Example for Illustrating Tables

▶ Here is the boring table

Year	1973	77	81	84	87	90	95	98	01	05	09	13	17
Price for 1 Mbit of DRAM memory (DM)	150.000	10.000	800	240	60	10	1	0,26	0,11	0,05	0,014	0,008	0,003

● And here is an interesting way for illustrating the same data
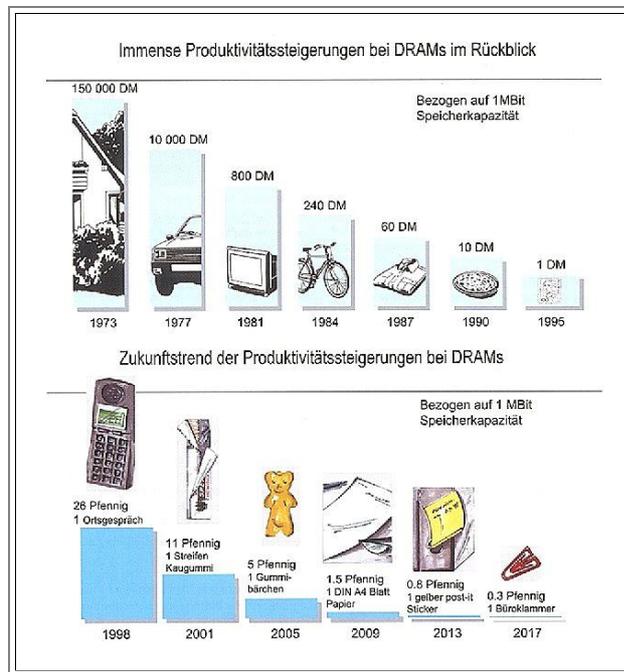
Example for Skeleton Foil

Sorry, it's in German; but the idea should be clear

The original had a little hand colouring; the "markers" (the circles, stars, cartouches) had a specific colour and a specific meaning

- Circles denote headlines of are main topics
- Stars are major points and facts
- Cartouches indicate actions:
  - "Folie **1**" means that here an illustrative viewgraph will be shown; after that this foil comes back
  - "Muster" means that a specimen is passed around or hold up to see.

Otherwise the speaker talks freely to the topics on the foil, following his own lead.

Illustration

```
SIEMENS                                          4 M - DRAM
_____

   ⬤  Das MEGA - Projekt

      ★  Aufholen    bei   1 M – Technologie  ⎫   gemeinsam
         Gleichziehen bei 4 M – Technologie   ⎬   mit Philips
                                              ⎭

      ★  ca. 1200 Mannjahre
         ca. 1,5 GDM Kosten
         ca. 250 Neueinstellungen in München P
         ca. 350 neue Arbeitsplätze in Regensburg

      ★  zwei 6" – Linien und Labor / Bürobauten in Mch P

   ( Folie 1 )     Mikroelektronik - Zentrum in Mch P

      ★  Zeitplan  4 M – DRAM

         "Erstes Silizium"   -----> 3/87    ⎫  Ziele
         Kundenmuster        -----> 1988    ⎬  erreicht oder
         Fertigungsanlauf    -----> 1989    ⎭  erreichbar

   ( Muster )      Erste funktionsfähige 4 M – DRAM`s

_____
1. Einleitung                                    HLT 3 / Fö
```

What are "Electronic Materials"

Ask Google, and you get this answer:

Illustration

# People forget

People do forget things. But often it is just an excuse for major blunders, used if you simply didn't *know* the issue, didn't feel like *looking it up*, or just plain *guessed*. If you forgot some of the topics needed for the course:

- In engineering, guessing is generally a bad idea. In case of doubt: *Look it up!*

Your mistakes are potentially dangerous. You will not just make a fool out of yourself like the "creative" genius (In Germany all advertising people call themselves "Kreative") who did the add shown below. I wonder if (s)he ever noticed.
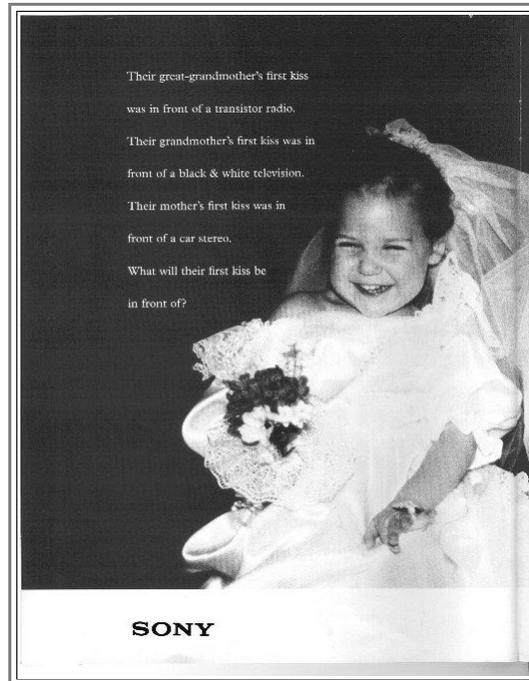
We do know, of course, that people behind advertising quite generally have a somewhat disturbed relation to the truth. But here we see that they are also very generous when it comes to recent technical history.

- Above, the left part of a two-page add is shown that appeared for quite some time in all major magazine in the **US** (around **1998**). If one assumes that the **SONY** people look at their adds before the are printed, this beauty demonstrates very nicely that the really fundamental human achievements in this century did not make a deep impression on our "creative thinkers".

- The great-grandmother alluded too above lived about **80** years ago, i.e. around **1910 - 1920**. That the quantum theory, the base of transistors was not yet quite invented, must be seen as an irrelevant detail. Unfortunately, however, the transistor itself was not invented before **1947** (by John **Bardeen**, Walter **Brattain** and William **Shockley**) - tough luck! "Transistors", meaning battery powered mobile radios, only hit the market in the sixties. Great-grandma, by the way, did not listen to the radio at all - it didn't exist then.

- Grandmother too, hardly enjoyed her first kiss in front of the black-and-white **TV**. It just barely existed, but not many people could afford it or lived in areas where there was actual broadcasting.

- Mother, that much could be true, may have listened to the stereo in the car while making-out; car radios and stereos did exist about **20 - 30** years back.

Colour **TV** it appears, was not so impressive as to be mentioned. And vacuum tubes obviously never existed at all in the world of our "creative" geniuses.

Silicone vs. Silicon

The fundamental difference between the materials **silicone** and *silicon*, though unknown to the media professionals, is best illustrated by the major application of *silicone*, which has nothing to do with the *silicon* used for *micro*electronics, but with rather *macro*scopic applications leading to soft products not easily confused with hard and brittle chips.

Illustration

Requirements for Chip Metallization

The metal lines connecting transistors or other components on a **Si** chip must meet many, partially conflicting, requirements. Below is a list, including some materials that do *not* meet the particular requirement very well.

● Can you guess the winner?

Desired Property	Materials **not** meeting requirement
Very good conductivity	All but **Ag**, **Cu**
High eutectic temperature with **Si** (**> 800 ºC** would be good)	**Au, Pd, Al, Mg**
Low diffusivity in **Si**	**Cu, Ni, Li**
Low oxidation rate; stable oxide	Refr. Metals, **Mg, Fe, Cu, Ag**
High melting point	**Al, Mg, Cu**
Minimal interaction with **Si** substrate	**Pt, Pd, Rh, V, Ni , Mo, Cr** (form silicides easily)
Minimal interaction with poly **Si**	Same as above
No interaction with **SiO$_2$**	**Hf, Zr, Ti, Ta, Nb, V. Mg, Al**
But must stick well to **SiO$_2$**	?
Must also comply with other substrates, e.g. **TiN**	? (see example for **Al**)
Chemical stability, especially in **HF** environments	**Fe, Co, Ni, Cu, Mg, Al**
Easy structuring	**Pt, Pd, Ni, Co, Au**
Electromigration resistant	**Al, Cu**
.... and many more,...	

The winner is: *Aluminum* (with **<1%** of **Si** and **Cu** added).

● **Al**, in fact, is pretty bad - but all others are worse!

● Presently (**2001**) a switch to **Cu** takes place (the better conductivity is definitely needed). The industry will pay several **10^9** Dollars to develop the new material technology and change the production facilities.

# Do Not Forget the Temperature Dependence of the Specific Resistivity!

Advanced

The discovery of high temperature superconductors in **1986** immediately lead to proposals to use these materials for interconnects on chips instead of the **Al** that was common than (and for about **15** more years).

- The reason was that the finite resistivity of **Al** together with parasitic capacitances (e.g. between two conducting lines on a chip) limits the maximum frequency to

$$f_{max} = \frac{1}{R \cdot C}$$

- With R = resistance of the longest connection line on the chip and C = parasitic capacitance "seen" by this line.

- For $R = 0\ \Omega$ as we have it for a superconductor, the maximum frequency is no longer limited by $R \cdot C$, no matter how large the parasitic capacitances are. Instead, the limit comes from
$f_{max} = (L \cdot C)^{-1/2}$
with L = inductance of the line, and this is just another way of saying that the signal propagation is limited by the speed of light.

$$f_{max} = (L \cdot C)^{-1/2}$$

Given the resistivity of **Al** (at room temperature!), a sizeable advantage was seen for the integrated circuits then envisioned.

- However, comparing the performance of a chip run with **Al** at room temperature to a chip run at liquid N_2 temperature (**77 K**), is not the right comparison. After all, you can cool down the conventional chip, too - and that will decrease R_{Al} by a factor of **6 - 8**.

- The comparison then is quite different. The graph shows the minimum switching time $\tau = 1/f_{max}$ as a function of the length of a standard interconnect line about **1 µm^2** cross section.

Whereas superconductors would already make an interesting difference for lengths of a few **mm** (typical line length) in the *wrong* comparison, the correct comparison only shows an advantage for about **1 cm** and larger - line lengths easily avoided by clever design.
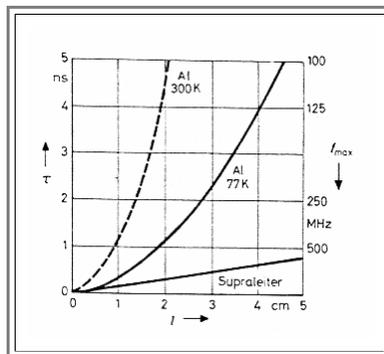
The Li Ion Battery

The Issue in Short

Presently (Oct. **2009**) the world at large is in the throes of the financial crisis; before and after it was (and will be) shaken by the **energy crisis**. The articles "Terawatt challenge" and "Powering the planet" provide some background of particular interest to Material Science and Engineering students.

- Every budding engineer knows, of course, that automobiles in the near future will run **electrically**, powered by **batteries** - at least this is the unavoidable conclusion if one just reads a newspaper occasionally or listens to news.

- Is that true? Are we all going to drive around in electrical cars (or at least serious hybrids) in a few years that have about the same cost / performance relationship than present gasoline powered cars? This module will provide a few essentials for pondering this question.

First, we realize that the energy source in a future car will be a **Li** ion battery? Why is that? We will find out by recalling some basic facts about cars and doing a little quiz.

Before you read on, you should try to figure out the answers yourself by doing the extremely simple but highly illuminating quizzes (far too simple to be called "exercise") provided in the links.

<div align="center">

Quiz 1

How much energy is contained in **1 liter** of gasoline?
Find out by using data you know about your car.

</div>

- What you could get is shown in the following table.

Known Property	SI units	Stupid units
Mileage	**10 km/l**	**23.5** miles/gallon
Range with full tank	**500 km**	**311** miles
Engine Power P	**100 kW**	**135 PS** or horse powers
Average speed in going 500 km	**120 km/h**	**74.6 miles/h**
Average capacity of engine used	**50 %**	
Average efficieny η **of engine used**	**0,3** or 33%	
Time t **to cover 500 km**	**4.17 h**	
Energy E **consumed = 0,5**Pt	**208 kWh**	
Energy E_G **contained in 1 l of gasoline = E/50 l·η**	**12.6 kWh/l**	

Not bad! The "official" number is $E_G \approx$ **10 kWh/l**.

- The "≈" sign alludes to the (small) differences between premium, diesel, and so on. Who cares. We are only concerned about orders of magnitude here.

Is a specific energy of around **10 kWh /l** a *large* or *small* number? Find out yourself in the next quiz:

<div align="center">

Quiz 2

How large or small are **10 kWh /l**
- in comparison to known energy (densities).

</div>

- Here are some answers: **1 kWh** energy is stored or used up in

  - **0,1 l** gasoline
  - Large (**85 Ah**) truck battery.
  - **0,25 kg** dry wood
  - **7,3 t** H_2O in a reservoir with **50 m** height difference.
  - A weight of **367 t** lifted to **1 m**.

- **9,5 l** brought to a boil (**100 ºC**) from **10ºC**.
- **100 h** of bicycling at **100 W** uses up the **10 kWh**, moves you about **2.000 km**, and works off about **17** Big Mac's.

In other words: The chemical energy contained in gasoline is *absolutely huge* compared to typical mechanical energies we can directly relate to! It is, by the way, larger than the energy stored in **1 kg** of a solid high explosive.

So what is the energy density of a decent battery? Well - it depends. Do you mean energy *per liter* or per *kilogram*? There is a big difference from the view point of the user.

Quiz 3
This and That

If you think about electric cars, the **weight** of the battery is what you are concerned with. The volume is not all that important. You have plenty of space because you do no longer need a bulky engine, transmission, drive train and so on. Electric motors are much smaller than comparable gasoline counterparts.

If you want to power your submarine, it's the the other way around. If the batteries are too light weight, you have trouble to "sink" it. If you want to power your cell phone, it's volume you are concerned about. If you want to store huge amounts of energy (e.g. to get through the night if your major energy source are solar cells), weight and volume are not confining - the price is!

Let's look at both specific energy densities in one diagram
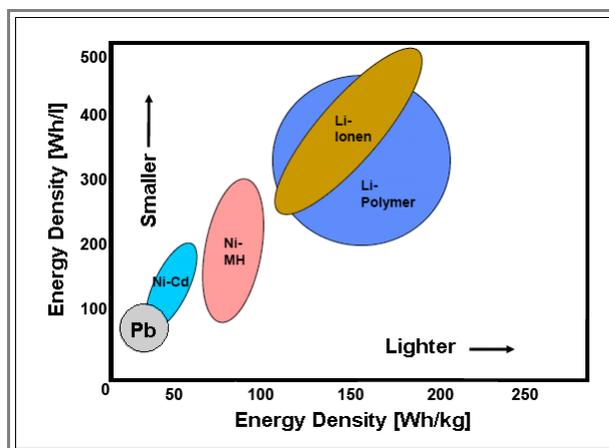
It looks like the best we can come up with is at present (Oct. **2009**) the **Li** ion battery with a specific capacity around **0.5 kWh** *per liter* or **0,15 kWh** *per kg*. In other words: **1 l** of gasoline beats the best battery we have by a factor of **20** with respect to the specific volume and by more than a factor of **100** with regard to the specific weight.

OK - that simply means we have to find room for a **Li** ion battery with a volume of **1000 l** or **1m x 1m x 10 cm** to run a car. That should be possible in a decent sized car.

Unfortunately, if we look at the figure, the weight of such a battery would be around **3 000 kg** or so (and the price would be totally prohibitive). Twice the weight of your old-fashioned standard car!

The conclusion is easy:

If cars are to be powered by batteries in the near future,
we need to improve batteries at at least by a
factor of 5 or so with respect to the energy density.

As a material scientist you now wonder what exactly determines the energy density of a battery. For finding out we need to look at the basic working principle of a battery.

Working Principle of a Battery

The energy stored in a battery is chemical energy, i.e. the energy released by a chemical reaction. We will only consider **Li** based batteries here, so we have a reaction of the type:

$$\text{Li} + \text{F} \Leftrightarrow \text{LiF} + 5{,}4 \text{ eV}$$

So take a piece of **Li** and a "piece" of **F**, separate it by an electrolyte that cannot pass electrons but only ions, put it into a box with contacts to the **Li** and the **F** - you have a battery.

  It's not so easy, of course. The general principle of forcing the electrons to go through an outer circuit from one reaction partner to the other one, while the ions move through the electrolyte is certainly correct. But:

  1. How do you keep and contact an (extremely corrosive) gas like F_2?
  2. How do you keep your **Li** from reacting with the oxygen in the air?
  3. Will the reaction actually take place? Will a piece of metallic **Li** in a F_2 atmosphere start to react without being "triggered" somehow (like $H_2 + O_2$?
  4. Can you reverse the reaction by running a current through your battery, i.e. charge it again?
  5. and so on. and so forth.

Making a real battery with "*Li ions*" is not all that easy - Point **2** will always a problem, for example, demanding airtight sealing and a lot of security features.

  So let's look at the working principle of a **Li ion battery** in a very general way.
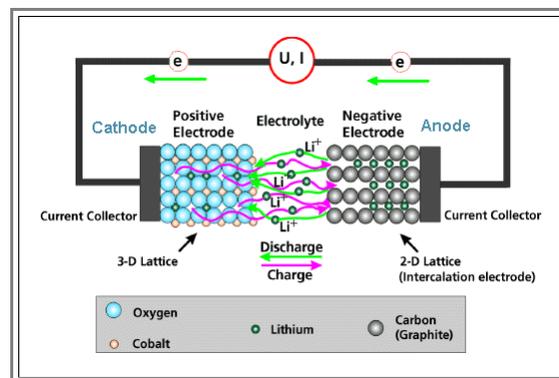
We have a **negative electrode**, also called **anode**, where **Li** is present as a "metal".
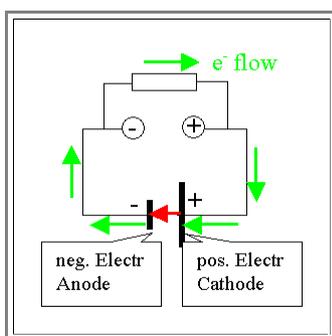
  The term *negative electrode* is clear. The **Li** atoms incorporated or **intercalated** in the electrode material must leave an electron back so that they can move as **Li$^+$** ion through the electrolyte if the battery is discharged and thus supplying energy to the outside world.

  But why is it also called *anode*? Isn't an anode always the positive pole towards which the electrons flow?

  Yeah - but only *outside* the battery as shown on the diagram. *Inside* the battery the electrons (or negative charges) must flow from *plus to minus*. The battery, after all, is a electron pump that moves the electrons "up" to a high energy level from which they can "flow down" towards the positive pole

  Of course, it's not electrons flowing from plus to minus inside the battery but positively charged **Li$^+$** ions in our case. But if you replace the battery by a generator, your electrons flow indeed in the "wrong" direction inside the generator.

  The general definition of an anode is therefore: An anode excepts electrons; it provides for a general oxidation reaction. The polarity is positive seen from an external user and negative as seen from inside a generator. In the picture you see that the internal electron (or negative charge) current does indeed flow into the anode (red arrows).

We have a **positive electrode** also called **cathode** (now we know why) where **Li** reacts to whatever and is incorporated as **Li⁺**.

- The chemical reaction to "whatever" - e.g. **LiCoPO₄** - provides the energy that drives the whole process.

Between the electrodes is an **electrolyte** that allows **Li⁺** ions to pass but does not conduct electrons. That's why we have a battery. The electrons can only get from the anode to the cathode by flowing through electron conductors in the external circuit.

The two electrodes must be intimately connected to some **current collector** (a metal like **Cu**) that conducts the electrical current aut of the battery to the terminals.

- This is not a simple issue! If you want to run a **100 kW** motor with a **3 V** battery, you are going to draw **100 000/3 A = 33 333 A** which is a lot of current. Even if you switch battery cells in series to achieve **300 V**, you still run **333 A** through the current collectors and wires.

What kind of properties are we asking for concerning the electrode materials? It's a long list; most important for us at this point are

- **General Properties:**

  - Specific capacity or how much **Li** (in **kg**) can you incorporate in **1 kg** or **1 l** of the the electrode material.
  - Electrochemical potential.
  - Conductivity; connection to current collector.
  - Long term stability; survives how many charge / discharge cycles?
  - Hazard potential (does it explode / burn if exposed to air?).
 - Price.
  - Ecological topics.

Negative Electrode/Anode

- In principle one could use **Li** metal. In practice, however, one cannot, for many reasons. Consider just recharging after all your **Li** has been used up and is now incorporated in the cathode. You now have a "hole" on your anode side. How do you get your **Li** back?

- We therefore use an anode material that ideally can incorporate a lot of **Li** easily, *and* can release most of that incorporated **Li** easily. In other words, it shouldn't take much energy to get it out again. That implies that no strong bonds between the anode material and the **Li** must develop.

