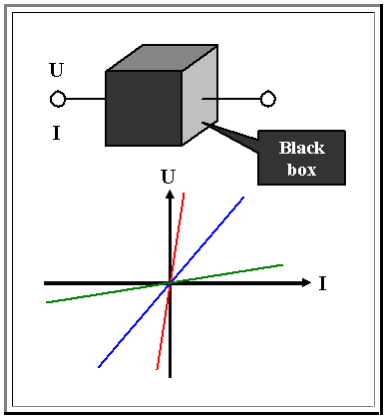
This Module comes from "Introduction to Materials Science II"; where you will find the most recent version. The link takes you there.

# Required Reading

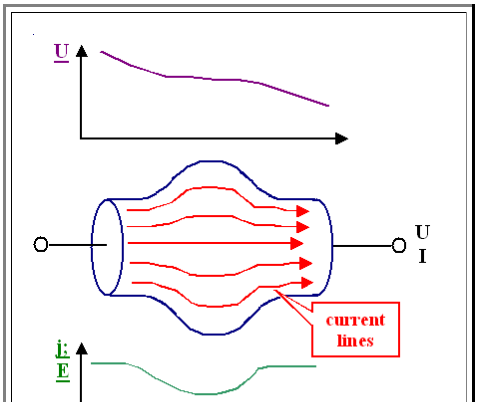
## 1.3.2 Ohms Law and Materials Properties




- In this subchapter we will give an outline of how to progress from the simple version of **Ohms "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**.
  - That is illustrated in the picture: As long as the voltage-current characteristic you measure between two terminals of the black box is linear, the black box is called an (ohmic) resistor).
  - Neither the slope of the ***I-U***-characteristics matters, nor the material content of the box.
- The*Materials Science* point of view is quite different. Taken to the extreme, it is:
  - Tell me what kind of material is in the black box, and I tell you:
    1. If it really is an *ohmic* resistor, ***i.e.*** if the current relates *linearly* to the voltage for reasonable voltages and *both* polarities.
    2. What its (specific) resistance will be, including its temperature dependence.
    3. And everything else of interest.
- In what follows we will see, what we have to do for this approach. We will proceed in **3** steps
  - In the first two steps, contained in this sub-chapter we simply reformulate Ohms law in physical quantities that are related to material properties. In other words, we look at the properties of the moving charges that produce an electrical current. But we only *define* the necessary quantities; we do not calculate their numerical values.
  - In the third step - which is the content of many chapters - we will find ways to actually *calculate* the important quantities, in particular for semiconductors. As it turns out, this is not just difficult with classical physics, but simply impossible. We will need a good dose of quantum mechanics and statistical thermodynamics to get results.

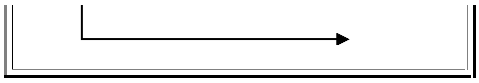
### 1. Step: Move to *specific* quantities

- 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* $\underline{j}$ would be parallel to the normal vector $\underline{f}$ of the reference area considered: it also may differ locally. So in full splendor we must write

$$\underline{j}(x,y,z) = \frac{I(x,y,z)}{F} \cdot \underline{f}$$

The "global" field strength is

$$E = \frac{U}{l}$$

- With $l$ = length of the body. If we want the *local* field strength $\underline{E}(x,y,z)$ as a vector, we have, in principle, to solve the Poisson equation

$$\nabla \cdot \underline{E}(x,y,z) = \frac{\rho(x,y,z)}{\epsilon\epsilon_0}$$

- With $\rho(x,y,z)$ = ***charge density***. For a homogeneous materisl with constant cross section, however, $\underline{E}$ is parallel to $\underline{f}$ and constant everywhere, again which is clear without calculation.

So. to make things easy, for a homogenous material of length $l$ with constant cross-sectional area $F$, the field strength $\underline{E}$ and the current density $\underline{j}$ do not depend on position - they have the same numerical value everywhere.

- For this case we can now write down Ohms law with the new quantities and obtain

$$j \cdot F = I = \frac{1}{R} \cdot U = \frac{1}{R} \cdot E \cdot l$$

$$\underline{j} = \frac{l}{F \cdot R} \cdot \underline{E}$$

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

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

- and $\rho$ is the **specific resistivity**. In words: A $1\ cm^3$ cube of homogeneous material having the specific resistivity $\rho$ has the resistance $R = (\rho \cdot l)/F$
- Of course, we will never mix up the *specific resistivity* $\rho$ with the *charge density* $\rho$ or *general densities* $\rho$, because we know from the context what is meant!
- The *specific resistivity* obtained in this way is necessarily identical to what you would define as specific resistivity by looking at some rectangular body with cross-sectional area $F$ and length $l$.
- The *specific conductivity* has the dimension $[\sigma] = \Omega^{-1}cm^{-1}$, the dimension of the *specific resistivity* is $[\rho] = \Omega cm$. The latter is more prominent and you should at least have a feeling for representative numbers by remembering

| | | |
|---|---|---|
| **ρ (metal)** | ≈ | **2 μΩcm** |
| **ρ (semicoductor)** | ≈ | **1 Ωcm** |
| **ρ (insulator)** | ≈ | **1 GΩcm** |

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

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

- Ohms law in this *vector form* 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 the equation given above *locally*.

