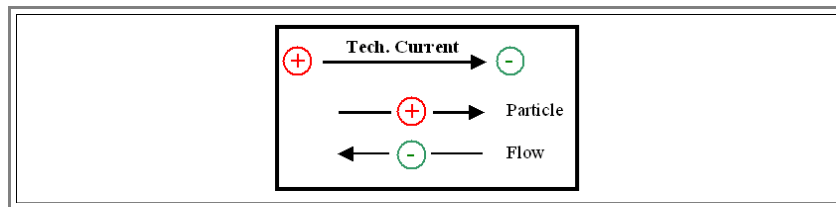
● In words: A technical current *I* flowing from **+** to **–** may be obtained by *negatively* charged carriers flowing in the *opposite* direction (from **–** to **+**), by *positively* charged carriers flowing in the *same* direction, or from both kinds of carriers flowing at the same time in the proper directions.

● The particle currents of *differently* charged particles then must be *added*! Conversely, if negatively charged carriers flow in the same directions as positively charged carriers, the value of the partial current flowing in the "wrong" direction must be subtracted to obtain the external current.

3. The flow of particles through a reference surface as symbolized by one of arrows above, say the arrow in the **+x** - direction, must be seen as an *average* over the **x** -component of the velocity of the individual particles in the wire. Instead of one arrow, we must consider as many arrows as there are particles and take their average. A more detailed picture of a wire thus looks like this
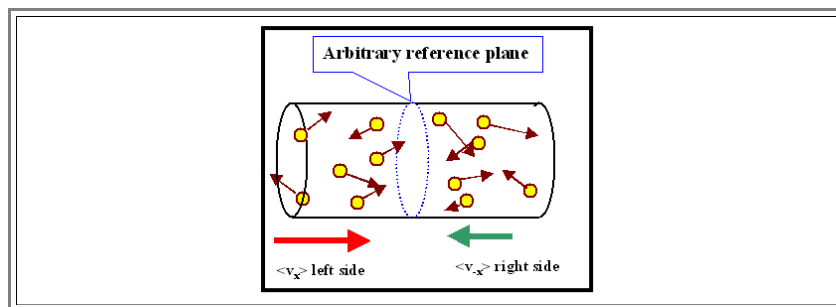
● If we want to obtain the net flow of *particles* through the wire (which is obviously proportional to the net *current* flow), we could take the average of the velocity components $\langle v_x \rangle$ pointing in the **+x** direction (to the right) on the left hand side, and subtract from this the average $\langle v_{-x} \rangle$ of the velocity components pointing in the **–x** direction (to the left) on the right hand side.

● We call this *difference* the **drift velocity** of the *ensemble* of carriers. If there is no driving force, e.g. an electrical field, the velocity vectors are randomly distributed and $\langle v_x \rangle = \langle v_{-x} \rangle$; the net current is zero as it should be.

▸ Average properties of ensembles can be a bit tricky. Lets look at some properties by considering the analogy of a localized **swarm of summer flies** "circling" around like crazy, so that the ensemble looks like a small cloud of smoke. A more detailed treatment can be found in the advanced section.

● First we notice that while the *individual* fly moves around quite fast, its *vector* velocity $\underline{v_i}$ averaged over time *t*, $\langle \underline{v_i} \rangle_t$, must be zero as long as the swarm as an ensemble doesn't move.

● In other words, the flies, *on average*, move just as often to the left as to the right, etc. The net current produced by *all* flies at any given instance or by *one* individual fly after sufficient time is obviously zero for any reference surface.

▸ In real life, however, the fly swarm "cloud" often moves *slowly* around – it has a finite *drift velocity* which must be just the difference between the average movement in drift direction minus the average movement in the opposite direction.

● The *drift velocity* thus can be identified as the proper average that gives the net current through a reference plane perpendicular to the direction of the drift velocity.

● This drift velocity is usually much smaller than the average magnitude of the velocity $\langle v \rangle$ of the individual flies. Its value is the difference of two large numbers – the average velocity of the *individual* flies in the drift direction minus the average velocity of the *individual* flies in the direction opposite to the drift direction.

▸ Since we are only interested in the drift velocity of the ensemble of flies (or in our case, carriers) we may now simplify our picture as follows:
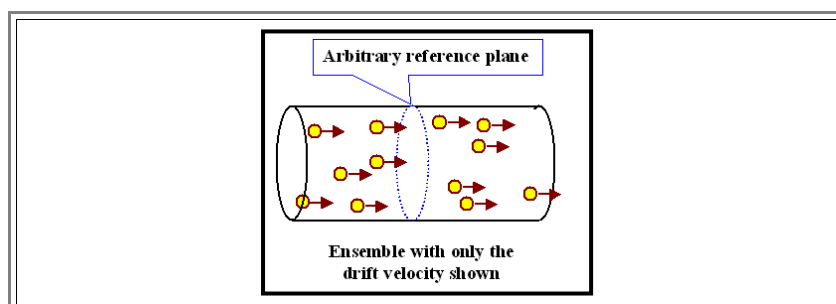
We now equate the *current density* with the *particle flux density* by the basic law of current flow:

- Current density $\underline{j}$=number N of particles carrying the charge q flowing through the cross sectional area F (with the normal vector $\underline{f}$ and $|\underline{f}|=1$) during the time interval t, or

$$\underline{j} = \frac{q \cdot N}{F \cdot t} \cdot \underline{f}$$

- In scalar notation, because the direction of the current flow is clear, we have

$$j = \frac{q \cdot N}{F \cdot t}$$

- With $n = N/V =$ density of carriers in a volume V, and $V = F \cdot d$ with d being the required certain length of the wire needed to obtain V, we now must consider how many carriers contained in the volume V will flow through the reference plane F.
- The trick is to take

$$d = v_D \cdot t$$

- This makes sure that *all* carriers contained in this length will have reached F after the time t has passed, and thus all carriers contained in the volume $V = F \cdot v_D \cdot t$ will contribute to the current density. We can write the current equation as follows:

$$j = \frac{q \cdot N}{F \cdot t} = \frac{q \cdot n \cdot V}{F \cdot t} = \frac{q \cdot n \cdot F \cdot d}{F \cdot t} = \frac{q \cdot n \cdot F \cdot v_D \cdot t}{F \cdot t}$$

This was shown in excessive detail because now we have the fundamtental law of electrical conductivity (in obvious vector form)

$$\underline{j} = q \cdot n \cdot \underline{v}_D$$

This is a very general equation relating a *particle current* (density) via its *drift velocity* to an *electrical current* (density) via the charge q carried by the particles.

- Note that it does not matter at all *why* an ensemble of charged particles moves on average. You do not need an electrical field as driving force anymore. If a concentration gradient induces a particle flow via diffusion, you have an electrical current, too, if the particles are charged.
- Of course, if you have different particles, with different density, drift velocity, and charge, you simply sum up the individual current contributions (following the sign convention as pointed out above).

All we have to do now is to compare this equation to Ohm's law:

$$\underline{j} = q \cdot n \cdot \underline{v}_D = \sigma \cdot \underline{E}$$

- We then obtain

$$\sigma := \frac{q \cdot n \cdot v_D}{E} = \textbf{constant}$$

This implies *by necessity*

$$\frac{v_D}{E} = \text{constant}$$

- A simple, but far reaching equation!
- What it means is that *if* v_D/E= const. holds for *any* (reasonable) field *E*, the material will show ohmic behavior. *We have a first condition for ohmic behavior expressed in terms of material properties*.
- If, however, v_D/E is constant (in time) for a *given* field, but with a value that depends on *E*, we have σ=σ(*E*); the behavior will *not be ohmic*!

The requirement v_D/E=const. for *any* electrical field requires a constant average velocity in field direction for the particle which is directly proportional to *E*. This leads to a simple conclusion:

- Since a constant electrical field exerts a constant force on a charged particle, without some kind of *friction* its velocity would grow to infinity. We thus conclude that there must exist some mechanism that acts like a frictional force on all accelerated particles, and that this frictional force in the case of ohmic behavior must be in a form where *the average drift velocity obtained is proportional to the driving force*.

Since v_D/E=constant must hold for all ohmic materials under investigation, we may give it a name:

- It is called the **mobility** μ of the carriers, with the unit
  [μ]=(m/s)/(V/m)=m^2/V · s.
- The *mobility* μ (Deutsch: **Beweglichkeit**) then is a *material constant* ; it is determined by the "friction", i.e. the processes that determine the average velocity for carriers in different materials subjected to the same force *q · E*.
- Thinking ahead a little bit, we realize that μ is a material constant *even in the absence of electrical fields* – it simply expresses how fast carriers give up surplus energy to the lattice; and it does not matter how the got the surplus energy. It is therefore no suprise if μ pops up in all kinds of relations, e.g. in the famous Einstein–Smoluchowski equation linking *diffusion coefficients* and mobility of particles.

We now can write down the *most general form of Ohm's law* applying to all materials meeting the two requirements: *n*=const. and μ =const. everywhere. It is expressed completely in particle (=material) properties:

$$\sigma = q \cdot n \cdot \mu$$

Sinc we like to have σ as a positive number, we always take only the magnitude of the charge *q* carried by a particle.

- However, if we keep the sign, e.g. write σ=–*e · n ·* μ_e for electrons carrying the charge *q*=–e (**e**= elementary charge), we now have an indication if the particle current and the electrical current have the *same* direction (σ > 0) or opposite directions σ < 0) as in the case of electrons.
- But it is entirely a matter of taste if you like to schlepp along the signs all the time, or if you like to fill 'em in at the end.

Everything more detailed then this is no longer universal but specific for certain materials. The remaining task is to calculate *n* and μ for given materials (or groups of materials).

- This is not too difficult for simple materials like metals, where we know that there is one (or a few) free electrons per atom in the sample – so we know *n* to a sufficient approximation. Only μ needs to be determined.
- This is fairly easily done with classical physics; the results, however, are flawed beyond repair: They just do not match the observations and the unavoidable conclusion is that classical physics must not be applied when looking at the behavior of electrons in simple metal crystals or in any other structure – we will show this in the immediately following section **2.1.3**.

We obviously need to resort to **quantum theory** and solve the **Schrödinger equation** for the problem.

- This, surprisingly, is also fairly easy in a simple approximation. The math is not too complicated; the really difficult part is to figure out what the (mathematical) solutions actually *mean*. This will occupy us for quite some time.