- The standard material at present is *graphite*. **Li** atoms are simply "intercalated" between the hexagonal **C**-layers. Another, very interesting material for anodes is **Si**. We will come back to that.

Positive Electrode/Cathode Properties

- In principle same thing as above, except that we must produce a lot of energy whenever **Li⁺** is incorporated.

- What we use are metal oxides (**MO**) like **LiCoO₂**, **LiNiO₂**, **LiMn₂O₄**, **LiFePO₄**, **LiNiₓCoᵧMn_zO₂**.

The over-all reaction then is like this:

$$Li_xC_6 \ + MO \quad \Leftrightarrow \quad C_6 \ + Li_xMO + \text{several eV}$$
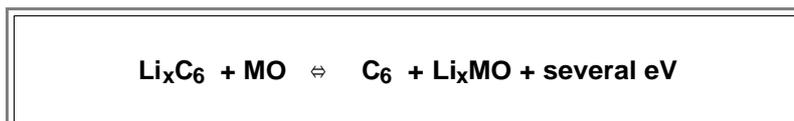
All we do, in simple terms, is to "shuttle" **Li** back and forth between the two electrodes, gaining energy in one direction (discharge) and using energy (charge) in the other.

Capacity of a Battery

What determines the capacity of a given **Li** ion battery? Easy. We first do a quiz to get some ideas.

> ## Quiz 4
> Battery capacity
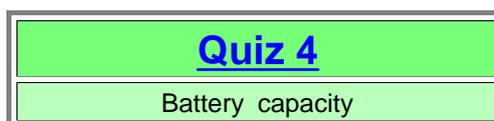
What we see is that about **90 g** of **Li** would be enough for a capacity of **1 kWh**. But the diagram above shows that presently we need at least **5.000 g** for that. How can that be?

- Well - besides the **Li**, you need the two electrodes that contain it, an electrolyte, current collectors, and a housing; not to mention security features.

- If we want to improve the gravimetric energy density by at least a factor of **5** as we must, we realize that there is a lot of work out there for enterprising Material Scientists. What we have to work at are the electrodes (and everything else). The crucial question is: What is the specific capacity (in **mAh/g**) of an electrode. In other words: How much **Li** (in **g**) can I incorporate into **1 g** of the electrode material.

- The reference would be metallic **Li**, where one obviously can have "**1 g Li** in **1 g Li**" with a specific capacity of **3 800 mAh/g**. It also takes a voltage of **0 V** to get **Li** "out", i.e. to drive the reaction **Li/Li$^+$** because we use that as the zero point of the potential scale.
- The relevant voltages are shown for various reactions in the figure. The differnce between the high end and the low end is what you get as the battery voltage. With a **Si/Li** anode and a **Li$_x$CoO$_2$** standard cathode, you should obtain around **3.5 V**.

Let's look what else we have

Material	Specific capacity [mAh/g]	U vs. Li/Li$^+$ [V]	Comments
Graphite	330 - 370	0,1 - 0,6	Present standard anode
Li$_4$Ti$_5$O$_{12}$	155	1,6	
Si	> 4 000	0,1 - 0,5	Volume change factor 4!!!
Li	3 800	0	Not practical
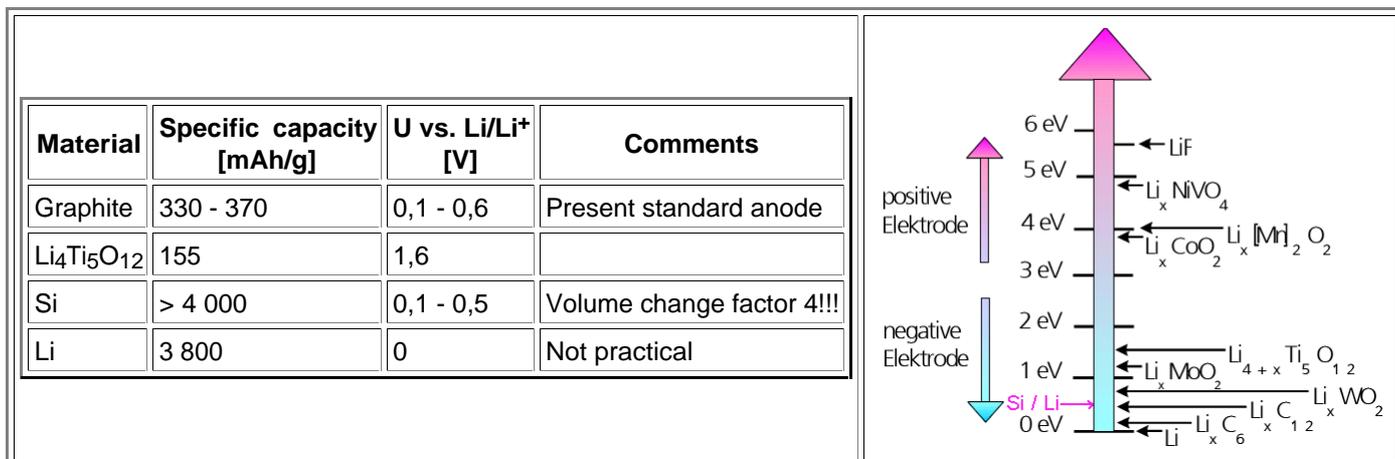
Now you should be a bit surprised. How can you have more **Li** in **Si** than in **Li** itself?

- Yes - you can. By forming alloys like **LiSi**, **Li$_{12}$Si$_7$**, **Li$_7$Si$_3$**, **Li$_{13}$Si$_4$** and **Li$_{22}$Si$_5$**.

So why don't we have **Si** anodes as a matter of course in our **Li** ion batteries?

- Because the volume of the **Si** expands by a factor of **4** when **Li** in high concentrations is incorporated. What that means is that your piece of **Si** anode will have fractured to fine dust if you load it just once with **Li**. This is obviously not practical.
- Nevertheless it can be done. The keyword are "**nanowires**".Overcoming that problem by using **Si** nanowires instead of bulk **Si** is not only a story in itself but brings you to the heart of "hot" research in materials science and engineering as it is going on right now (Oct. **2009**).

The Si Nanowire Anode

The pictures below show **Si** nanowire anodes. On the left we have a **Si** nanowire array as made by anodic pore etching and chemical over-etching: On the right we see a **Si** nanowire anode with a **Cu** backing after it has been used in a few charge and discharge cycles in a battery.
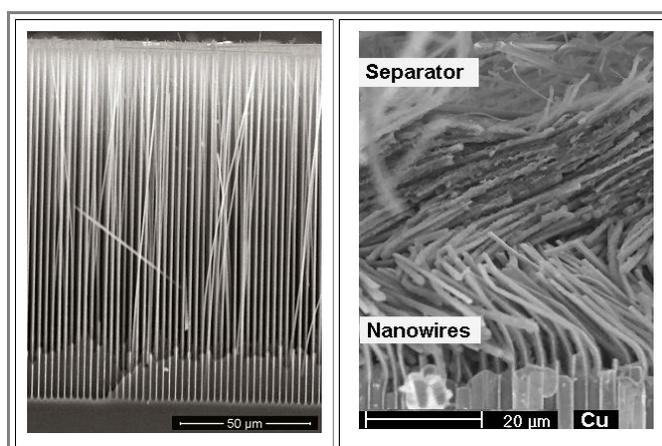
- It works! No destruction of the **Si** nanowires is visible.
- If you want to know more about this, refer to these two short papers:

  - The Stanford paper that started it all in **Jan 2008**.
  - The Kiel paper that makes it practical (and was co-authored by a student presently (fall term **2009/10**) taking this course).

Tunnelling effect

This was actually a exercise in "Matwiss I". The <u>Link</u> takes you there.

Advanced

Thermoelectric effects

Seebeck Effect

First of all, in considering thermoelectric effects, we have to realize that we are dealing with a *non*-equilibrium situation.

- A general theory of non-equilibrium is beyond our means, suffice it to say that Lars **Onsager**, with a paper entitled "*Reciprocal relations in **irreversible processes***" induced some fundamental insights as late as **1930**; he received the Nobel price for his contribution to non-equilibrium thermodynamics in *1968* - for chemistry, of all things.

However, what we should be aware of, is the essential statement of non-equilibrium theory:

- As long as there is no equilibrium, we always have *currents* of something trying to establish equilibrium by reducing a gradient in something else that is the actual cause of the non-equilibrium. A gradient in the electrical potential, e.g., causes our well-known electrical currents, and a gradient in a concentration causes diffusion currents.

- But we must abstract even more, and consider things like entropy currents as well as all kinds of combinations of gradients and currents.

While Onsager discovered some quite general relations between gradients and currents, we will not delve into details here, but only look a bit more closely at what causes the Seebeck effect.

For that, we still treat the thermoelectric effect with equilibrium thermodynamics, simply assuming that *locally* we are not very far from equilibrium and thus can still use band structure models with a Fermi energy (which is only a well defined quantity for equilibrium) and resulting carrier distributions.

- In the simplest possible case, what we will get for a long bar of metal, hot at one end and cold a the other, is something like this:
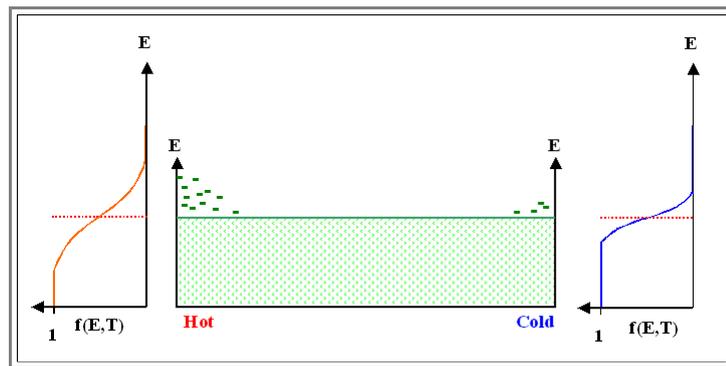
At the hot end, the Fermi distribution is "soft", and we have a noticeable concentration of electrons well above the Fermi energy. At the cold end, the Fermi distribution is sharp, and we have fewer electrons above the Fermi energy.

- The drawing, of course, grossly exaggerates the real situation. Note also that the total concentration of electrons a both ends is the same - even so the drawing does not show this because the holes below the Fermi energy are not included.

- Note too, that the Fermi energy is constant throughout the material (we neglect any possible effects of the temperature on the Fermi energy, as we have it, for example, in doped semiconductors).

- As always, electrons go to where the energy is lower; the electrons would tend to move from the hot end to the cold end, thereby transporting energy and thus equilibrating the temperature eventually. Equilibrium, with a constant temperature everywhere will be achieved.

- An equally valid alternative interpretation just looks at the concentration gradient of the electrons in energy space, which would automatically drive a kind diffusion current until the concentration (and thus the temperature) is equalized.

- Yet another way of looking at it is to consider that the average momentum of the electrons at the hot end is larger than that of the electrons at the cold end. They would therefore "run away" faster (taking energy with them) than the electrons from the other end would "run in".

However, since we keep the *temperature difference* constant, all this *cannot happen*. We will have to maintain constant but different temperatures and therefore different energy distributions at both ends of the metal bar.

- If nothing happens, we will loose the electrons with large momentum faster than we gain electrons with smaller momentum; and a temperature gradient cannot be maintained. The only way to change that, is to lower the potential at the hot end somewhat, i.e. make the ends positively charged, and to raise it at the cold end.

- The potential difference must built up until it is large enough to exactly counteract the net loss of "hot" electrons due to momentum imbalance.

This is essentially the reason why we find a **thermovoltage**.

- Note that the junction is not directly essential. However, if you just plug a wire from one material into your Voltmeter and heat up the middle part, leaving the two ends cold (and at the same temperature), your potential along the wire may change, but at the two ends you have the same potential, and it is the potential difference between the two ends you measure

- Plucking the hot end into your Voltmeter is a bit unpractical, so you necessarily end up with a junction to some other material. The other material now will also have a hot end and a cold end, and thus develop a potential difference.

- Since the potential at the other end can only have *one* value, you will now get a potential difference between the *two* cold ends which depends, of course, somehow on the choice of materials.

Still, there is a potential difference between the hot and cold end of one piece of material, and even so it cannot be measured directly, we can measure it indirectly somehow and tabulate the values.

- We can do this, with somewhat more involved but similar reasoning not only for metals, but also for semiconductors. The table below gives some absolute values and shows that semiconductors are good candidates for actual thermocouples, because their **Seebeck voltage** is fairly large. The values are for about room temperature, or about **700 ºC** for the last three materials

| Material	Al	Cu	Ag	W	$(Bi,Sb)_2Te_3$	$Bi_2(Te,Se)_3$	ZnSb	InSb	Ge	TiO_2
Seebeck voltage [µV/K] (V_{hot} - V_{cold})	-0,20	+3,98	+3,68	+5,0	+195	-210	+220	-130	-210	-200

Surprise! There are positive (as expected) *and* negative values of the voltage. What does it mean?

- Simply that you are looking at *positively charged* carriers being reponsible for the Seebeck effect - **holes**, in other words.

- Not so surprising for semiconductors, perhaps, but somewhat unexpected for **Al**. But, as we should know, conduction in **Al** relies heavily on holes, as evidenced, e.g., in its positive Hall coefficient while most other metals have a negative one

Peltier Effect

Understanding qualitatively the Seebeck effect does not help much to understand the Peltier effect.

- Again, lets look at some simple junction, this time an ohmic conduct of a metal to a semiconductor.
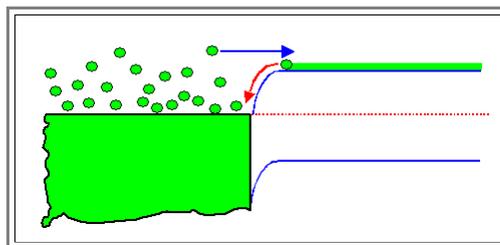
- Shown is an equilibrium situation, where the Fermi energy is constant throughout, and the flow of electrons across the junction must be equal in both directions. Note that only the high-energy end electrons oft the Fermi distribution in the metal makes it across the junction, whereas all electrons of the semiconductor can flow into the metal.

- The electrons of the metal thus also transport some thermal energy out of the metal, but in equilibrium exactly the same amount is gained by the semiconductor electrons, which are high-energy electrons in the metal.

Now consider some external voltage driving some net current through the junction in either direction.

- If this current is an electron current flowing from the metal into the semiconductor, it *still* transports some thermal energy out of the metal, but since it is now much larger than the electron current flowing back, we have a *net transport of thermal energy* out of the metal, which therefore *must cool down*. The semiconductor part heats up, of course.

- If the current is reversed, the flow of thermal energy reverses, too, and now the semiconductor part cools down.

- It is conceivable then (also far from clear) that the total effect in terms of temperature differences is proportional to the current *I* flowing.

Note, however, that as a completely independent process, you always have ohmic heating (or Joule heating) which is simply given by the total power *P* dumped into the system via

$$P = U \cdot I = R \cdot I^2$$

- with $U =$ voltage applied, $R =$ total series resistance of the system.
- Since this general heating of the whole device is proportional to I^2, it can easily overwhelm any cooling effect that might be there.
- If you want to use the Peltier effect as an elegant way of cooling something, you must not only choose your materials very carefully, but also optimize your system design and working points.
- That this is possible is evidenced by the successful marketing of **Peltier cooling elements**, mostly for scientific applications. Here is a table with technical data from a major supplier (EURECA Messtechnik GmbH, Am Feldgarten 3 D-50769 Köln, GERMANY)

Micro Peltier Elements

Module	I_{max} [A]	Q_{max} [W]	U_{max} [V]	dT_{max} [K]	Dimensions					Unit Price [Euro]
					A [mm]	B [mm]	C [mm]	D [mm]	H [mm]	
TECM-4-4-1b/69	1,4	0,7	0,9	69	4,3	4,3	4,3	4,3	2,95	28,75
TECM-4-5-1/67	0,7	0,4	1,0	67	3,4	3,4	3,4	5,0	2,30	29,50
TECM-5-7-1/67	0,7	0,9	2,2	67	5,0	5,0	5,0	6,6	2,30	38,50
TECM-7-8-2/67	0,7	1,7	3,9	67	6,6	6,6	6,6	8,3	2,30	52,50
TECM-9-12-4/67	0,7	3,5	8,0	67	9,1	9,9	9,1	11,5	2,30	66,25
TECM-12-6-4/69	1,7	4,4	4,3	69	6,0	12,0	6,0	12,0	2,75	57,50

In this class you will find elements with various geometries and electrical parameters. For this reason, these elements are suited for very different and partly exotic requests as you have in the research. Our support will help you with the selection and the startup of the elements in consideration of your particular requests.

Generally you will receive these elements in small quantities from stock.

Averaging Vectors

Lets look at bit closer at the averages one can take by considering a (localized) swarm of summer flies "circling" around like crazy, so that the ensemble looks like a small cloud of smoke.

- "Localized" means that the swarm maintains a defined form (on average), so all flies are always inside this defined volume in space.
- In the case of the charge carriers in a piece of metal, it simple implies that the carriers stay inside the piece of metal.

First we notice again that while the *individual* fly moves around quite fast, its average *vector velocity* $\langle \underline{v}_i \rangle_t$, averaged over time 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 flowing through some surface produced by *all flies at any given instance*, or by *one individual fly after sufficient time* is obviously zero for *any* reference surface you care to chose. This is illustrated schematically below.
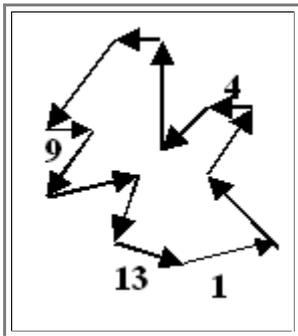
- Shown are **13** velocity vectors of an individual fly; the chain of vectors closes so $\langle \underline{v}_i \rangle_t = 0$.

The average of the *magnitude* of the velocity of an *individual* fly, $\langle |\underline{v}_i| \rangle_T = \langle v_i \rangle_t$, however, is obviously *not* zero - the fly, after all, is buzzing around at high (average) speed. *Note the details in the equation above:* Only the underlining of **v** is different!

- If we define $\langle v_i \rangle_t$ as follows, we have a simple way of obtaining the average of the magnitude (we take only the positive root, of course) .

$$\langle v_i \rangle_t \;=\; +\, \langle (\underline{v}^2_i)^{1/2} \rangle_t$$

- $\underline{v}^2$ is a scalar, and the (positive) square root of $\underline{v}^2$ gives always the (positive) magnitude of $\underline{v}$; i.e. $|\underline{v}|$

- This is an elegant and workable definition, but beware: $\langle (\underline{v}^2)^{1/2} \rangle$ is *not* the same as $(\langle \underline{v}^2 \rangle)^{1/2}$! Lets try it with a few arbitrary numbers ⇒

$|\underline{v}|$ =	3	4	6
$\langle (\underline{v}^2)^{1/2} \rangle$ =	$(3 + 4 + 6)/3 = 13/3 = 4{,}333...$		
$(\langle \underline{v}^2 \rangle)^{1/2}$ =	$[(9 + 16 + 36)/3]^{1/2} = 20{,}33^{1/2} = 4{,}51$		

If we have $\langle v \rangle_t = \langle (\underline{v}^2)^{1/2} \rangle_t$, we may also calculate the average (over time) of the velocity *components* in **x**, **y**, and **z**-direction, $\langle v_x \rangle_t$, $\langle v_y \rangle_t$, $\langle v_z \rangle_t$, of an individual fly *for a truly random movement*. (*We drop the index "i" now to make life easier*).