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

  - Of course, obtaining the external current ***I*** flowing for the external voltage ***U*** now needs summing up the contributions of all the little cubes, i.e. integration over the whole volume, which may not be an easy thing to do.
- Still, we have now a much more powerful version of Ohms law! But we should now harbor a certain suspicion:
  - There is no good reason why $\underline{\boldsymbol{j}}$ must always be *parallel* to $\underline{\boldsymbol{E}}$. This means that for the most general case σ is not a *scalar* quantity, but a *tensor*; $\sigma = \sigma_{ij}$.
    *(There is no good way to write tensors in html; we use the $_{ij}$ index to indicate tensor properties*.
  - Ohms law then writes

$$j_x = \sigma_{xx} \cdot E_x + \sigma_{xy} \cdot E_y + \sigma_{xz} \cdot E_z$$

$$j_y = \sigma_{yx} \cdot E_x + \sigma_{yy} \cdot E_y + \sigma_{yz} \cdot E_z$$

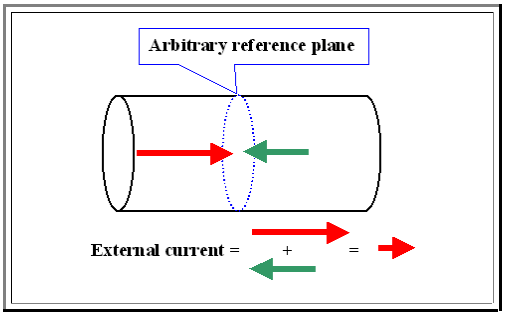
$$j_z = \sigma_{zx} \cdot E_x + \sigma_{zy} \cdot E_y + \sigma_{zz} \cdot E_z$$

- 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 Ohms law.
  - Note that this is *not* so general as to be meaningless: We still have the basic property of Ohms law: The local current density is directly proprotional to the local field strength (and not, for example, to **exp– [const. · $\underline{\boldsymbol{E}}$]** ).
- Our goal now is to find a relation that allows to calculate $\sigma_{ij}$ for a given material (or material composite); i.e. we are looking for
  - $\sigma_{ij} = \sigma_{ij}$**(material, temperature, pressure, defects... )**

## 2. Step: Describe $\sigma_{ij}$ in Terms of the Carrier Properties

- Electrical current needs *mobile* charged "things" or *carriers* that are *mobile*. Note that we do not automatically assume that the charged "things" are *always* electrons. *Anything* charged and mobile will do.
- What we want to do now is to express $\sigma_{ij}$ in terms of the *properties* of the carriers present in the material under investigation.
  - To do this, we will express an electrical current as a "mechanical" stream or current of (charged) particles, and compare the result we get with Ohms 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*.

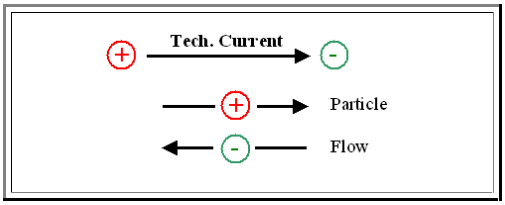
- In short: the *net* current is the difference of two *partial* currents flowing in opposite directions:




- Do not take this point as something simple! 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:

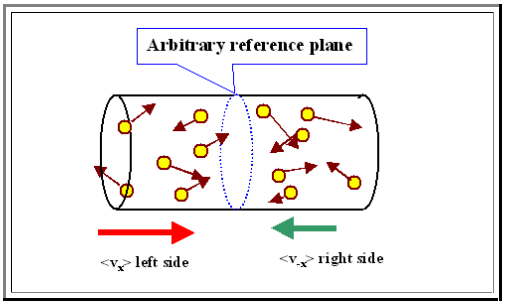
- The *electrical* current is (for historical reasons) defined as flowing from **+** to **–**. For a *particle* current this means:




- 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 at *a given instant* thus looks like this




- An instant later it looks entirely different *in detail*, but exactly the same *on average*!
- 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* in velocities the **drift velocity** $\underline{v}_D$ 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 drift velocity and thus net current is zero as it should be.