- Again, the vector averages $\langle v_x \rangle$ and so on of the *vector* components must be **= 0** because in a truly random movement the components in **+ x** and **- x** direction and so on must cancel on average.
- Since the magnitude $|\underline{A}|$ of a vector $\underline{A}$ is given by the square root of the scalar product of the vector with itself . We have

$$\underline{A} \cdot \underline{A} \;=\; A_x \cdot A_x + A_y \cdot A_y + A_z \cdot A_z = A^2$$

$$A \;=\; |\underline{A}| \;=\; (\underline{A}^2)^{1/2}$$

- Since

$$\langle v^2 \rangle_t = \langle v_x^2 \rangle_t + \langle v_y^2 \rangle_t + \langle v_z^2 \rangle_t \quad ,$$

- and since in a *truly random movement* we have

$$\langle v_x \rangle_t = \langle v_y \rangle_t = \langle v_z \rangle_t \quad ,$$

- we end up with

$$\langle v^2 \rangle_t = 3 \langle v_x^2 \rangle$$

$$\langle v_x^2 \rangle_t = = 1/3 \langle v^2 \rangle \quad .$$

- From this we finally get

$$\langle v_x \rangle_t = \langle (v_x^2)^{1/2} \rangle_t = (1/3)^{1/2} \cdot \langle (v^2)^{1/2} \rangle_t = \frac{\langle v \rangle_t}{3^{1/2}}$$

In real life, however, the fly swarm "cloud" often moves slowly around - it has a finite **drift velocity $\underline{v}_D$**.

$$\underline{v}_D = \langle \underline{v}_i \rangle_t$$

- In consequence, $\langle \underline{v}_i \rangle_t$ is not zero, and $\langle v_{i,+x} \rangle_t$ (= average velocity component in **+x** direction) in general is different from $\langle v_{i,-x} \rangle_t$.
- Note that the drift velocity by definition is an average over vectors; we do not use the $\langle \rangle$ brackets to signify that anymore. Note also, that the drift velocity of the *fly swarm* and the drift velocity of an *individual fly* must be identical if the swarm is to stay together.
- Without prove, it is evident that $v_{D,i,x} = \langle v_{i,+x} \rangle_t - \langle v_{i,-x} \rangle_t$ and so on. In words: The magnitude of the component of the average drift velocity of fly number **i** in **x**-direction is given by the difference of the average velocity components in **+x** and **−x** direction.

This induces us to look now at the *ensemble*, the swarm of flies. What can we learn about the averages taken for the *ensemble* from the known averages of *individual* flies?

- As long as every fly does - on average - the same thing, the *vector* average over time of the ensemble is identical to that of an individual fly - if we sum up a few thousand vectors for *one* fly, or a few million for *lots* of flies does not make any difference. However, we also may obtain this average in a different way:
- We do not average *one fly in time* obtaining $\langle \underline{v}_i \rangle_t$, but at any given time *all flies in space*.
- This means, we just add up the velocity vectors of all flies at some moment in time and obtain $\langle \underline{v}_e \rangle_r$, the **ensemble average**. It is evident (but not easy to prove for general cases) that

$$\langle \underline{v}_i \rangle_t = \langle \underline{v}_e \rangle_r$$

- i.e. *time average = ensemble average*. The new subscripts "**e**" and "**r**" denote ensemble and space, respectively. This is a simple version of a very far reaching concept in stochastic physics known under the catch word "**ergodic hypothesis**w1".

This means that in "normal" cases, it doesn't matter how averages are taken. This is the reason why text books are often a bit unspecific at this point: It is intuitively clear what a drift velocity is and we don't have to worry about how it is obtained. It also allows us to drop all indices from now on whenever they are not really needed.

- In our fly swarm example, the drift velocity $\langle v_D \rangle = \langle \underline{v}_i \rangle$ is usually much smaller than the average $\langle v_i \rangle$ of the velocity magnitudes of an individual fly.
- The magnitude of $\langle v_D \rangle$ 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.
- This induces an *asymmetry*: From a knowledge of the drift velocity *only*, *no inference whatsoever* can be made with regard to $\langle v_{i,+x} \rangle$, $\langle v_{i,-x} \rangle$ or $\langle v_i \rangle$ whereas knowlegde of $\langle v_{i,+x} \rangle$ and $\langle v_{i,-x} \rangle$ tells us all there is to know in **x**-direction

This teaches us a few things:

1. Don't confuse $\langle \underline{\mathbf{v}} \rangle$ with $\langle \mathbf{v} \rangle$. The first quantity - for our flies - is zero or small, whereas the second quantity is large; they are totally different "animals".

2. This means in other words: Don't confuse the property of the *ensemble* - the drift velocity $\mathbf{v_D}$ of the ensemble or swarm - with the properties of the *individuals* making up the ensemble.

Simple Exponential functions

With this JAVA module you can plot exponential (or other) functions

Her are a few examples for writing equations

cos(x)	**exp(x)**
cos(x*2)	**exp(1/x)**
cos(x/40)	**x^2**
cosh(x)	**1/x^2**
cosh(40*x)	**1/(x^3+10)**
	1/(exp(x-20)+1)

Here are a few results for exponentials:

$y = e^x$

$y = e^{-x}$

$y = e^{1/x}$

$y = e^{-1/x}$
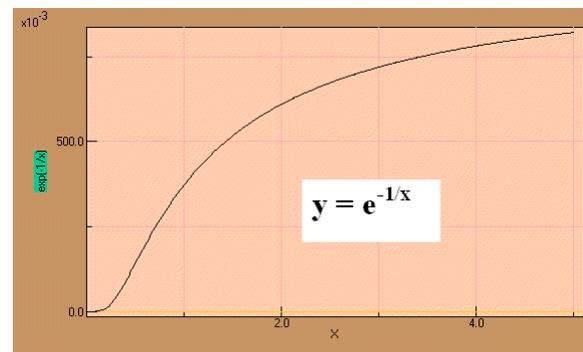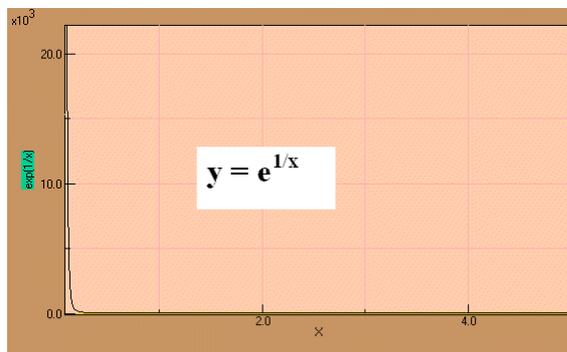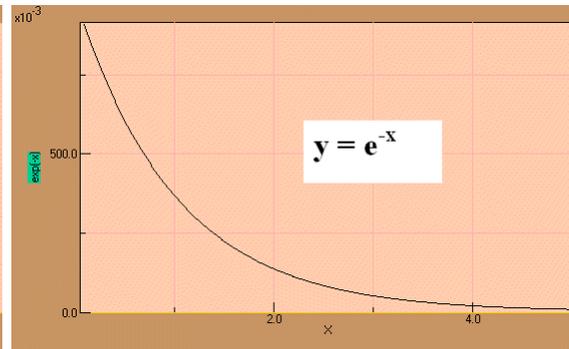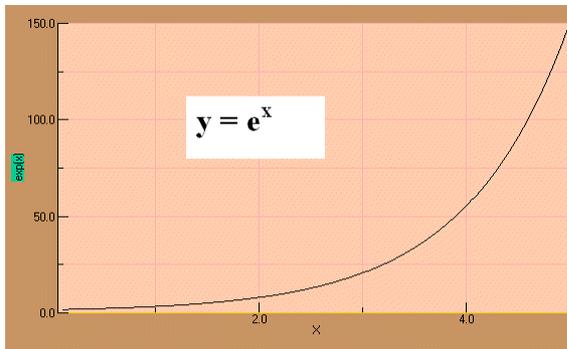
Multiple Choice Test

2.1.1 Ohms Law and Materials Properties

Start Multiple Choice

Multiple Choice Test

2.1.2 Ohms Law and Classical Physics

Start Multiple Choice

Multiple Choice Test

2.1.3 Hall effect

Start Multiple Choice

Multiple Choice Test

2.2.1 Metals

Start Multiple Choice

Multiple Choice Test

2.2.2 Alloys

Start Multiple Choice

Multiple Choice Test

2.2.3 Non-Metals

Start Multiple Choice

Multiple Choice Test zu

2.2 All of Materials and Conductivity

Start Multiple Choice

Multiple Choice Test

2.4 Electron Emission

Start Multiple Choice

Multiple Choice Test

2.4.3 Thermoelectric Effects

Start Multiple Choice

Multiple Choice Test

2.4 All of Special Applications

Start Multiple Choice

Multiple Choice Test zu

2.5 All of Ionic Conductors

Start Multiple Choice

Multiple Choice Test zu

MC 2. All of Conductors

Start Multiple Choice

Exercise 2.1-1

Derive and Discuss numbers for µ

Calculate numerical values for the *mobility* **µ** of some typical metals.

- Take typical (metal) values for specific conductivity σ and concentrations of electrons **n** and then *calculate* typical numbers for the mobility **µ** - do not take the values from the table! I you do not understand the German link, use this one.

- Consider typical field strengths for metals by picking suitable current densities, and then derive typical values for the *drift velocity* v_D.

Solution

Exercise 2.1-2

Derive numbers for v_0, v_D, τ, and l

▸ Show that the claims made in the backbone text are actually true (for room temperature = **300 K**). Use the following equations taken from the backbone

● For the average velocity v_0 of a particle zooming around in the crystal:

$$v_0 = \left(\frac{3kT}{m} \right)^{1/2}$$

● For the mean time τ between scattering:

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

● For the drift velocity v_D

$$v_D = - \frac{E \cdot e \cdot \tau}{m}$$

● For the minimal mean free path length l_{min} obtained for $v_D = 0$:

$$l_{min} = 2 \cdot v_0 \cdot \tau$$

▸ Of course, you need numbers for the concentration n of the free carriers and for the specific conductivity σ

● Since we are essentially considering metals, you assume for a start that you have **1** free electron per atom if you want to find a number for n. Here are a few data needed for the calculation:

Atom	Density $[kg \cdot m^{-3}]$	Atomic weight $\times 1{,}66 \cdot 10^{-27}$ kg	Conductivity σ $\times 10^5$ $[\Omega^{-1} \cdot m^{-1}]$	Conzentration Atoms n $[m^{-3}]$???
Na	970	23	2.4	
Cu	8.920	64	5.9	
Au	19.300	197	4.5	

▸ You may run into some trouble with the dimensions. Just look at conversions from, e.g. **[eV]** to **[J]**, from Ω to **V** and **A**, and at the relations beween Volt, Ampere, Watts and Joule.

Solution

Exercise 2.1-3

What does it take to build a 4 GHz Microprocessor?

A typical **MOS** transistor of **200x (x = 0 .... 5)** vintage has a "gate length" (= distance between source an drain of about **0.5 µm** and is run at about **3 V**

1.) What is the mobility the material (= semiconductor) must have? Discuss the result for known mobility values and consider the following points

- Transistor speed = device speed ??
- Mobility range for a given material ??
- Could we have powerful **PCs** without micro- or nanotechnology ??

2.) How could you increase the speed for a given material

- In principal?
- Considering that there limits. e.g. to field strengths?

Solution

"Exercise 2.2-1": Quizzes to Li Ion Battery

Quiz 1: How much energy is contained in **1 liter** of gasoline?
Find out approximately by using data you know about your car.

- Consider what you know about your car or some average car: Mileage (let's say **10 km/l**), how far you get on this (**500 km**), engine power (**100 kW**), engine efficiency (??? - think) how long it takes you to go the **500 km** and how much percent of the engine power you use for this on average (you are not always going full throttle!).

- Energy, by the way, is power times time.

Quiz 2: How large or small are **10 kWh /l** - in comparison to known energy (densities).

- How far up do you have to drag you body to gain **10 kWh**? Potential energy, by the way, is $E_{pot} = mgh$.

- You store energy by pulling up a ball of lead in your (now unused) chimney (diameter = **20 cm**). How far up do you have to pull it to store the **10 kWh?** (Specific density of lead = **11,4 g/cm^3**).

- How much water can you bring from **10 ºC** to a boil? The specific heat capacity of water is **4.2 kJ/kgK**. A Joule **J**, as we know, is equal to **1 Nm** or **1 Ws**

- Your power output on a bicycle for some length of time is **??? kW**. Mine is at best ≈ **100 W**. How far and / or how long do you have to ride you bike before you used up **10 kWh**? How many Big Mac's have you worked off then (a Big Mac of about **120 g** contains **2071,74 kJ = 494,94 kcal.**

- How much energy do you convert into heat if you wrap your car around a tree at **100 km/h**. In other words: **1/2mv^2 = ??? KWh** (without the gasoline burning). Your car weighs about **1 500 kg** + passengers

- How fast do you need to hit the tree so that the kinetic energy contained in **50 l** ≈ **50 kg** of gasoline equal the kinetic energy?

Quiz 3: This and That

- Why do you have plenty of room in an electric car for the battery?

- Why do you want you batteries not to be extremely light weight in a submarine?

- Why is the current collector in a powerful battery not to be sneered at? Hint: Your electric car has a **100 kW** motor; a battery cell has a voltage of about **3 V**.

- You want to be able to run your **100 kW** electric motor car for **5** hours at half the capacity? What is the required battery size? How long does it take you to recharge that battery from your standard outlet (**230 V AC; 16 A**)?

- Take a **1 kWh Li** ion battery with a voltage of **3V**. How much charge Q must be stored in it when it is fully loaded?

- How much **Li** atoms would that be? What is their weight? Compare to the energy density figure and discuss.

Quiz 4:

- --- To be written ----

Solutions are found in the Li Ion Battery module

Exercise 2.4-1 Richardson Equation

Illustration

Link to the solution

Exercise 2.5.1 Field Screening

Consider a capacitor made of parallel metal plates in air with an area of **1 cm^2** at a distance of **1 cm**.

1. How many electrons per **cm^2** do you need on the surface to provide for some field **E** ending there?

2. What would be the maximum charge density for reasonable field strengths up to an ultimate limit of about **10 MV/cm**? (For higher field strengths you will get violent discharge).

3. How does this number compare to the average *volume* density of electrons in metals. Consider, e.g., from how far away from the surface you have to collect electrons to achieve the required surface density, if you allow the volume density in the afflicted volume to decrease by **x %**?

Link to the <u>solution</u>

Illustration

Solution to Exercise 2.1-1

Derive and Discuss numbers for μ

First Task: Derive numbers for the mobility **μ**.

● First we need typical conductivities and electron densities in *metals*, which we can take from the table in the link.

● At the same time we expand the table a bit

Material	ρ [Ω cm]	σ [Ω^{-1} cm^{-1}]	Density $d \times 10^3$ [kg m^{-3}]	Atomic weight w [× 1u = 1,66 · 10^{-27} kg]	$n = d/w$ [m^{-3}]
Silver Ag	$1,6 \cdot 10^{-6}$	$6.2 \cdot 10^5$	10,49	107,9	$5,85 \cdot 10^{28}$
Copper Cu	$1,7 \cdot 10^{-6}$	$5.9 \cdot 10^5$	8,92	63,5	$8,46 \cdot 10^{28}$
Lead Pb	$21 \cdot 10^{-6}$	$4.8 \cdot 10^4$	11,34	207,2	$3,3 \cdot 10^{28}$

For the mobility **μ** we have the equation

$$\mu = \frac{\sigma}{q \cdot n}$$

With q = elementary charge **= 1,60 10^{-19} C** we obtain, for example for **μ$_{Ag}$**

$$\mu_{Ag} = \frac{6,2 \cdot 10^5}{1,6 \cdot 10^{-19} \cdot 5,85 \cdot 10^{28}} \frac{m^3}{C \cdot \Omega \cdot cm} = 66,2 \frac{cm^2}{C \cdot \Omega}$$

The unit is a bit strange, but rembering that **[C] = [A · s]** and **[Ω] = [V/A]**, we obtain

$$\mu_{Ag} = 66,2 \frac{cm^2}{Vs}$$

$$\mu_{Cu} = 43.6 \frac{cm^2}{Vs}$$

$$\mu_{Pb} = 9,1 \frac{cm^2}{Vs}$$

Second Task: Derive numbers for the drift velocity v_D by considering a reasonable field strength.

The mobility **μ** <u>was defined</u> as

$$\mu = \frac{v_D}{E}$$

or

$$v_D = \mu \cdot E$$

So what is a reasonable field strength in a metal?

Easy. Consider a cube with side lengt **l = 1 cm**. Its resistance **R** is given by

$$R = \frac{\rho \cdot l}{F} = \rho \; \Omega$$

A **Cu** or **Ag** cube thus would have a resistance of about **1,5 ·10^{-6} Ω.** Applying a voltage of **1 V**, or equivalently a field strength of **1 V/cm** thus produces a current of **$I = U/R \approx$ 650 000 A** or a current density **j = 650 000 A/cm^2**

That seems to be an awfully large current. Yes, but it is the kind of current *density* encountered in integrated circuits! Think about it!

Nevertheless, the wires in your house carry at most about **30 A** (above that the fuse blows) with a cross section of about **1 mm^2**; so a reasonable current density is **3000 A/cm^2**, which we will get for about **U = 1,5 ·10^{-6} Ω · 3000 A = 4,5 mV**.

For a rough estimate we then take a field strength of **5 mV/cm** and a mobility of **50 cm^2/Vs** and obtain

$$v_D = 50 \cdot 5 \; \frac{mV \cdot cm^2}{cm \cdot V \cdot s} = 0{,}25 \; \frac{cm}{s} = 2{,}5 \; \frac{mm}{s}$$

That should come as some surprise! The electrons only have to move v e r y s l o w l y *on average* in the current direction (or rather, due to sign conventions, against it).

Is that true, or did we make a mistake?

It *is* true! However, it does *not* mean, that electrons will not run around like crazy inside the crystal, at very high speeds. It only means that their *net* movement in current anti-direction is very slow.

Think of an single fly in a fly swarm. Even better <u>read the module</u> that discusses this analogy in detail. The flies are flying around at high speed like crazy - but the fly swarm is not going anywhere as long as it stays in place. There is then no drift velocity and no net fly current!

Solution to Exercise 2.1-2

Derive numbers for v_0, v_D, τ, and l

First Task: Derive a number for v_0 (at room temperature). We have

$$v_0 = \left(\frac{3kT}{m}\right)^{1/2} = \left(\frac{8{,}6 \cdot 10^{-5} \cdot 300}{9{,}1 \cdot 10^{-31}} \frac{eV \cdot K}{K \cdot kg}\right)^{1/2} = 1{,}68 \cdot 10^{14} \cdot \left(\frac{eV}{kg}\right)^{1/2}$$

⬤ The dimension "square root of **eV/kg**" does not look so good - for a velocity we would like to have **m/s**. In looking at the energies we equated kinetic energy with the classical dimension **[kg · m²/s²] = [J]** with thermal energy **kT** expressed in **[eV]**. So let's convert **eV** to **J** (use the link) and see if that solves the problem. We have **1 eV = 1,6 · 10^{-19} J = 1,6 · 10^{-19} kg · m² · s⁻²** which gives us

$$v_0 = 1{,}68 \cdot 10^{14} \cdot \left(\frac{1{,}6 \cdot 10^{-19}\, kg \cdot m^2}{kg \cdot s^2}\right)^{1/2} = 5{,}31 \cdot 10^4\ m/s = 1{,}91 \cdot 10^5\ km/hr$$

Possibly a bit surprising - those electrons are no sluggards but move around rather fast. Anyway, we have shown that a value of $\approx$ **10^4 m/s** as postulated in the backbone is really OK.

⬤ Of course, for $T \to 0$, we would have $v_0 \to 0$ - which should worry us a bit ???? If instead of room temperature (T = **300 K**) we would go to let's say **1200 K**, we would just double the average speed of the electrons.

Second Task: Derive a number for τ. We have

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

First we need some number for the concentration of free electrons per **m³**. For that we complete the table given, noting that for the number of atoms per **m³** we have to divide the density by the atomic weight.

Atom	Density [kg · m⁻³]	Atomic weight × 1,66 · 10⁻²⁷ kg	Conductivity σ × 10⁵ [$\Omega^{-1} \cdot m^{-1}$]	No. Atoms [m⁻³] × 10²⁸
Na	970	23	2,4	2,54
Cu	8.920	64	5,9	8,40
Au	19.300	197	4,5	5,90

⬤ So let's take **5 · 10^{28} m⁻³** as a good order of magnitude guess for the number of atoms in a **m³**, and for a first estimate some average value σ = **5 · 10^5 [$\Omega^{-1} \cdot m^{-1}$]**. We obtain

$$\tau = \frac{5 \cdot 10^5 \cdot 9{,}1 \cdot 10^{-31}}{5 \cdot 10^{28} \cdot (1{,}6 \cdot 10^{-19})^2}\ \frac{kg \cdot m^3}{\Omega \cdot m \cdot A^2 \cdot s^2} = 3{,}55 \cdot 10^{-16}\ \frac{kg \cdot m^2}{V \cdot A \cdot s^2}$$

Well, somehow the whole thing would look much better with the unit **[s]**. So let's see if we can remedy the situation.

⬤ Easy: Volts times Amperes equals *Watts* which is power, e.g. energy per time, with the unit **[J · s⁻¹] = kg · m² · s⁻³**. Insertion yields

$$\tau = 1{,}42 \cdot 10^{-28} \; \frac{kg \cdot m^2 \cdot s^3}{kg \cdot m^2 \cdot s^2} = 3{,}55 \cdot 10^{-16} \, s = 0.35 \, fs$$

The backbone thus is right again. The scattering time is in the order of femtosecond which is a short time indeed. Since all variables enter the equation linearly, looking at somewhat other carra ier densities (e.g. more than **1** electron per atom) or conductivities does not really change the general picture very much.

Third Task: Derive a number for v_D . We have (for a field strength E = 100 V/m = 1 V/cm)

$$|v_D| = \frac{E \cdot e \cdot \tau}{m} = \frac{100 \cdot 1{,}6 \cdot 10^{-19} \cdot 3{,}55 \cdot 10^{-16}}{9{,}1 \cdot 10^{-31}} \; \frac{V \cdot C \cdot s}{m \cdot kg} = 6{,}24 \cdot 10^{-3} \; \frac{V \cdot A \cdot s^2}{m \cdot kg}$$

$$= 6{,}24 \cdot 10^{-3} \; \frac{kg \cdot m^2 \cdot s^2}{m \cdot kg \cdot s^3} = 6{,}24 \cdot 10^{-3} \, m/s = 6{,}24 \, mm/s$$

This is somewhat larger than the value given in the backbone text.

- However - a field strength of **1 V/cm** applied to a *metal* is huge! Think about the current density j you would get if you apply **1 V** to a piece of metal **1 cm** thick.
- It is actually $j = \sigma \cdot E = 5 \cdot 10^7 \, [\Omega^{-1} \cdot m^{-1}] \cdot 100 \, V/m = 5 \cdot 10^9 \, A/m^2 = 5 \cdot 10^5 \, A/cm^2$!
- For a more "reasonable" current density of $10^3 \, A/cm^2$ we have to reduce E hundredfold and then end up with $|v_D| = 0{,}0624 \, mm/s$ - and that is slow indeed!

Fourth Task: Derive a number for l. We have

$$l_{min} = 2 \cdot v_0 \cdot \tau = 2 \cdot 5{,}31 \cdot 10^4 \cdot 3{,}55 \cdot 10^{-16} \, m = 3{,}77 \cdot 10^7 \, m = 0{,}0377 \, nm$$

- Right again! If we add the comparatively miniscule v_D, nothing would change. Decreasing the temperature would lower l to eventually zero, or more precisely, to $2 \cdot v_D \cdot \tau$ and thus to a value far smaller than an atom..

Solution to Exercise 2.1-3

What does it take to build a 4 GhZ Microprocessor?

First Task: What is the mobility the material (= semiconductor) must have? Discuss the result in considering the following points

- Transistor speed = device speed ???
- Mobility range for a given material ??
- Could we have powerful **PCs** without micro- or nanotechnology ??

The essential equation is

$$t_{SD} = \frac{I_{SD}^2}{\mu \cdot U_{SD}} \approx \frac{1}{f_{max}}$$

The necessary mobility thus is given by

$$\mu = \frac{I_{SD}^2}{t_{SD} \cdot U_{SD}} = \frac{f_{max} \cdot I_{SD}^2}{U_{SD}} = \frac{4 \cdot 10^9 \cdot 2.5 \cdot 10^{-13}}{3} \cdot \frac{m^2}{s \cdot V} = 0.33 \cdot 10^{-3} \frac{m^2}{s \cdot V} = 3.3 \frac{cm^2}{s \cdot V}$$

What is the mobility of typical semiconductors? Finding values in the Net is not too difficult; if you just turn to the Hyperscript "Semiconductors" you should find this link

- Well, all "useful" semiconductors seem to be OK, their mobilities are much larger than what we need. But perhaps we are a little naive?

- Yes, we are! If a device combining some **10.000.000** transistors is to have a limit frequency of **4 Ghz**, an individual transistor "obviously" must be much faster. If you don't see the obvious, think about the routing of many letters by the mail through a few million post offices (with different routes for every letter) and compare the individual and (average) total processing times.

- Bearing this in mind, mobilities of about a factor of **100** larger than the one we calculated do not look all that good anymore!

The mobility table in the link shows large variations in mobility for a given material - obviously **μ** is not really a material constant but somehow depends on the detailed structure.

- We do not need to understand the intricacies of that table - we already know that **μ** is directly proportional to the mean free path length **l** and thus somehow inversely proportional to defect densities.

- It is very clear, then, that for high-speed devices we need rather perfect crystals! So let's try to have single crystals, with no dislocations (or at least only small densities, meaning that the crystal must *never* plastically), and the minimum number of extrinsic and intrinsic point defects.

- Quite clear - but do you see the *intrinsic* problem? A more or less perfect crystal is *not* a device! To make a device from a crystal, we must do something to the crystal. And whatever you do to a *perfect* crystal - the result can only be a less perfect crystal!

- In other words: Making a device means to start with very good crystals and only induce the minimum of defects that is absolutely necessary.

Could we have **4 GHz** without microelectronics?

- Well, take for I_{SD} a value **100** times larger, and your highest frequency will be **10.000** times smaller - **400 kHz** in the example. Of course, the **4 GHz** of modern processors is not only determined by mobility values of the materials used, but the argument is nevertheless valid.

- So, without microelectronics (or by now nanoelectronics) life would by much different, because you can just about forget everything you do as a direct (and indirect!) present-day "user" of electronics. But would it be worse? The answer is a definite: Yes - it would be worse! Trust me - I have been there! It's not that long ago that **400 kHz** was considered a pretty high frequency.

> **Second Task: How could you increase the speed for a given material**
>
> - In principal
> - Considering that there limits. e.g. to field strength

⬤ In principal it is simple: Make I_{SD} smaller and / or U_{SD} larger.

⬤ It is so simple, that you now should wonder, why it's not done immediately? Why not make a **40 GHz** or **400 GHz** microprocessor now - always, of course, only as far as it concerns the mobility?

Well, there are limits that are not so easily overcome. To name just two:

⬤ Things are structured by "painting" with light. And just as much as you can't make a line thinner than than the size of your brush or pencil, you can't make structures smaller than the wavelength of the light you use, which is in the **0.5 µm** range.

⬤ Funny coincidence to the I_{SD} we used, don't you think so?

OK, so we increase the voltage; let's say from **3 V** to **300 V**.

⬤ This increases the field strength from **3/5 · 10^5 V/cm** to **3/5 · 10^7 V/cm** or **600.000 V/mm**.

⬤ In other words: A **1 mm** thick layer of your material should be able to isolate a high-voltage cable carrying **600.000 V**. Seems a bit strange, given the fact that they still hang lousy **300.000 V** cables high up on poles to have many meters of air (a very good insulator) because otherwise you would have to use many **cm** of some really good insulating solid.

⬤ To put it simple: no material withstands field strength of more than **10 MV/cm** (give or take a few **MV**). If you try to exceed that value, you will get interesting and very loud fire works. Whenever mother nature tries it, we call it a thunderstorm.

⬤ And only a few very good *insulators* will even come close to that number. Semiconductors, not being insulators, by necessity, can take far less. Our **60.000 V/cm** are pretty much the limit. So forget about higher voltages, too.

Does this mean **4 GHz** is the end of the line?

⬤ No it's not. It just means it is not easy to go beyond. It take a lot of knowledge, understanding, and skills to make existing devices "better". It take highly qualified engineers and scientists to do the job. It takes what you will be in a few more years if you keep to ít!

Solution to Exercise 2.4.1

Illustration

Solution to **Exercise 2.5.1**

1. How many electrons per **cm^2** do you need on the surface a capacitor made of parallel metal plates in air with an area of **1 cm^2** and distance **1 cm** to provide for some field **E** ending there?

The relation between the field **E** resulting from a homogeneous two-dimensional charge distribution and the charge density ρ_{area} is

$$E = \frac{Q}{\epsilon_0 \cdot A} = \frac{\rho_{\text{area}}}{\epsilon_0}$$

- with **Q =** charge in **[C]**, **A =** area considered, ρ_{area} **=** areal density of the charge.

- Compare the two formulas for the capacity **C** of the capacitor formed by the parallel plates if you are not sure about the equation above. We have:

$$C = \frac{\epsilon_0 \cdot A}{d} = \frac{Q}{U} \quad \text{and} \quad E = \frac{U}{d}$$

2. What would be the maximum density for reasonable field strengths up to an ultimate limit of about **10 MV/cm**? (For higher field strengths you will get violent discharge).

Lets look at some numbers (ϵ_0 = 8,854 · 10^{-14} **C/Vcm**)

Field strength	10^3 V/cm (rather low)	10^5 V/cm (breakdown limit of "normal dielectrics")	10^7 V/cm (close to ultimate breakdown limit)
ρ_{area}	8,85 · 10^{-11} C/cm^2	8,85 · 10^{-9} C/cm^2	8,85 · 10^{-7} C/cm^2

3. How does this number compare to the average volume density of electron in metals. Consider, e.g., from how far away from the surface you have to collect electrons to achieve the required surface density, if you allow the volume density in the afflicted volume to decrease by **x %**?

The average volume density of electrons in metals is about **1** electron/atomic volume.

- Lets keep thing easy and take for the size d_{atom} = 1 Å, which gives **1 Å^3 = 10^{-3} nm^3** for the volume of one atom. The *volume density* of atoms or electrons per **cm^3** is thus ρ_{volume} = 10^{24} **electrons/cm^3**.

- The *areal density* is whatever is contained in a volume with an extension of just one atom diameter in one direction, i.e.

$$\rho_{\text{areal}} = \rho_{\text{volume}} \cdot d_{\text{atom}} = 10^{-17} \text{ electrons/cm}^2$$

- If we want to collect a surplus charge of Q_{surplus} = 8,85 · 10^{-7} C/cm^2, the maximum charge from above, from a volume V_{surplus} by reducing the concentration of **10^{-24} electrons/cm^3** by **x %**, we have

$$Q_{\text{surplus}} = \frac{\rho_{\text{volume}} \cdot d}{100 \cdot x}$$

$$d = \frac{100 \cdot x \cdot Q_{\text{surplus}}}{\rho_{\text{volume}}} = \frac{x \cdot 8,85 \cdot 10^{-5}}{10^{24}} \text{ cm} = x \cdot 8,85 \cdot 10^{-29} \text{ cm}$$

In words: Whatever value we like for **x**, we only have to change the volume concentration of the electrons in an extremely thin layer a tiny little bit to produce *any* areal charge densities needed - in *metals*, that is!

Al Grain Structure on Different Substrates

Illustration

Around the late eighties, the necessity came up to use a **diffusion barrier** between the **Al** - metallization and the **Si** substrate becasue the rection of **Al** with the **Si** in contact holes with cross sections **< 1 μm^2** became a problem. One material of choice was **TiN**, another one **Ta**.

- The grain structure of the **Al** layer (and with it other properties, e.g. the electromigration resistance, depends significantly on the substrate).

- Below you can see the representative pictures (identical scale) that illustrate this point.

Aluminium layer on top of a **Ta** layer	Aluminium layer on top of a **TiN** layer
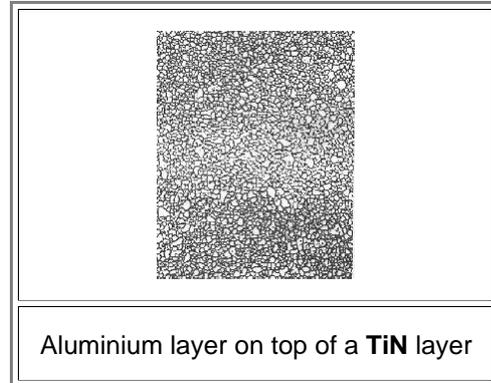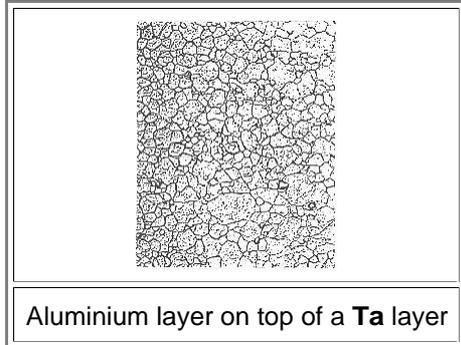
Close examination revealed that the substrate influences:

- Grain size

- Grain size distribution

- Texture

- Degree of **Si** precipitation

- Macroscopic stress

- Microscopic stress

All of these properteis may influence the performance ot the **Al** conductor - and this gives you an idea of what it means to introduce a new material into a fine-tuned product.

Specific Resistivity as a Function of Temperature

Here is a plot of the specific resistivity vs. temperature for some metals.

- The resistivity seems to go to **0** for **0 K**. This is not really true, cf. the detailed curve for Na.

- Still, simple free electron theory predicts zero resistance at **0 K**, and trying to see if that is true was one of the driving forces behind the discovery of superconductivity by **Kammerlingh Onnes** in **1911**.
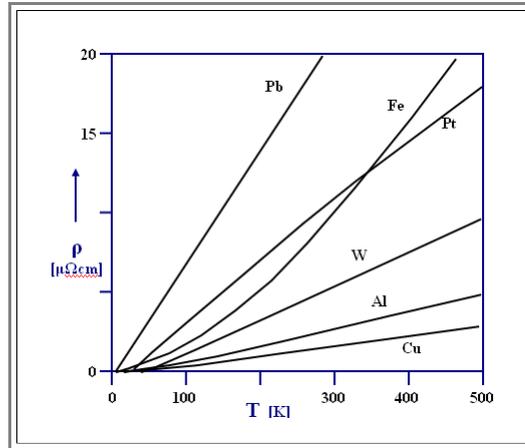
Material for Heating Elements

Illustration

The figure shows some materials for heating elements and the maximal temperature they can endure.

- Note that the maximum temperature, while more or less scaling with the melting point, is usually well below the melting point - because most materials start to develop all kinds of problems long before they melt.

CuNi 44
600 °C

NiCr 2520   8020
1050 °C   1200 °C

CrAl 25 5
1300 °C

Pt   PtRh   Mo   W
1000 °C   1300 °C   1500 °C 1700 °C

MoSi$_2$, SiC   C
1600 °C   3000 °C

Some Properties of Metals

The following table lists important metal properties (at room temperature).

- Specific resistivity ρ
- Density **d**
- Temperature coefficient α_ρ of the specific resistivity
- Thermal conductivity λ

Illustration

Group	Metal	ρ $\mu\Omega$cm	d g/cm^3	α_ρ %/^{o}C	λ W/cm^{o}C
Ia	Na	4,2	0,97		1,4
	K	6,2	0,86		0,9
Ib	Cu	1,7	8,9	0,43	4,0
	Ag	1,6	10,5	0,41	4,1
	Au	2,2	19,3	0,40	3,1
IIa	Mg	4,5	1,7	0,41	1,4
	Ca	3,9	1,5	0,42	
IIb	Zn	5,9	7,2	0,42	1,1
	Cd	6,8	8,6	0,42	1,0
	Hg	97	13,5	0,08	0,08
IIIa	Al	2,7	2,7	0,43	2,3
IVa	Sn	12	7,3	0,43	0,7
	Pb	21	11,3	0,35	0,4
VIIIb	Fe	9,7	7,9	0,65	0,7
	Co	6,2	8,9	0,60	0,7
	Ni	6,8	8,9	0,69	0,9
Vb/VIb	Ta	13	16,6	0,38	0,5
	Cr	14	7,2	0,30	0,7
	Mo	5,2	10,2	0,40	1,4
	W	5,5	19,3	0,40	1,6
VIIIb	Rh	4,5	12,5	0,42	0,9
	Pd	9,8	12,0	0,38	0,7
	Pt	9,8	21,4	0,39	0,7

Residual Resistivity and Defects

Shown here are measured curves of the low temperature resistivity of **Na** with different defect concentrations

- The resistivity is constant for very small temperatures.

- In the "bend" it shows T^5 characteristics.

- For most of the temperature range it is proportional to T.

Defects clearly do increase the residual resistance (the upper two curves are for **Na** with defects, the lower one for rather perfect **Na**); the effect can be much large in other metals or for larger defect densities.
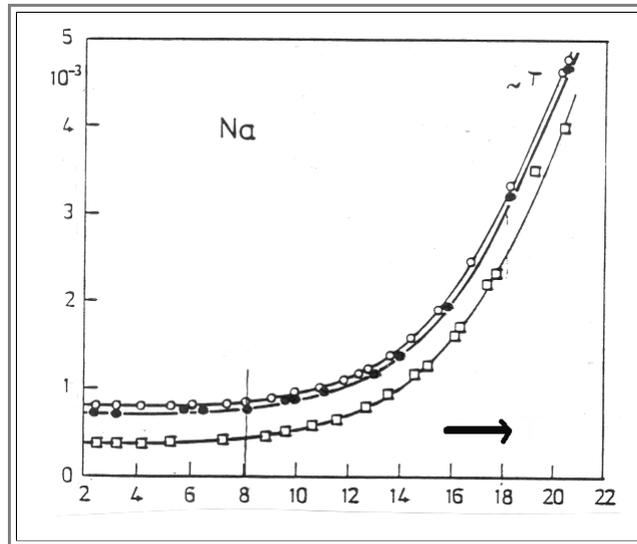
Illustration

Some Properties of Cu Alloys

The following table lists just a few of the existing **Cu** based alloys for specific uses.

Illustration

Alloy	Essential Advantage	σ 10^{-4} S/cm [1]	Uses
Cu + 0,2% Ag	relatively hard	57	Collector lamellae
Cu + 0,5% Te	easy machinable	55	precision parts
Cu + 1,2% Cd	high strength	52	Overhead wires for trains
Cu + 0,6% Cr	can be hardened	48	Welding electrodes
Cu + 1,7% Be	can be hardened	18	Contact springs

[1] **S = Siemens = 1/Ω**

Some Properties of Ag Based Contact Materials

▶ The following table lists just a few **Ag** based alloys that are obtained by a *sintering process* for specific contact uses

● The melting point is always around **960 ºC**

Illustration

Alloy	ρ [$\mu\Omega$cm]	Brinell Hardness [kp/mm^2]	Uses
Ag (60 .... 90) % Ni (40 ... 10) %	2,8...2,0	50 ... 130	Low Voltage circuit breakers
Ag 88% CdO 12%	2,4	60 ... 70	Circuit breakers
Ag 95% SnO$_2$ 5%	2,5	50 ..60	High load relays
Ag 98 % C 2 %	2,5	35 ... 45	Welding resistant contacts
Ag (10 ... 30) % W (90 ... 70) %	5,0 ... 4,0	105 ... 230	Low voltage high power switches

▶ The next table lists just a few **Ag** based alloys that are obtained by *melting* the constituents

● The melting point varies from **(800 - 1030) ºC**

Alloy	$\rho\mu\Omega$cm	Brinell Hardness (kp/mm^2)	Uses
Ag 85 % Cd 15 %	4,8	40...78	Welding resistant DC contacts
Ag (72 ...97) % Cu (28...3) %	1,8 ... 2,1	40...140	Heavy duty relay contacts
Ag 95% Ni 5%	1,9	50	Contacts in communication technology
Ag (70..50) % Pd (30...50) %	15,6...32	70...190	Contacts in communication technology
Ag 20 % Au 80 %	10	37...90	Fine contacts
Cu ca. 95 % Co (...2,5) % Be (1..3) %	3,5...10	100...400	Brushes, pantographs

[1] S = Siemens = 1/Ω

Phase Diagram Ag - Cu

For illustration purposes the **Cu - Ag** phase diagram is shown, demonstrating a miscibility gap.
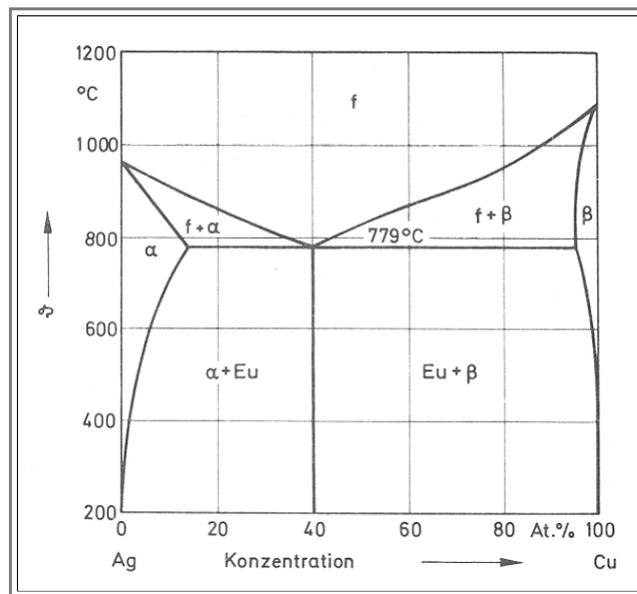
Illustration

Conducting Polymers

Shown below is the conductivity of a polymer (cis-polyacethylene) doped with **AsF$_6$**$^-$ or **I** $^-$

About **1%** of doping materials incorporated into the polymer increases the conductivity by **5** orders of magnitude!