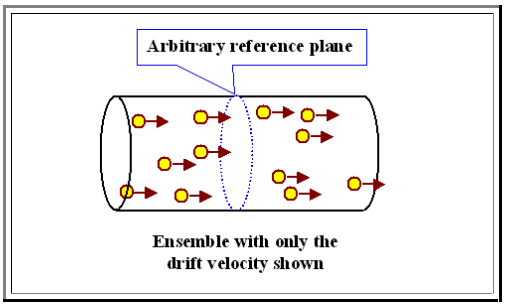
Average properties of ensembles can be a bit tricky. Lets look at some properties by considering the analogy to a localized **swarm of summer flies** "circling" around like crazy, so that the ensemble looks like a small cloud of smoke. A more detailed treatment can be found in 1.3.5.

- 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 $\langle \mathbf{v} \rangle$ 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

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

The problem with this formula is $N$, the *number* of carriers flowing through the cross section $F$ every second.

- $N$ is not a basic property of the material; we certainly would much prefer the carrier *density* $n = N/V$ of carriers. The problem now is that we have to chose the volume $V = F \cdot l$ in such a way that it contains just the right number $N$ of carriers.
- Since the cross section $F$ is given, this means that we have to pick the length $l$ in such a way, that all carriers contained in that length of material will have moved across the internal interface after **1** second.
- This is easy! The trick is to give $l$ just that particular length that allows *every* carrier in the defined portion of the wire to reach the reference plane, i.e.

$$l = v_D \cdot t$$

- 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 now write the current equation as follows:

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

This was shown in excessive detail because now we have the *fundamental 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.
  - Note also that electrical current flow *without* an electrical field as primary driving force as outlined above is *not* some odd special case, but at the root of most electronic devices that are more sophisticated than a simple resistor.
  - Of course, if you have different particles, with different density drift velocity and charge, you simply sum up the individual contributions as pointed out above.
- All we have to do now is to compare our equation from above to Ohms law:

$$\underline{j} = q \cdot n \cdot \underline{v_D} := \sigma \cdot \underline{E}$$

  - We then obtain

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

- If Ohms law holds, σ must be a constant, and this implies *by necessity*

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

  - And this is a simple, but far reaching equation saying something about the driving force of electrical currents (= electrical field strength ***E***) and the drift velocity of the particles in the material.
  - What this means is that *if* $v_D/E = \text{const.}$ 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 $\sigma = \sigma(E)$; the behavior will *not be ohmic*!
- The requirement $v_D/E = \text{const.}$ for *any* electrical field thus requires a drift velocity in field direction for the particle, which is directly proportional to ***E***. This leads to a simple conclusion:
  - This is actually a rather strange result! A charged particle in an electrical field experiences a constant force, and Newtons first law tells us that this will induce a constant accelerations, i.e. its velocity should increase all the time! Its velocity therefore would grow to infinity - if there wouldn't be some kind of friction.
  - 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 $v_D/E = \text{constant}$ must obtain for all (ohmic) materials under investigation, we may give it a name:

$$\frac{v_D}{E} = \mu = \text{Mobility} = \text{Material constant}$$

  - The **mobility** ***μ*** of the carriers has the unit
    **[μ] = (m/s)/(V/m) = $m^2/V \cdot s$**.
  - 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 $q \cdot \underline{E}$.
  - **Friction**, as we (should) know, is a rather unspecified term, but always describing energy transfer from some moving body to the environment.
  - Thinking ahead a little bit, we might realize that **μ** is a basic material constant *even in the absence of electrical fields*. Since it is tied to the "friction" a moving carrier experiences in its environment - the material under consideration - it simply expresses how fast carriers give up surplus energy to the lattice; and it must not matter how they 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 Ohms law* applying to all materials meeting the two requirements: ***n* = const.** and **μ = const.** everywhere. It is expressed completely in particle (= material) properties.

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

  - The task is now to calculate ***n*** and **μ** from first priciples, i.e. from only knowing what atoms we are dealing with in what kind of structure (e.g. crystal + crystal defects)
  - This is a rather formidable task since σ varies over a extremely wide range, cf. a short table with some relevant numbers.
- In order to get acquainted with the new entity "mobility", we do a little exercise:

**Exercise 1.3-1**

Derive and dicuss numbers for **μ**

- Since we like to give 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 $\sigma = -e \cdot n \cdot \mu_e$ 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 ($\sigma > 0$) or opposite directions ($\sigma < 0$) 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 subchapter **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.

**Questionaire**

**Multiple Choice Questions to 1.3.2**