Illustration
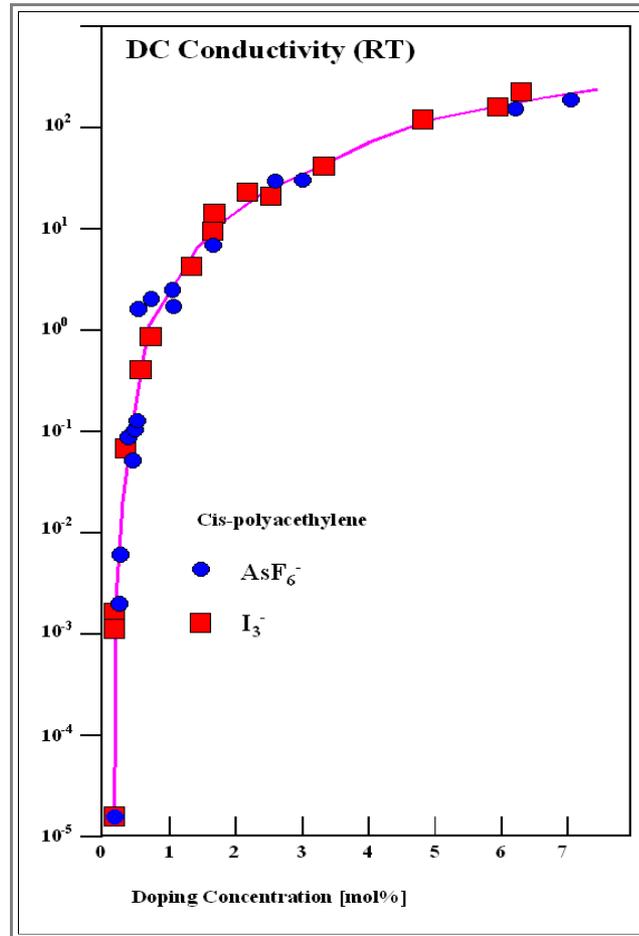
Overview of Heating Materials

The diagram shows the temperature range and the resistivity of typical materials for heating elements.

- Do not forget that humble **1500 ºC** (roughly the melting point of iron) means that it is *really* hot! Mankind had to invent pretty tricky crafts for about **2000** years because nobody could reach the melting point of iron.

- Beyond **2000 ºC** there are not many usable materials left. Essentially you are stuck with graphite (not in the figure).

Illustration
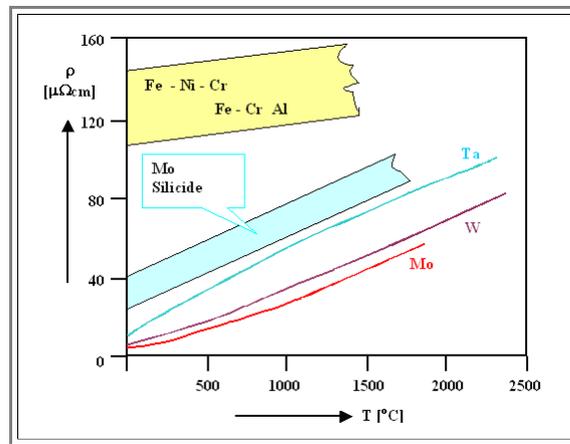
Example for MoSi$_2$ Heater

Here the "News" concerning **MoSi$_2$** heating elements from a German company im **2004**.

Illustration

Elektrische Heizelemente aus MoSi$_2$ für Industrie- und Laboröfen

06.07.04: Neu in der MolyCom-Serie sind die MolyTec-1600-Heizpaneele, elektrische, modular aufgebaute Beheizungssysteme bis *1600 Grad Celsius*. Einsatzfeld der hoch effizienten MolyTec-Elemente sind Schmelzwannen und Feeder in der Glasindustrie und anderen Hochtemperaturbranchen. MolyTec-Paneele bestehen aus MolyCom-Heizelementen, die in hochtemperaturfesten UltraBoard-Mullitfaserplatten eingebettet sind. UltraSiC-Rohre verstärken die Paneele für eine sichere Aufhängung im Zielsystem.

Die M. E.-SCHUPP-Marke MolyCom fasst elektrische Heizelemente mit einem sehr günstigen Preisleistungsverhältnis zusammen. Ihr Einsatzbereich reicht bis *1800 Grad Celsius*. Sie setzen sich aus Molybdändisilizid und einigen Keramik-Komponenten zusammen. Über 900 Grad Celsius bildet sich auf ihrer Heizleiteroberfläche eine dichte, aber dünne Quarzglas-Schicht. Sie schützt das MoSi$_2$- Glühteil vor Oxidation. MolyCom hat sich als technisch gleichwertige, aber kostengünstigere Alternative zu den marktführenden Heizelement-Produkten auf MoSi$_2$-Basis etabliert.

Durch die Hot-Bending-Technologie (MolyCom-Ultra) können im neuen Werk des Produktionspartners von M. E. SCHUPP nun auch komplexere Heizelemente hergestellt werden, zum Beispiel flache oder zylindrische Multishank-Module, wie sie in den MolyTec-Heizpaneelen zum Einsatz kommen. Ebenfalls möglich sind jetzt größere gebogene Heizelemente mit 90 Grad-Winkeln mit Standarddurchmessern von 3/6 mm bis 12/24 mm.

usw.

Strange words

The somewhat unusual word "*ken*" is best remembered by a variant of a famous English poem:

The Star or **Twinkle, Twinkle, Little Star**
by *Jane Taylor*, **1806**

Original:

Twinkle, twinkle, little star,
How I wonder
what you are.
Up above the world so high,
Like a diamond in the sky.

Physicists Version:

Twinkle, twinkle little star.
I don't wonder
what you are,
'cause by spectroscopic *ken*
I know you are hydrogen.

Ken (Scottish) To know, to recognize (German "Kennen"); To have an understanding of something.

Paul Langevin

Paul Langevin (**1872 – 1946**) was one of the fathers of magnetism.

- In the "miracle year" **1905**, when Einstein published three revolutionary papers, Langevin published his theory of para- and diamagnetism.
- Considering that quantum theory had yet to be discovered, and that statitical thermodynamics was in its infancy, his contribution was of amazing insight.
- As far as paramgnetism was concerned, he first established the treatment we used in the text for orientaiio polarization (which is formally indenticl to paramagnetism).

The resulting function of the form **L(a) = −1/*a* + coth(*a*)** is therfore called teh Langevin functions (or sometime Langevin-Debye function, since Debye used the same procedure somerwhat later for polar molecules).

Langevin also worked in the field of Brownian motion (like Einstein). His work concerning ultrasonic sound during world war I was the base for sonar technology .

Beer and Relaxation

Around **1970** I was an auxiliary teacher at my old High School, earning some money needed to see me through my study of physics.

- Just before christmas, I always conducted a lot of "fun" experiments, including an experiment the students did (I provided the material): Measure the decay of the froth on top of a mug of beer.

- Everbody always got the exponential decay law, learned a bit about relaxation phenomena, and just had plain old fun.

Little did I know then that this could have gotten me the **(Ig)-Nobelprize**!

- Arnd **Leike** of the University of Munich, won the **2002** physics Ig Nobel prize for demonstrating that beer froth obeys the mathematical Law of Exponential Decay. [REFERENCE: "Demonstration of the Exponential Decay Law Using Beer Froth," Arnd Leike, European Journal of Physics, vol. 23, January 2002, pp. 21-26.] INTERDISCIPLINARY

- Here is a link to this groundbreaking paper, showing that relaxation with beer may have more meanings than you would have imagined.

Frequency Dependence of Orientation Polarization

How do we get to the time- and frequency dependence $P(t)$ and $P(\omega)$, respectively, of the orientation polarization without "cutting corners" as in the backbone?

- While in principle each function is just the Fourier transform of the other, it is not so easy to actually do the required math. It is probably best, to start with the differential equation that describes the system.

Within the "relaxation time approximation" always used for those cases we have

$$\frac{dP(t)}{dt} = -\frac{P}{\tau} + S(t)$$

- $S(t)$ is some disturbance or signal or input - whichever term you prefer - that has some time dependence. We need it because otherwise the system would be "dead" and not doing anything after at most one decay if we pick suitable starting conditions.

Whatever happens, we can always write $P(t)$ and $S(t)$ as a <u>Fourier series, or, more general, as Fourier integral</u> of the correlated $P(\omega)$ and $S(\omega)$ "spectra" of the time functions. Doing this we have

$$P(t) = \int_{-\infty}^{\infty} P(\omega) \cdot \exp(i\omega t) \cdot dt$$

$$S(t) = \int_{-\infty}^{\infty} S(\omega) \cdot \exp(i\omega t) \cdot dt$$

- $P(\omega) \cdot \exp(i\omega t)$ and $S(\omega) \cdot \exp(i\omega t)$ are the Fourier "coefficients" (with values for every ω, not just harmonics as in Fourier series) for the time functions.

We now have a linear differential equation that is solved by some $P(t)$ which can be expressed as a Fourier transform and that implies that all Fourier coefficients (and any superposition thereof) also solve the differential equation. Inserting the Fourier coefficients directly gives

$$\frac{d\{P(\omega) \cdot \exp(i\omega t)\}}{dt} = i\omega \cdot P(\omega)\exp(i\omega t) = -\frac{P(\omega) \cdot \exp(i\omega t)}{\tau} + S(\omega) \cdot \exp(i\omega t)$$

- From this we obtain

$$P(\omega) \cdot (i\omega + 1/\tau) = S(\omega)$$

If we define $\omega_0 = 1/\tau$ (or $= A/\tau$ if we want to be more general) we now have a simple relation between the Fourier components of input S and output P:

$$P(\omega) = \frac{1}{\omega_0 - i\omega} \cdot S(\omega)$$

The dielectric function $\epsilon(\omega)$ that we are trying to calculate is simple the relation between the output $P(\omega)$ and the input $S(\omega)$, what we get is

$$\epsilon(\omega) := \frac{P(\omega)}{S(\omega)} = \frac{1}{\omega_0 - i\omega}$$

- Considering that the disturbance $S(\omega)$ must have the dimension of an electrical field, forces us to conclude that it actually must be an electrical field, and we could just as well write $\underline{E}(\omega)$. What we have then is essentially the dielectric function as [discussed in the backbone](#).

Cooking with Microwaves

When you heat up food with a **microwave oven**, all you do is to jiggle the water molecules with a frequency where the dielectric losses are large.

- Lets look at the **dielectric function of water**:
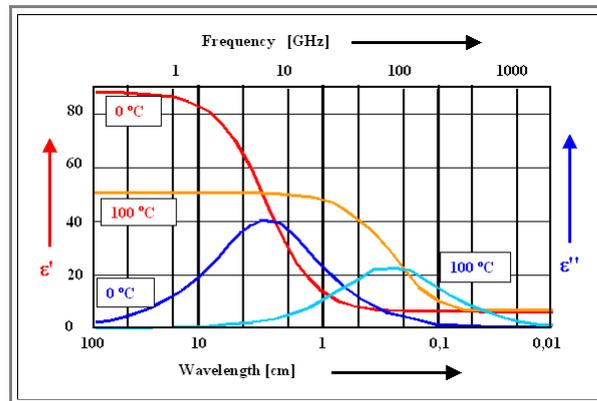
First, we see that the general graph of the frequency dependence is exactly as we would expect from the theory.

- There is a noticeable change of ϵ' and ϵ'' with the temperature. This is as it should be, we had a temperature dependence for the polarization .

$$\langle P \rangle = \frac{N \cdot \mu^2 \cdot E}{3kT}$$

- Changing the temperature from about **300 K** to **400 K** thus should reduce **'(300 K)** $\approx$ **80** by about ¾; i.e. to ϵ'**(400 K) = 60**. The observed reduction is somewhat more severe, because we did not take into account that the water dipoles interact to some extent; and at low temperature this interaction is stronger than at high temperatures.

The maximum of the dielectric losses occurs roughly between **5 GHz - 100 GHz**., i.e. in the microwave region of the spectrum

- Most microwave ovens work at **2.45 GHz**, well below the region of maximum losses. This is intentional to ensure that the radiation is not totally absorbed by the first layer of water it encounters but may penetrate further into the foodstuff, heating it more evenly.
- Radiation passing through the food items is mostly reflected back, due to the design of the microwave oven, and absorbed on later passes.

If the water is frozen, i.e. you have ice, you have problems. The **DK** of ice at the microwave frequency is only about **3**, and little energy is absorbed

If your water is salty, the **DK** goes down, too. On the other hand, the **Na$^+$** and **Cl** ions are jiggled by the electrical field; too (without producing dipoles and thus a **DK**), producing frictional heat and increasing the heating rate.

- Thus whereas ice is a very poor microwave absorber, and water becomes a poorer microwave absorber with rising temperature, a lossy salty food such as salt meat becomes a better microwave absorber with rising temperature.
- This is particularly noticed on thawing. It may take forever to thaw your frozen butter or steak, but after it happened it only takes a short time to turn it liquid or mushy, respectively

Piezo Electricity

It will take a while befor this page will be ready.

- Until then, Wikipedia has a quite good article on the topic. Here is the link:
http://en.wikipedia.org/wiki/Piezoelectric

Advanced

PZT or Lead-Zirconate-Titanate

PZT is short for Lead (= **P**b) zirconate (= **Z**r) titanate (= **T**i) or **Pb[Zr$_x$Ti$_{1-x}$]O$_3$**. It is mixture of **PbTiO$_3$** and **ZrTiO$_3$**

Both constituents are Perowkites as described in the [backbone](). For temperatures below the Curie temperature we have spontaneous polarization as indicated in the phase diagram (adopted form Wikipedia).
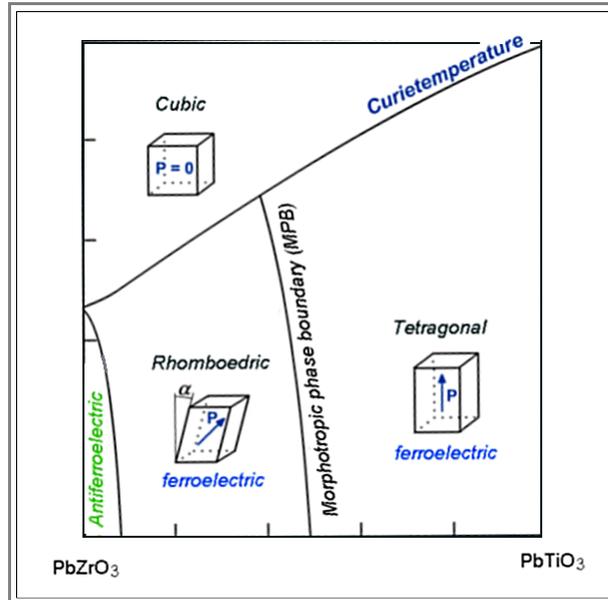
Both lattice pictures in the phase diagram are hugely exaggerated. Drawn to scale, the eye would not see a difference to a perfect cube. The relation of the axis' in the tetragonal case is about **1,06**, and the angle α in the rhomboedric structure, for example, is around **0.3⁰**.

This rather small distortions are large enough, however, to produce major permanent polarization effects.

The interesting part is the "**morphological phase boundary**" (*MPB*) where the structure changes - but not the constituents. Several properties, most interesting for us the "dielectric constant", show pronounced maxima on the **MPB**; "theoretically" they could diverge to infinity.

More down to earth, a mixture of tetragonal and rhomboedric crystals have all together **14** possible directions for spontaneous polarization. In other words, no matter what the external field direction might be, there is always an "easy" direction available in the **PZT** that is not too steeply inclined to the field direction.

As always, optimizing the mixture and adding some other "dopants" or better alloying elements, can produce a large range of properties.

Gauss Law or Integral Theorem

Basics

▶ **Gauss law** relates the *charge* contained inside a volume **V** bounded by a surface **S** to the *flux of the electrical field*.

- The **flux of the electrical field** through a surface **S** is the integral over the components of **E** perpendicular to the surface.
- The most simple way to visualize this is to equate the flux with the number of field lines running through the surface.
- The charge is usually expressed in terms of charge density ρ(**x,y,z**).

▶ Gauss law then states:

$$\iint\limits_{S} \underline{E} \cdot \underline{n} \cdot \mathrm{d}a \;=\; \frac{1}{\epsilon_0} \cdot \iiint\limits_{V} \rho(x,y,z) \cdot \mathrm{d}V$$

- With **n** = normal vector of the surface **S**, **d**a **=** surface increment, **d**V **=** volume increment.

▶ Lets apply Gauss law to a capacitor with or without a dielectric inside. We have the following situation:
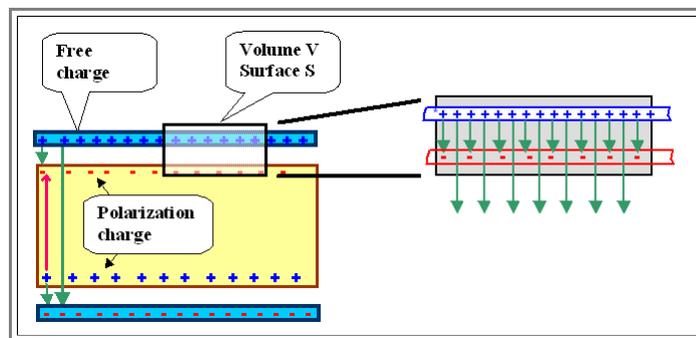
- *Without* a dielectric, *all* green field lines starting at the positve charges of the capacitor plates would run through the interior of the capacitor (and thus through the *lower* surface of the probing volume for applying Gauss' law).
- *With* a dielectric inside, only the "*long*" field lines from all field lines starting at the positive charges on the upper electrode will contribute to the *flux of* **E** because some of the green ones will end at the charges on the surface of the dielectric as shown in the enlargement of the probing volume.

▶ The number of green field lines ending at the surface charge of the dielectric is identical to the number of field lines that we would have inside the dielectric for the given polarization - where green and red ones meet, they cancel each other.

- We see that only the lower surface of our probing volume carries field lines, so the *flux* on this surface is *number of field lines = field times one major area* (= **A**) of the volume **V**.
- *Without* the dielectric, the flux would be larger because *all* flux lines starting at a positive charge would then contribute. The flux **D** in this simple case would be ,

$$D = E_{ex} \cdot A$$

With **A** = that part of the surface **S** that contains field lines and E_{ex} **=** field caused by the external charges only.

- *With* the dielectric, the flux is smaller as reasoned above. We conclude, using Gauss law, that the *amount of charge inside the volume* **V** must be reduced by the dielectric, which is quite obvious when we look at the picture.

▶ For a quantitative description lets compare the case *with* and *without* dielectric, realizing that the integrations called for in the formulations of Gauss law as given above are now simple multiplications:

Without dielectric	With dielectric
Electrical flux with Gauss law	

$$D_0 = E_0 \cdot A = A \cdot \frac{U}{d} = \frac{Q_0}{\epsilon_0}$$

Gauss law

$$D_{di} = E \cdot A = \frac{Q_0 + Q_{pol}}{\epsilon_0}$$

Gauss law

with E_0 = Field without the dielectric,
U = voltage applied to the capacitor,
d = distance between plates;
Q_0 = charge on the plate within V,
A = area of the relevant side of V.
(Only one surface of V contributes)

with E = field inside the capacitor.

$$\frac{Q_{pol}}{A} \quad \text{is the polarization } P \text{ by definition.}$$

Electrical flux with Maxwell Definition

Rewriting the equations gives

$$\frac{Q_0}{A} = \epsilon_0 \cdot E_0 := D_0$$

Maxwell definition

$$Q_0 + \frac{Q_{pol}}{A} = D_{di}$$

$$= \frac{Q_0}{A} + P$$

$$= D_0 + P$$

$$:= \epsilon_0 \cdot \epsilon_r \cdot E$$

Maxwell definition

This is the *definition* of D, the electrical flux density

This is the *definition* of ϵ_r, the **(relative) dielectric constant**

Capacitance

The capacitance C is defined as $C = Q/U = Q/E \cdot d$. Using the equations from above we have

$$C = \frac{Q_0}{E_0 \cdot d} = \frac{A \cdot \epsilon_0 \cdot E_0}{E_0 \cdot d} = \frac{A \cdot \epsilon_0}{d}$$

$$C = \frac{Q}{E \cdot d} = \frac{A \cdot \epsilon_0 \cdot \epsilon_r \cdot E}{E \cdot d} = \frac{A \cdot \epsilon_0 \cdot \epsilon_r}{d}$$

This is of course exactly what we would have expected

Linking the two systems

With $P = \epsilon_0 \cdot \chi \cdot E_0$ it follows

$$D_{di} \quad = \quad \epsilon_0 \cdot E_0 + \epsilon_0 \cdot \chi \cdot E_0$$

$$= \quad \epsilon_0 \cdot (1 + \chi) \cdot E_0$$

$$:= \quad \epsilon_0 \cdot \epsilon_r \cdot E_0$$

$$\epsilon_r \quad := \quad 1 + \chi$$

We thus obtain two simple equations connecting the old-fashioned "**_D_** and ϵ_r" world with the modern "**_P_** and χ" world

$$D_{di} = D_0 + P$$

$$\epsilon_r = 1 + \chi$$

**OK** - so it is tedious and boring. And the result is simple and we all know it.

Still, try at least once in your life to understand *completely* the reasoning behind this. Similar stuff will come up all the time!

Spherical Coordinates

For many mathematical problems, it is far easier to use spherical coordinates instead of Cartesian ones.

- In essence, a vector *r* (*we drop the underlining here*) with the Cartesian coordinates (*x,y,z*) is expressed in spherical coordinates by giving its distance from the origin (assumed to be identical for both systems) |*r*|, and the two angles φ and Θ between the direction of *r* and the *x*- and *z*-axis of the Cartesian system.
- This sounds more complicated than it actually is: φ and Θ are nothing but the geographic *longitude* and *latitude*. The picture below illustrates this.
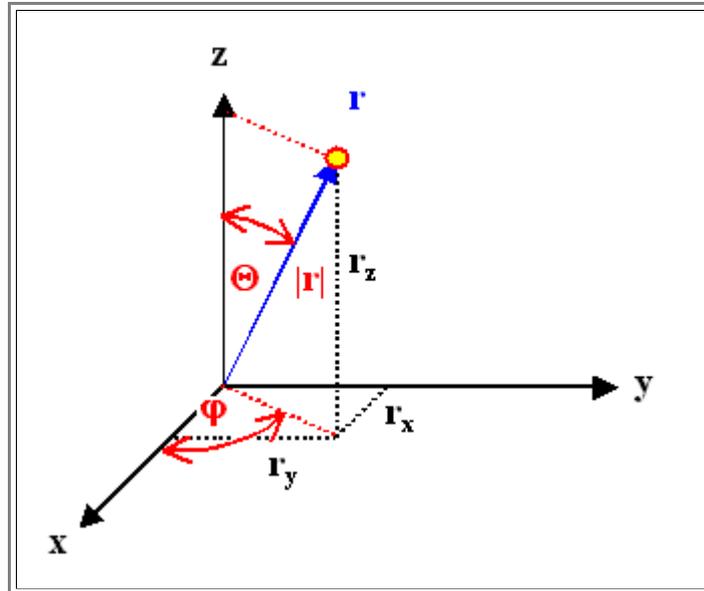
This is simple enough, for the translation from one system to the other one we have the equations

$$x = r \cdot \sin\Theta \cdot \cos\varphi \qquad r = (x^2 + y^2 + z^2)^{1/2}$$

$$y = r \cdot \sin\Theta \cdot \sin\varphi \qquad \varphi = \text{arctg}\,(y/x)$$

$$z = r \cdot \cos\Theta \qquad \Theta = \text{arctg}\,\frac{(x^2 + y^2 + z^2)^{1/2}}{z}$$

Not particularly difficult, but not so easy either.

Note that there is now a certain ambiguity: You describe the *same* vector for an ∞ set of values for Θ and φ, because you always can add **n·2π (n=1,2,3...)** to any of the two angles and obtain the same result.

- This has a first consequence if you do an integration. Lets look at the ubiquitous case of normalizing a wave function ψ **(x,y,z)** by demanding that

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \psi\,(x,y,z) \cdot dx\,dy\,dz = 1$$

In spherical coordinates, we have

$$\int_{0}^{\infty} \int_{0}^{2\pi} \int_{0}^{\pi} \psi\,(r,\varphi,\Theta) \cdot dr\;d\varphi\,d\Theta = 1$$

- You no longer integrate from **-∞** to ∞ with respect to the angles, but from **0** to **2π** for φ and from **0** to π for Θ because this covers all of space. *Notice the different upper bounds!*

Lets try this by computing the volume V_R of a sphere with radius **R**. This is always done by summing over all the differential volume elements **dV** inside the body defined by some equation

In Cartesian coordinates we have for the volume element **dV=dxdydz**, and for the integral:

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \textit{???} \, \mathbf{dxdydz}$$

Well, if you can just *formulate* the integral, let alone solving it, you are already doing well!

In spherical coordinates we first have to define the volume element. This is relatively easily done by looking at a drawing of it:
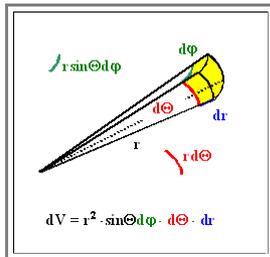
An incremental increase in the three coordinates by **dr**, **dφ**, and **dΘ** produces the volume element **dV** which is close enough to a rectangular body to render its volume as the product of the length of the three sides.

Looking at the basic geometry, the length of the three sides are identified as **dr**, **r · dΘ**, and **r · sinΘ · dφ**, which gives the volume element

$$dV \ = \ r^2 \cdot \sin\Theta \cdot dr \cdot d\Theta \cdot d\varphi$$

The volume of our sphere thus results from the integral

$$V_r \ = \ \int_0^{\infty} \int_0^{2\pi} \int_0^{\pi} r^2 \cdot \sin\Theta \cdot dr \, d\varphi d\Theta = \ 2\pi \cdot \int_0^{\infty} \int_0^{\pi} r^2 \cdot \sin\Theta \cdot dr \, d\Theta \ = 2\pi \cdot [-\cos \pi + \cos 0] \cdot \int_0^{\infty} r^2 \cdot dr$$

$$V_r = \ 2\pi \cdot [2] \cdot 1/3R^3 \ = \ (4/3) \cdot \pi \cdot R^3 \qquad \textit{q.e.d.}$$

Not extremely easy, but no problem either.

Next, consider **differential operators**, like **div**, **rot**, or more general, ∇ and ∇^2 (=Δ).

Lets just look at Δ to see what happens. We have (for some function **U**)

<div align="center">

Cartesian coordinates

$$\Delta = \frac{\partial^2 U}{\partial x^2} + \frac{\partial^2 U}{\partial y^2} + \frac{\partial^2 U}{\partial z^2}$$

</div>

<div align="center">

Spherical Coordinates

$$\Delta = \frac{\partial^2 U}{\partial r^2} + \frac{2}{r} \cdot \frac{\partial U}{\partial r} + \frac{1}{r^2 \cdot \sin^2 \Theta} \cdot \frac{\partial^2 U}{\partial \varphi^2} + \frac{1}{r^2} \cdot \frac{\partial^2 U}{\partial \Theta^2} + \frac{\cot g \, \Theta}{r^2} \cdot \frac{\partial U}{\partial \Theta}$$

</div>

- Looks messy, **OK**, but it is still a lot easier to work with this Δ operator than with its Cartesian counterpart for problems with spherical symmetry; witness the solution of Schrödingers equation for the Hydrogen atom.

Looking back now on our treatment of the orientation polarization, we find yet another way of expressing spherical coordinates for problems with particular symmetry:

- We use a **solid angle** Ω and its increment **d**Ω.

- A *solid angle* Ω is defined as the ratio of the area on a unit sphere that is cut out by a cone with the solid angle Ω to the total surface of a unit sphere (**=4πR^2==4π** for **R=1**).

- A solid angle of **4π** therefore is the same as the total sphere, and a solid angle of π is a cone with a (plane) opening angle of **120°** (figure that out our yourself).

An incremental change of a solid angle creates a kind of ribbon around the opening of the cone defined by Ω. This is shown below
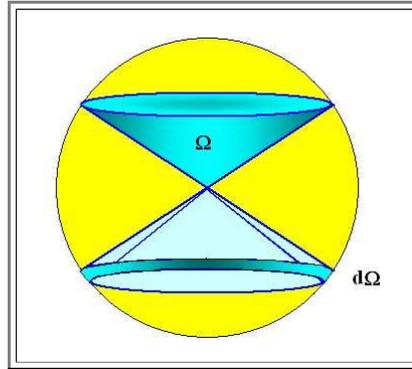
Relations with spherical symmetry where the value of Θ does not matter - i.e. it does not appear in the relevant equations - are more elegantly expressed with the solid angle Ω.

- That is the reason why practically all text books introduce Θ in the treatment of the polarization orientation. And in order to be compatible with most text books, that was what we did in the main part of the Hyperscript.

- Of course, eventually, we have to replace Θ and **d**Θ by the basic variables that describe the problem, and that is only the angle δ in our problem (same thing as the angle φ here).

Expressing **d**Θ in terms of δ is easy (compare the picture in the main text)

- The radius ot the circle bounded by the **d**Θ ribbon is **$r \cdot \sin\delta = \sin\delta$** because we have the unit sphere, and its width is simply **d**δ.

- Its incremental area is thus the relation that we used in the main part.

$$d\Theta = 2\pi \cdot \sin\delta \cdot d\delta$$

The Driven, Damped, Harmonic Oscillator

Basics

In this module we just recall the essentials of the driven and damped harmonic oscillator - for full details see any textbook of physics, e.g. the **Feynman** lectures I-21 - I-25.

- We are looking at a system that can be visualized as shown
  .
- We have a mass *m* hanging on a spring in the gravitational potential of the earth. We assume in addition that the mass is carrying a fixed charge *q*.
- The system is **harmonic**, if the force law for he spring is *linear*, i.e. **Hooke's law** applies:

$$F = k_S \cdot x$$
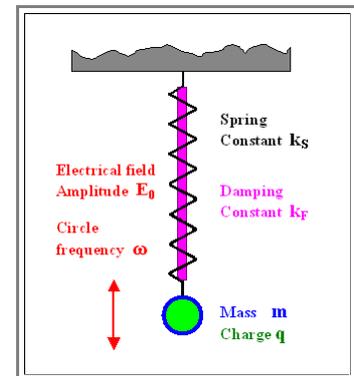
- With *F =* force acting on the spring, *x* = elongation caused by *F*, and k_S = spring constant.
- In other words: The potential *U* that *m* "sees" must be parabolic since we always have $F = -dU/dx$.
- We also assume that the system is *damped*, e.g. by a "shock absorber" that is inside the spring like in the suspension system of your car. This is described by damping constant k_F ("**F**" signifies "friction") and makes sure that an oscillation, once started, will not go on forever.

Finally, we *drive* the system, i.e. we apply a periodically changing driving force - in this example by an oscillating electrical field characterized by its amplitude E_0 and its (circle) frequency ω.

We are interested in two things, as shown below:

- **1.** The amplitude x_0 of the oscillation as a function of the system parameters, in particular as a function of the frequency of the driving force.
- **2.** The phase of the oscillation relative to the phase of the driving force.
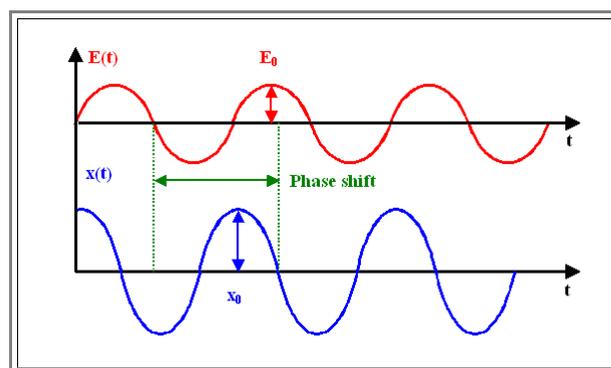
We can rephrase these questions by describing the amplitude of the oscillations as a sum of two sinus function, one exactly in phase with the driving fore, and the other one shifted by **90⁰** (which simply makes it a **cosine** function relative to the in-phase **sin** function)

In this case we ask for the in-phase amplitude x_0' and the out-of-phase amplitude x_0''. The total amplitude x_0 then follows most easily from the "pointer" diagram as shown on the right, we have (with ϕ = phase angle)

$$x = \left(x' + x'' \right)^{1/2} = \frac{x''}{\sin \phi} = \frac{x'}{\cos \phi}$$
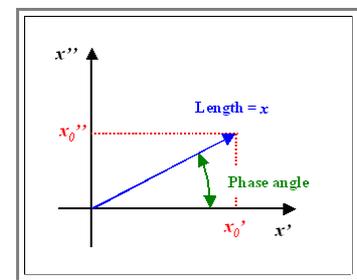
By now you realize (it is hoped) that this leads up to the complex notation generally employed for periodic phenomena (otherwise read up on complex numbers and pointer diagrams, or use the (German) link).

Anyway, first we have to write down the differential equation for the system. It follows (almost) straight from Newtonian mechanics, we have

$$m \cdot \frac{d^2x}{dt^2} + k_F \cdot m \cdot \frac{dx}{dt} + k_S \cdot x = q \cdot E_0 \cdot \cos(\omega t)$$

This is simply the force equilibrium and the only non-trivial force in this equation is the term $k_F \cdot m \cdot dx/dt$

- This is the damping or friction term, we simply assume that it is proportional to the mass m and its velocity dx/dt. The proportionality constant is our damping constant k_F *times the mass*.
- Often the friction term is just written as $k^*_F \cdot dx/dt$, i.e. the mass is included in k^*_F, but our approach has a certain advantage as we will see below.
- While all other terms come from ironclad first principle physical law (always assuming harmonic potentials), the friction term is a bit arbitrary; its exact formulation depends on the specific problem.
- However, if you have a system where the amplitude "decays" exponentially after the driving force is switched off, you must have a damping term as given. Essentially you are back to the very general model of relaxation into the ground state as employed for the frequency dependence of the orientation polarization.

We are now stuck with solving a linear second order differential equation - and we know how that is done.

- Usually, we would move step by step, first looking at a simplified system without damping and driving forces, and then adding the complications.
- What we would find for the simplified system is that there is a special frequency ω_0 called the **resonance frequency** or "Eigenfrequency", which is the simply the frequency with which the system will oscillate by itself if started once. The resonance frequency without damping we call ω_0'; it is given by

$$\omega_0' = \left(\frac{k_S}{m} \right)^{1/2}$$

- With damping added, the resonance frequency changes somewhat, and the amplitude will decrease with time after some initial push started an oscillation. This is described by the following equations

$$x(t) = x_0 \cdot \cos(\omega_0 t) \cdot \exp - \frac{k_F}{2} \cdot t$$

$$\omega_0 = \left(\frac{k_S}{m} - \frac{k_F{}^2}{4} \right)^{1/2}$$

If, for a moment, we apply these equations to an ion sitting in a lattice, we will notice two interesting points:

1. The "spring constant" follows from the binding potential. It is - of course - related to Youngs modulus **Y** which tells us how much the length of a specimen changes under an applied force, or more precisely, how *stress* applied to a material creates (elastic) *strain*. For a homogeneous isotropic material we actually have

$$k_S = Y \cdot a_0$$

- With a_0 = bond length $\approx$ lattice constant. In other words, we know a lot about the spring constant for the systems we are treating here.
- What that means is that we also have a good idea for the order of magnitude of the resonance frequency. It will come out to be roughly **10^{13} Hz**.

2. The damping or friction constant k_F for a single atom, which is coupled by "bond springs" to some other atoms, which are coupled by bond springs ... and so on, is far more difficult to assess. Off hand, most of us probably do not have the faintest idea about a possible numerical value, or if k_F relates somehow to some quantities we already know, like the spring constant.

- However, realizing that the dimension of the damping constant is **$[k_F] = 1/s$**, and that it takes just a few reciprocal k_F's before the oscillation dies out, we can make an *educated guess*:
- If you "snap" just *one* atom of a huge collection of more or less identical atoms, all connected by more or less identical springs, pretty soon all atoms will oscillate. And the original energy, initially contained in the amplitude of the "snapped" atom, is now spread out over all atoms - which means that their amplitudes will be far smaller than the original one. To get the idea, just look at the picture.
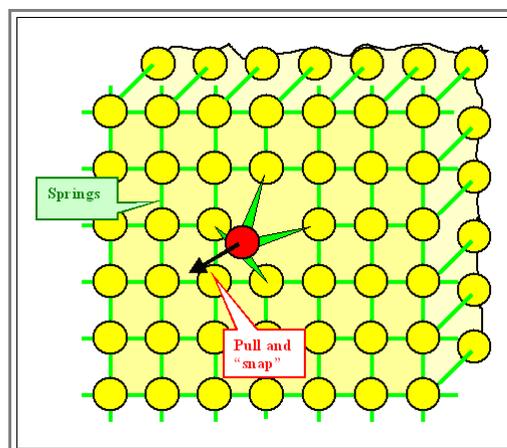
- In other words: There is no doubt that it will just take a few - say **5** or maybe **50** - oscillations of the primary atom, before the *orderly* energy contained in the oscillation of that one atom will have spread and became *diluted* and *disordered*.
- In yet other words: excess energy contained in the oscillations of one atom will turn into thermal energy (= random vibrations of *all* the atoms); it becomes *thermalized* rather quickly - in the time it takes to oscillate back and forth a few times.
- $k_{F\omega}$ is thus tied to ω_0, we expect it to be very roughly in the order of $5\omega_0 \dots 50\omega_0$.

So far so good. But now we must go all the way and switch on "driving", in our example an electrical field that pulls at the charged mass with a force that oscillates with some arbitrary frequency ω

- However, we will not even try to write down the solution the full differential equation given above in "straight" terms - it is too complicated, and there is a better way. We will, however, consider the solution *qualitatively*.
- We (should) know that the mass oscillates with the frequency of the driving force and an amplitude that depends on the frequency (and the damping constant and so on), and that there will be a phase shift between the driving force and the oscillating mass that also depends on the frequency, and so on.
- We also (should) know what all of this looks like - qualitatively. Here it is:
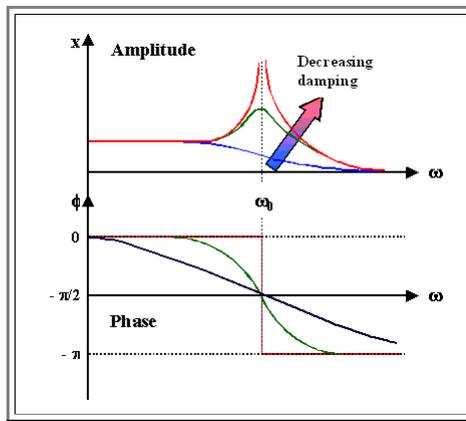
What we are going to do, of course, is to describe the driven damped harmonic oscillator in **complex notation**. The basic equation than is

$$m \cdot \frac{d^2 x}{d t^2} + k_F \cdot m \cdot \frac{d x}{d t} + k_S \cdot x = q \cdot E_0 \cdot \exp(i\omega t)$$

The solutions are most easily obtained for the in-phase amplitude x_0' and the out-of-phase amplitude x_0''.

● The total amplitude x_0 and the phase shift ϕ are contained in these amplitudes. If we want to have them, we simply calculate them as outlined above.

The solution we will obtain is

$$x(\omega, t) = x(\omega) \cdot \exp(i\omega t)$$

$$x(\omega) = \frac{q \cdot E_0}{m} \left(\left(\frac{\omega_0^2 - \omega^2}{(\omega_0^2 - \omega^2)^2 + k_F^2 \, \omega^2} \right) - i \cdot \left(\frac{k_F \, \omega}{(\omega_0^2 - \omega^2)^2 + k_F^2 \, \omega^2} \right) \right)$$

$$x'(\omega) = \frac{q \cdot E_0}{m} \left(\frac{\omega_0^2 - \omega^2}{(\omega_0^2 - \omega^2)^2 + k_F^2 \, \omega^2} \right)$$

$$x''(\omega) = \frac{q \cdot E_0}{m} \left(\frac{k_F \, \omega}{(\omega_0^2 - \omega^2)^2 + k_F^2 \, \omega^2} \right)$$

● This looks complicated, but is, in fact, far more elegant than the description without complex numbers. If we plot $x'(\omega)$ and $x''(\omega)$, we obtain the following curves
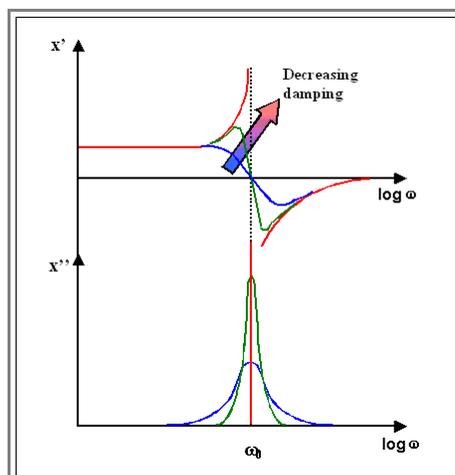
These curves are purely qualitative. A quantitative rendering can be obtained by the JAVA module below

⬤ Instead of the spring constant, you may enter Youngs modulus directly. Typical numbers (in **GPa**) are:

- Diamond: 1000
- Carbides, Oxides, Nitrides: ≈ 300 - 600
- Glas: 70
- Quartz: 100
- Alkali halides: 15 - 70
- Wood: 10
- Polymers: 1 - 10
- Rubber: 0.001 - 0.1

⬤ The damping constant enters with its reciprocal value normalized to ω, i.e. roughly the number of cycles it takes to dampen out an oscillation.

⬤ You can compare two sets of parameters, because the last curve will always be shown with the new curve.

⬤ You can also enlarge any portion of the diagram by simply drawing a window on the part you like to see enlarged.

Fourier Series and Transforms

Fourier Series

Every (physically sensible) *periodic* function $f(t) = f(t + T)$ with $T = 1/\nu = 2\pi/\omega$ and ν, ω = frequency and angular frequency, respectively, may be written as a *Fourier series* as follows

$$f(t) \approx a_0/2 + a_1 \cdot \cos \omega t + a_2 \cdot \cos 2\omega t + ... + a_n \cdot \cos n\omega t + ..$$
$$+ b_1 \cdot \sin \omega t + b_2 \cdot \sin 2\omega t + ... + b_n \cdot \sin n\omega t + ..$$

and the Fourier coefficients a_k and b_k (with the index $k = 0, 1, 2, ...$) are determined by

$$a_k = 2/T \cdot \int_0^T f(t) \cdot \cos k\omega t \cdot dt$$

$$b_k = 2/T \cdot \int_0^T f(t) \cdot \sin k\omega t \cdot dt$$

This can be written much more elegantly using complex numbers and functions as

$$f(t) = \sum_{-\infty}^{+\infty} c_n \cdot e^{in\omega t}$$

The coefficients c_n are obtained by

$$c_n = \int_0^T f(t) \cdot e^{-in\omega t} \cdot dt = \begin{cases} \tfrac{1}{2}(a_n - ib_n) & \text{for } n > 0 \\ \\ \tfrac{1}{2}(a_{-n} + ib_{-n}) & \text{for } n < 0 \end{cases}$$

The function $f(t)$ is thus expressed as a sum of sin functions with the **harmonic frequencies** or simply *harmonics* $n \cdot \omega$ derived from the fundamental frequency $\omega_0 = 2\pi/T$.

The coefficients c_n define the **spectrum** of the periodic function by giving the amplitudes of the harmonics that the function contains.

Fourier Transforms

A nonperiodic function $f(t)$ ("well-behaved"; we are not looking at some ***abominable*** functions only mathematicians can think of) can also be written as a Fourier series, but now the Fourier coefficients have some values for all frequencies ω, not just for some harmonic frequencies.

Instead of a spectrum with defined lines at the harmonic frequencies, we now obtain a **spectral density** function $g(\omega)$, defined by the following equations

$$f(t) = \int_{-\infty}^{+\infty} g(\omega) \cdot e^{i\omega t} \cdot d\omega$$

$$g(\omega) \ = \ (1/2\pi) \cdot \int_{-\infty}^{+\infty} f(t) \cdot e^{-\,i\omega t} \cdot dt$$

The simplicity, symmetry and elegance (not to mention their usefulness) of these **Fourier integrals** is just amazing!

Complex Notation

Please refer to the corresponding module (in German) in the Hyperscript "Introduction to Materials Science I" via the link

Basics

Multiple Choice Test zu

3.1.1 Dielectrics General

Start Multiple Choice

Multiple Choice Test zu

3.2.1 Polarization Mechanisms

Start Multiple Choice

Multiple Choice Test zu

3.2.2 Electronic Polarization

Start Multiple Choice

Multiple Choice Test zu

3.2.3 Ionic Polarization

Start Multiple Choice

Multiple Choice Test zu

3.2.4 Orientation Polarization

Start Multiple Choice

Multiple Choice Test zu

3.2.5 Dielectrics - Summary and Generalization

Start Multiple Choice

Multiple Choice Test zu

3.2.7 Polarization Mechanisms - Summary

Start Multiple Choice

Multiple Choice Test zu

3.3.4 Complete Frequency Dependence of a Dielectric Material

Start Multiple Choice

Multiple Choice Test zu

3.4.1 Dielectric Losses

Start Multiple Choice

Multiple Choice Test zu

3.5.1 Dielectric Breakdown

Start Multiple Choice

Multiple Choice Test zu

# 3.6.1 Piezo and Ferroelectricity

Start Multiple Choice

Multiple Choice Test zu

3.1.1 Dielectrics General

Start Multiple Choice

Exercise 3.2-1 Maximum Polarization of Water

Looking into some standard reference book with numbers, e.g. the *"CRC Handbook of Chemistry and Physics"*, you find that the structure of a water molecule and its dipole moment is
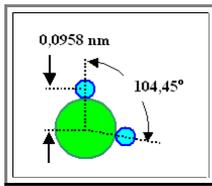
$$\mu_{water} = 1{,}87 \cdot 10^{-18} \text{ e.s.u.}.$$

1. How large would the *dielectric constant* of water be if *all* water dipoles are completely oriented into the field direction? Or, if you realize right away that this question does'nt make much sense:

1a. How large would the *polaization* of water be if *all* water dipoles are completely oriented into the field direction?

And what, for gods sake, are **e.s.u.**?

Link to the solution

Exercise 3.2-2 Interface Polarization

Look at a grain boundary in a simple ionic crystal. Take two grains, for example, that are only rotated with respect to each other and are joined along some grain boundary as shown below
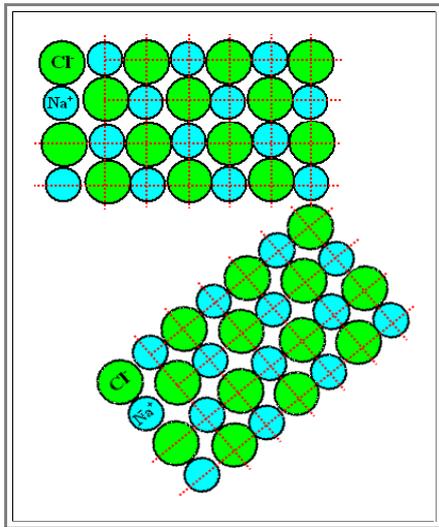
● Construct a grain boundary by filling in material

● Show that in most cases the boundary will be charged and contain dipoles

Link to the <u>solution</u>

Exercise 3.2-3 Electronic Polarization

Look at an atom with atomic number *z*.

How large is the distance *d* between the (center of gravity) of the positive and negative charges for reasonable field strengths and atomic numbers, e.g. the combinations of

- **1 kV/cm**
- **100 kV/cm**
- **10 MV/cm**
- , the last one being about the ultimate limit for the best dielectrics there are,

and

- *z* = **1** (H, Hydrogen)
- *z* = **50** (Sn, (= tin), ...)
- *z* = **100** (?)

Calculate the "spring constant" and from that the resonance frequency of the "elctron cloud" (assume the nucleus to be fixed in space).

Link to the solution

Solution to Exercise 3.2-1

Illustration

🔻 Sometimes, a question can be more tricky than originally intended. That is the case here - lets see why.

- 🔵 First lets get the **e.s.u** out of the way. It means "*electrostatic units*" which are sub-units of the old c.g.s (centimeter-gram-second) system, and still much in use.

- 🔵 Few things are more confusing than converting electric or magnetic **c.g.s.** units into the SI (Standard International) kilogram- meter- second-Ampère system. If you are not somewhat familiar with that, read up the basic modules accessible by the links to this topic.

🔻 In the case given here, you have to multiply with $|c|/10 = 3,3356 \cdot 10^{-10}$ ($c =$ vacuum speed of light) to obtain the charge in **[C]** (The magnitude signs | | simply mean hat you only take the number!); and since the dipole moment is charge times distance, the distance in *e.s.u* units must be **cm**.

- 🔵 We obtain
  $\mu_{water} = 1,87 \cdot 10^{-18}. \ 3,3356 \cdot 10^{-10} \ C \cdot cm = 6,24 \cdot 10^{-28} \ C \cdot cm$

- 🔵 Lets see if that is reasonable: A water molecule carries about one elementary charge $= 1,6 \cdot 10^{-19}$ C at the end of the dipole, and the distance will be about $1 \ Å = 10^{-8}$ cm. This would give a dipole moment of $1,6 \cdot 10^{-27}$ C·cm, so the number we got should be correct

🔻 Now to the tricky part. First it is important to realize that:

- 🔵 A material with *completely oriented natural dipoles* does not have a dielectric constant ϵ_r or dielectric susceptibility $\chi = \epsilon_r - 1$ anymore!

- 🔵 Consider: χ was the proportionality factor between the external field **E** and the induced polarization **P**

$$P = \epsilon \cdot {}_0 \chi \cdot E$$

- 🔵 If the field doubles, the polarization, and thus the degree of orientation into the field doubles.

- 🔵 However, if *all* dipoles are *fully aligned*, the polarization is at a maximum and will not respond to the field anymore; χ looses its meaning.

🔻 Nevertheless, we could take this fully polarized material, stick it into a plate capacitor, and just measure how the capacitance **C** changes . This would give us a value for ϵ_r simply by computing C_{after}/C_{before}. Lets see if we can do this.

- 🔵 For the capacity *before* we use our fully polarized dielectric we have with some applied voltage **U** and some corresponding charge Q_0

$$C_{before} = \frac{Q_0}{U}$$

- 🔵 For the capacity *after* we use our fully polarized dielectric we have
  $C_{after} = (Q_0 + Q_{pol})/U$,
  and this gives us

$$\frac{C_{after}}{C_{before}} = \epsilon_r = \frac{Q_0 + Q_{pol}}{Q_0}$$

🔻 This does not help, however, because we do not know Q_0. Lets try a different approach and look at $C_{after} - C_{before}$.

- 🔵 We obtain .

$$C_{after} - C_{before} = \epsilon_r \cdot C_{before} - C_{before} = C_{before} \cdot (\epsilon_r - 1) = C_{before} \cdot \chi = \frac{Q_0 + Q_{pol}}{U} - \frac{Q_0}{U} = \frac{Q_{pol}}{U}$$

$$\chi = \frac{Q_{pol}}{U \cdot C_{before}} = \frac{Q_{pol}}{Q_0}$$

● This looks better, but it is still not useful - we do not know Q_0. We still have the same problem: The changes are not *proportional* to what we had *before* the introduction of the dielectric, but *absolute* - we are, in effect, adding a fixed charge and thus switching a second capacitor in series.

Lets try a different approach. We know that $\chi(H_2O) \approx 80$. The polarization that goes with this value increases steadily as the field strength inducing the polarization increases - as long as we have $P = \chi \cdot E$

● For large field strength, however, this "law" must break down - we reach the absolute limit of polarization sooner or later.

● So lets compute in a first approximation the field strength needed (within the simple law) to induce the maximum polarization and compare the value obtained to field strengths usually encountered.

First, we compute the maximum polarization P_{max}. This is simply the the charge q_{H2O} on one end of the water dipole times the distance of the charges d_{H2O} divided by the (area) density of the dipoles, i.e. the (area density) of water.

● The dipole moment of water is given by

$$\mu_{water} \ = \ q_{H2O} \cdot d_{H2O} \ = \ 1{,}87 \cdot 10^{-18} \cdot 3{,}3356 \cdot 10^{-10} \ C \cdot cm$$

● We need d_{H2O} to compute q_{H2O}; from the picture in the question we find it to be $d_{H2O} = 0{,}0958$ nm $\cdot$ $\cos(104{,}45^o/2) = 0{,}0586$ nm.

● The (effective) charge q_{H2O} at the end of a dipole thus is

$$q_{H2O} \ = \ q_{H2O} = 6{,}24 \cdot 10^{-28} \ C \cdot cm \ / \ 0{,}0586 \cdot 10^{-7} \ cm = 1{,}065 \cdot 10^{-19} \ C$$

about 2/3 of an elementary charge.

The density of water is $\rho_{H2O} = 1$ **kg/l = 1g/cm^3** by definition.

● One mol of water is **1+ 1+ 16 = 18 g** which tells us that we have **1 mol = 6.022 $\cdot$ 10^{23}** water molecules in **18 cm^3**.

● The areal density ρ_{areal} of dipoles is therefore

$$\rho_{areal} \ = \ \frac{6.022 \cdot 10^{23} \cdot 0.0586 \ nm}{18 \ cm^3} \ = 1{,}96 \cdot 10^{14} \ dipoles/cm^2$$

● Converting *volume* densities to **areal** or **surface densities** may appear tricky. If you are not sure about how it is done, consult the link.

● The maximum polarization P_{max} thus is.

$$P_{max} \ = \ 1{,}065 \ 10^{-19} \cdot 1{,}96 \cdot 10^{14} C \ /cm^2 = 2{,}087 \cdot 10^{-5} \ C \ /cm^2$$

● If we want to generate this polarization with an electrical field and a susceptibility $\chi = 80$, we need a saturation field strength E_{sat} of

$$E_{sat} \ = \ P_{max}/80 \cdot \epsilon_0 = 2{,}087 \cdot 10^{-5}/80 \cdot 8{,}854 \cdot 10^{-12}(C/cm^2) \cdot (Vm/C) = 2{,}946 \cdot 10^6 \ V/cm$$

OK, that is a definite result. Now we have to ask ourselves, how we must compare a field strength of about $3 \cdot 10^6$ **V/cm** to "normal" field strengths.

● To some extent, we do that in sub-chapter 3.5.1, but common sense tells us that we would certainly use **1mm** or more of a dielectric to insulate a wire carrying **1000 V**, for example. This translates to a "typical" field strength of 1**0.000V/cm**.

● Many materials will be destroyed at field strengths of very roughly **100.000 V/cm**, so $3 \cdot 10^6$**V/cm** is very large, indeed.

● However, dielectrics in integrated circuits must be able to operate at field strength of this order of magnitude. Take **3 V** and a thickness of the dielectric of **10 nm** - a not atypical combination - and you have a field strength of $3 \cdot 10^6$**V/cm**, just what we calculated.

Anyway, if we take **100.000 V/cm** as a "normal value, we realize that the only **3,4%** of the dipoles need to be oriented in field direction, whereas the rest could be oriented at random. ($1 \cdot 10^5/2{,}946 \cdot 10^6 = 0{,}034$).

- This is not the physical reality, of course. A more physical interpretation is that all dipoles change whatever orientation they happen to have by about **3,4 %** in field direction. What that means precisely, we will leave open, the general meaning, however, is clear:

- The effect of polarization would hardly be noticeable by just looking at the distribution of the dipoles. It is a rather small effect, even for a material with a comparatively very large dielectric susceptibility.

Solution to Exercise 3.2-2

▸ Again, we have a question here that's a bit more tricky than it looks

  ● Let's look what we get if we construct a grain boundary along the lines suggested.
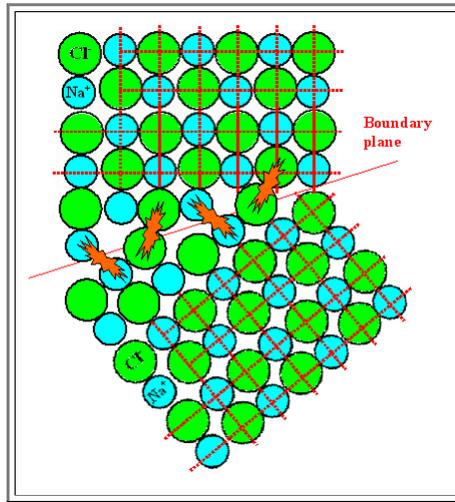
  ● In this example, some boundary plane was drawn in; then atoms were just added on regular positions to the top to bottom crystal as long as there was enough space.

  ● The result is not satisfying: We have mans "head-on" situations, were atoms with the same charge are in intimate contact. This would be a high-energy situation, and that is unlikely.

▸ The crystal for almost sure will be smarter than us, and arrange its atoms - ions, to be more precise - in a better way.

  ● Possibly, also atoms a bit away from the grain boundary need to be re-arranged a bit, for that goal.

▸ What do we learn from that? Two things:

  ● **1.** The precise atomic structure of grain boundaries in ionic crystal (or any crystals with ionic components in their bonding) is not easy to predict. In fact, even the precise structure of grain boundaries in simple metal crystals is far from being simple.

  ● **2.** Whatever kind of smart structure the crystal will realize, it is quite likely that there will be some charge imbalance in and around the grain boundary. That means that we also have an imbalance of dipoles - they do not nearly as nicely cancel each other as the neighboring dipoles in the undisturbed lattice.

  ● And that simply means that grain boundaries - or any kind of interface - will most likely contribute more than the perfect lattice to the polarization of the material. Of course, only for that part of the "volume" that it occupies

Solution to Exercise 3.2-3

How large will be the distance **d** between the (center of gravity) of the positive and negative charges for reasonable field strengths and atomic numbers, e.g. the combinations of

- **1 kV/cm**
- **100 kV/cm**
- **10 MV/cm**
- , the last one being about the ultimate limit for the best dielectrics there are,

- **z = 1** (H, Hydrogen)
- **z = 50** (Sn (= tin), ...)
- **z = 100** (?)

From the backbone we have a relation for **d** as a function of **z**,m the radius **R** of the atom, and the field strength **E**:

$$d_E = \frac{4\pi\epsilon_0 \cdot R^3 \cdot E}{ze}$$

We need to look up some number for the radius of the three atoms given (try this link), then the calculation is straight forward - let's make a table:

Atom	R	d(1 kV/cm)	d(100 kV/cm)	d(10 MV/cm)
z = 1				
z = 50				
z = 100				

- Compared to the radius of the atoms, the separation distance is tiny. No wonder, electronic polarization is a small effect *with spherical atoms*!

Calculate the "spring constant" and from that the resonance frequency of the "electron cloud" (assume the nucleus to be fixed in space).

If you don't know off-hand the resonance frequency of a simple harmonic oscillator - that's fine. If you don't know exactly what that is, and where you can look it up - you are in deep trouble.

- Anyway, in this link you get all you need. In particular the resonance (circle) frequency ω_0 of a harmonic oscillator with the mass **m** and the spring constant k_S is given by

$$\omega_0 = \left(\frac{k_S}{m}\right)^{1/2}$$

- How large are the spring constants? That is question already answered in the backbone, so we import the equation

$$k_S = \left(\frac{(ze)^2}{4\pi\epsilon_0 \cdot R^3}\right)$$

Again, let's make a table for the answers:

Atom	Spring constant	ω_0
$z = 1$		
$z = 50$		
$z = 100$		

Values for dielectric constants

Here are some values for dielectric constants:

- First, some of themore interesting materials with electronic polarization at work, at least to some noticeable extent.

Static ϵ_r for some semiconductors.			
Covalent bonding		Covalent and ionic bonding	
Electronic polarization is the main mechanism		Mix of electronic and ionic polarization	
C	5.7	**ZnO**	4.6
Si	12.0	**ZnS**	5.1
Ge	16.0	**ZnSe**	5.8
SiC	6.7	**CdS**	5.2
GaP	8.4	**CdSe**	7.0
GaAs	10.9	**BeO**	3.0
InP	9.6	**MgO**	3.0
The numbers are from "Solid State Physics" of Ashcroft / Mermin (an advanced text book).			

- Next, some numbers for ionic crystals. Besides the static $\epsilon_r(\omega = 0)$, the value $\epsilon_r(\omega = \infty)$ for very high frequencies is also given. This means that after ionic polarizaton "dies out", there is still some electronic polarization left.

Static and high-frequency ϵ_r for some ionic crystals		
Crystal	$\epsilon_r(\omega = 0)$	$\epsilon_r(\omega = \infty)$
LiF	9.01	1.96
NaF	5.05	1.74
KF	5.46	1.85
LiCl	11.95	2.78
NaCl	5.90	2.34
KCl	4.84	2.19
LiBr	13.25	3.17
NaBr	6.28	2.59
LiI	16.85	3.80
NaI	7.28	2.93
The numbers are from "Solid State Physics" of Ashcroft / Mermin (an advanced text book).		

Piezioelectric fuel injector

Illustration

▸ Here is a picture of a car engine (from Audi) with 4 fuel injectors in place. and a simplified cross-section through one fuel injector.

- The greyish cylinder on top is the stack of piezoelectric materials. It react very quickly to an applied voltage by elongating (more than 5 times faster than old "solenoid" technology) , thus allowing fuel to be pressed in the cylinder. Just as important, it exerts a very large fore, which is needed because injection takes place at huge pressures (around 1800 bar)

Copyright © 1996-2006 by AudiWorld. Source: www.audiworld.com/...
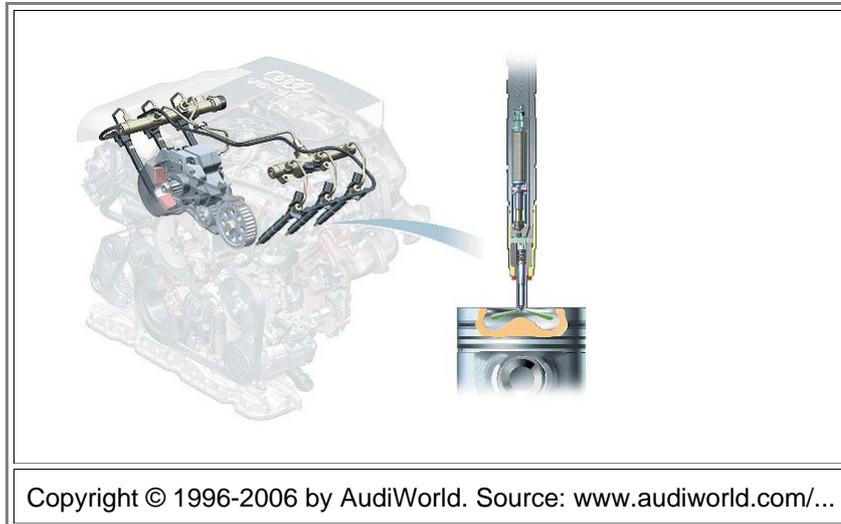
▸ In principle, the piezoelectric fuel injector is a result of Siemens research. Production began around 2000, in 2005 more than 5 Mio injectors had been delivered. Why? Well, the technology boosts performance while reducing fuel consumption up to **20%** and cutting carbon dioxide emissions.

- However, High-tech materials do not come cheap. Siemens (together with Bosch) has invested more than 5 Billion € in the technology so far.

Wrong Illustrations of Orientation Polarization

Some (undergraduate) text books like the "Atkins", "Barrett" or "Askeland" show simplified pictures to orientation polarization that are simply *wrong*.
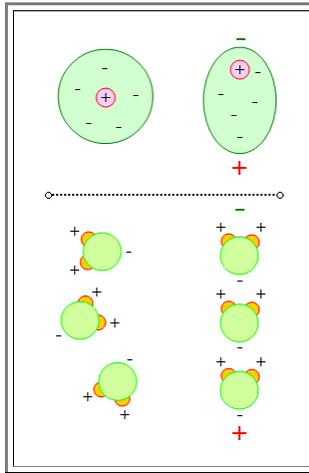
This figure reproduces roughly a picture from the (otherwise very good) "Askeland: The Science and Engineering of Materials". In the bottom part it is supposed to show water molecules without (left) and with (right) an electrical field.

Well - it is simply wrong. However, considering that this book only spends two pages on polarization mechanisms and dielectric constants, there simply is no room for the author to describe "details".

The same is true for the magnetic equivalent of orientation polarization: paramagnetism.

Here is a picture drawn after an illustration in the "Barrett"
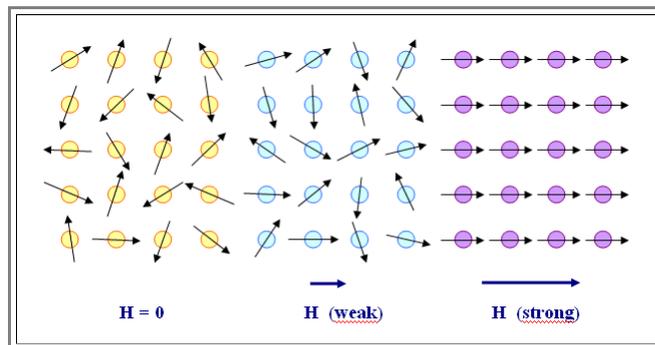
It is just as wrong as the picture above. However, the same "excuse" applies: This is Undergraduate stuff, much simplified, and without a discussion of the statistical nature of the orientation.

Dielectric Function of a Metal-Organic Molecule

Here is a curve of a dielectric function taken from a random scientific paper.
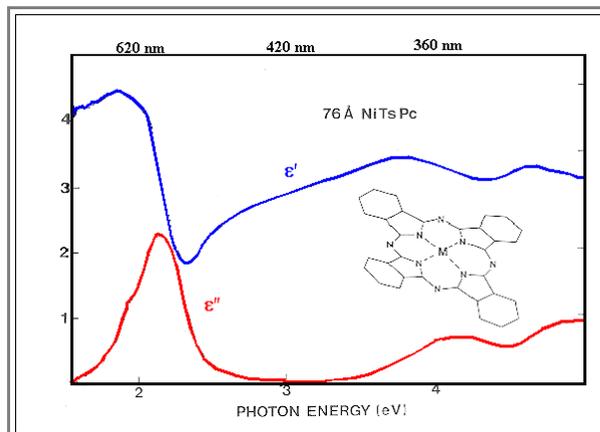
- The material is some kind of metal-organic molecule; shown in the inset.

- The real part (ϵ') and the imaginary part (ϵ'') as measured in a small range of frequencies (expressed as photon energy) is shown.

While the general structure clearly shows the effect of (a strongly damped) oscillation mechanism, there is some fine structure visible. This is easily understood in principle, because all kinds of oscillations are possible in contrast to the simple model with only one oscillating atom.

Ferromagnetic Materials

Here is a list of ferromagnetic (including **ferrimagnetic**) materials (from the "Kittel"). Besides the chemical formula, the Curie temperature T_C and the **magnetic moment** m_m of the molecules (in units of the Bohr magneton m_B) is listed

Material	T_C [K]	m_m
Fe	1043	2.22
Co	1388	1.72
Ni	627	0.606
Gd	292	7.63
Dy	88	10.2
CrO_2	386	2.03
MnAs	318	3.4
MnBi	630	3.52 + 3.6 Mn −0.15 Bi
EuO	69	6.8
NiO / Fe (Ferrit)	858	2.4
$Y_3Fe_5O_{12}$	560	5.0

The list could be much longer, but we see a number of interesting facts.

- There exist more *elemental* ferromagnets than just the common trio **Fe**, **Ni**, **Co** - but not at room temperature!

- Elements that do *not* form a ferromagnetic elemental crystal, may become from ferromagnetic crystals in combination with some other atoms. This is especially true for **Mn** and **Cr** compounds.

- There are many "strange" oxides or mixtures of oxides of non-magnetic elements (**EuO**) or magnetic elements that are ferri- or ferromagnetic. Most compounds with the composition **MOFe$_2$O$_3$** and **M** being some bivalent metal (including **Fe**) are *ferri*magnets.

- The total magnetic moment carried by the atoms or molecules can be rather large; it is a combination of the moments of the atoms (and, if applicable, whatever free electrons contribute). It is constructed from positive and negative contributions for ferrimagnets (as shown for the **MnBi** case), It is, however not obvious, if the total magnetic moment from some compound is "ferro" (all contributions same direction or sign) or "ferri" (different signs). While most oxides are "ferro", some (e.g. **CrBr$_3$**, **EuO**, **EuS**) are "ferro".

Here is a list of **anti-ferromagnetic materials**; T_C is now the Néel temperature

Material	T_C [K]
Cr	308
MnO	116
MnS	160
NiO	525
$FeCl_2$	24
FeO	198
$CoCl_2$	25

CoO	291
NiCl$_2$	50

- We find the by now usual suspects **Fe**, **Ni**, **Co**, **Mn**, **Cr** and their oxides, but also plenty of other compounds (mostly not listed).
- While anti-ferromagnetic ordering provides endless challenges for solid state physicists, it appears that there are no practical uses for this magnetic property at present.

Giant Magnetostriction

Here are a few "clippings" concerning giant magnetostriction. (Emphasizes are mine)

Announcement of a **NATO** conference; June **2000**

The phenomenon of *magnetostriction* was discovered more than 150 years ago (Joule J.P. Philosophical Magazine, 1847, **30,** p.76). Since that time there has been both study of the basic science, and application in such areas as the generators of sound, magnetoacoustic transformers, actuators for opto-electronic systems, devices for non-destructive control and remote detection and ranging. The recent development of modern technologies, such as microfabrication, and materials, such as rare earth based bulk materials and magnetic thin films, has produced new opportunities for the study and application of magnetostriction. Thus, *discovery of giant magnetostriction*, enables one, in particular, to generate ultrasound and extend the usage of the non-destructive control techniques; development of *cryogenic technologies* gives new insight to the forced magnetostriction, namely to its irreversible component, related to *magnetization reversal* and *thermoactivated processes* , which are involved in displacement of the *domain walls and flux lines*, i.e. stability of magnetic and superconducting devices, as well as to the giant magnetostriction in *rare-earth-magnets* (up to 10^{-2}). The new field of the interest in magnetostriction as the strain derivative of *magnetic anisotropy*, is relevant to *magnetic recording industry*, particularly as recorded densities go beyond 20 Gbits/in^2. As physical dimensions of devices are reduced the surface area to volume ratio increases, and surface anisotropy (magnetostriction) effects may become significant in terms of ultimate switching speeds or noise floor. Miniaturisation within the sensor/actuator sector also may invoke such complications, and also now make magnetostrictive materials competitive with piezoelectric materials. There has been a resurgence of interest in perovskite materials, particularly for their outstanding magnetoresistive properties. The fundamental mechanisms driving the observed effects are still being elucidated, but lattice distortions (Jahn-Teller) and significant magnetostrictions appear to play a part. There is an urgent need for coherent studies in this area.

Magnetic field induced *giant magnetostriction* has recently been discovered in high-temperature superconductors. The magnetoelastic strains may limit technical applications of this important group of materials.

Spread of the novel experimental techniques like *magnetic resonances, neutron scattering, modern X-ray facilities* to magnetostriction examination, allows high resolution *structural studies* of magnetostriction and the differentiation of its surface and bulk components. It is timely to review and explore the various possibilities offered here, and attempt to co-ordinate the use of large scale facilities to maximise the scientific output.

The goals of the proposed ASI were delivery of lectures on new achievements and discussion of the listed potentials for the study and application of magnetostriction study among experts from the different branches of science and industry, presenting the leading teams of the West and Eastern Europe. It is hoped that a more co-ordinated and focussed approach at both the level of fundamental science and demonstrator applications, moved the subject on significantly. Wide dissemination of the meeting via publications will be an important outcome. The recent opening up of Eastern Europe makes such a meeting practical, as before much expertise lay beyond the reach of western scientists. This ASI was the first forum on modern trends in magnetostriction study and application. Only a meeting of this kind, supported by NATO, allowed us to gather the worldwide acknowledged specialists in the related fields, capable to promote the solution of the existing problems and identify the future prospects.

Dec. **2000** News from Ames Lab - Iowa State University

Giant Magnetostrictive Materials
Just about everything you ever wanted to know about magnetostriction is covered in a new book by Goran Engdahl entitled Handbook of Giant Magnetostrictive Materials.
The book is a fairly thorough treatment of giant magnetostrictive materials, from basic theory and physics to applications. The book contains six chapters and four appendices. The first chapter is entitled "Physics of Giant Magnetostriction." It covers a wide range of topics from the physical origins of giant magnetostriction to manufacturing processes. Stops along the way include metallurgy and microstructure, crystallography, atomic and magnetic force microscopy images, designing materials, crystalline rare earth alloys, applications, and, of course, TERFENOL-D, among other materials. This chapter includes 85 figures, 50 equations, and 13 tables, all of which serve as excellent illustrative guides to understanding the subject.
The second chapter is devoted to modeling giant magnetostrictive materials. Linear models, finite element modeling, and nonlinear modeling are discussed in detail. Explanations and illustrations of stress and strain, coupling, equivalent circuits, resonance, wave propagation, eddy currents, hysteresis, among others, are included. As is expected, a large number of equations are necessary to explain the topics adequately, and over 230 equations are used throughout the chapter, accompanied by 38 figures.
Chapter 3 covers magnetostrictive design and contains discussions of magnetic, electrical, mechanical, electromechanical, and thermal design. Also included are physical data of TERFENOL-D, magnetic and mechanical operation ranges, 38 figures, and 54 equations.

Two methods of actuator characterization using magnetostrictive materials are presented in Chapter 4. The two methods are time domain methods and frequency domain methods. The discussion is accompanied by 14 figures, 23 equations, and one table.

Device applications are covered in Chapter 5, with emphases on sound and vibration sources, vibrational control, direct and indirect motional control, and materials processing. The final chapter discusses the materials, fabrication, and application of giant magnetostrictive thin films.

Hystereses Losses

Advanced

Finding the proper formula for the hystereses losses is most easily done by considering the following situation:
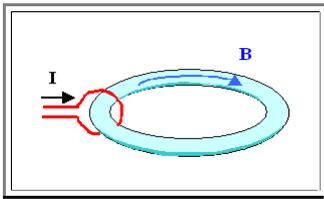
- We have a single loop of wire around a doughnut of magnetic material with **R =** (average) radius of the doughnut or torus of the magnetic material. A current **I** flows through the wire loop.
- The magnetic field **H** generated by this arrangement is given by

$$H = \frac{I}{2\pi R}$$

This formula follows straight from the Maxwell equations; it is known as **Ampères law**.

- The magnetic field **H** of the wire coil induces a magnetic flux **B** in the torus.
- If we now imagine that **I** changes suddenly , e.g. by ΔI in the time interval Δt, to a new constant value, the magnetic flux changes by ΔB, and a voltage **U** will be induced in the wire coil given by

$$U = \frac{A \cdot \Delta B}{\Delta t}$$

- With **A =** cross-sectional era of the torus

This is of course nothing but the well-known effect of self-inductance - you cannot turn on a current very quickly that is flowing through a large inductance.

- In our "experiment", however, we just keep the current at the new constant value - even against the effect of the induced voltage that opposes current flow in the wire.
- This requires that we cancel the effect of the induced voltage by raising the outside voltage accordingly. Since we are interested in power losses, we may also argue that we now need to supply power to the system for a while to be able to keep **I** fixed. Note that in this kind of "experiment" we can make the wire with zero resistance, so no power is fed into the system as long as **I** does not change

We need to maintain a current **I** against a voltage **U**; this requires the power $P_{\Delta B} = U \cdot I$.

- Using our formulas from above (using $I = 2\pi R \cdot H$) yields

$$P_{\Delta B} = 2\pi R \cdot H \cdot A \cdot \frac{\Delta B}{\Delta t}$$

Power is energy times time; for finding a useful material properties it is advantageous to calculate the energy **E** deposited in the magnetic material per unit volume

- Dividing by the volume $V = 2\pi R \cdot A$ and forming $E_{\Delta B} = P_{\Delta B} \cdot \Delta t$ gives

$$E_{\Delta B} = H \cdot \Delta B$$

The total energy deposited in an unit volume of the magnetic material during the time it takes to run through *one* cycle of the hystereses curve is obtained by integrating over a complete cycle, i.e.

$$E_{\text{cycle}} \ = \ \int_{?}^{?} H \cdot dB$$

⬤ With slightly unclear boundaries at present. Lets look at this

⬤ Since we are integrating over **B**; we rotate the hystereses curve to obtain the conventional "**y - x**" form:
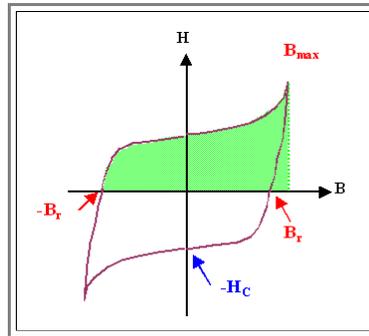
⬤ This is exactly the hystereses curve <u>used before</u>, we <u>just replaced</u> **M** by **B** which does not change the shape. For integrating once around the loop, we may start at the extreme **- B$_r$** and integrate to the other end, i.e. to **B$_{max}$**.

⬤ This gives us the area shown in green which corresponds to the energy needed to change **B** from **B$_r$** to **B$_{max}$**.

⬤ Now we continue the integration running backwards from **- B$_{max}$** to **B$_r$**. This gives us the small area corresponding to the green part outside the hystereses loop, however with a negative sign because we actually recover some energy stored in the magnetization of the material.

▌ In total we obtain just half of the area of the hystereses loop.

⬤ The complete integral thus is simply the area contained in the hystereses loop.

▌ For hard magnetic materials with a roughly rectangular hystereses loop, the area and thus the energy dispersed in *one* cycle per unit volume is than approximately

$$E_{\text{cycle}} \ = \ \int H \cdot dB \ \approx \ 2 \cdot H_C \cdot B_r$$

⬤ The total power loss than is the energy loss per cycle times the number of cycles, i.e.

$$P \ \approx \ 2 \cdot f \cdot H_C \cdot B_r$$

⬤ With **f =** frequency.

▌ This was the <u>formula used</u> in the main part.

Comparison of Dielectric and Magnetic Properties

Here is a quick and simple comparison of dielectric and magnetic *definitions* and *laws*

Basics

Dielectric Behavior			Magnetic Behavior
Charge **q**			*No equivalent*
Electrical field **E**			Magnetic field **H**
Electrical displacement **D**			(Magnetic) Induction **B**
Permittivity constant of vacuum ϵ_0			Permeability constant of vacuum μ_0
Relative dielectric constant of material ϵ_r			Relative permeability constant of material μ_r
From Maxwell equations			*From Maxwell equations*
Connection between dielectric flux density **D**, electrical field **E**, and relative dielectric constant ϵ_r	$D = \epsilon_0 \cdot \epsilon_r \cdot E$	$B = \mu_0 \cdot \mu_r \cdot H$	Connection between *magnetic flux density **B**, magnetic field **H**,* and *relative (magnetic) permeability* μ_r
Formulation with electrical Polarization **P** in the material caused by the electrical field	$D = \epsilon_0 \cdot E + P$	$B = \mu_0 \cdot H + J$	Formulation with *magnetic polarization **J*** in the material caused by the magnetic field
Justified by theory of polarization mechanisms		*Justified by theory of magnetization mechanisms*	
Material "law" describing **P** as response of a material to a field **E** and defining the dielectric susceptibility χ Note exception: *Ferroelectricity*	$P = \epsilon_0 \cdot \chi \cdot E$	$J = \mu_0 \cdot \chi_{mag} \cdot H$	Material "law" describing **J** as response of a material to a field **H** and defining the *magnetic susceptibility* χ_{mag} Note exception: *Ferromagnetism*
Relation between χ and ϵ_r	$\chi = \epsilon_r - 1$	$\chi_{mag} = \mu_r - 1$	Relation between χ_{mag} and μ_r
Definition of **P** as material property in terms of electrical dipole moment μ and density N_V	$P = \langle\mu\rangle \cdot N_V$	$J = \langle m \rangle \cdot N_V$	Definition of **J** as material property in terms of *magnetic moments **m*** and density N_V
		$M = J/\mu_0$	Definition of *magnetization **M***
		$M = \chi_{mag} \cdot H$	Relations between **M** and **H**

Next, let's compare mechanisms that lead to polarization

Dielectric Polarization			Magnetic Polarization
Electronic polarization			*Diamagnetism*
Induce dipole moments by displacing electrons and nuclei. Weak for spherical atoms. Stronger for covalent bonds. Important for optics.	$\epsilon_r \approx 1{,}0001 \ldots 30$	$\mu_r \approx 0{,}9999$	Induce precession of electrons. Always very weak and opposite to field. Not important.
Orientation polarization			*Paramagnetism*
Average small orientation of fluctuating existing dipoles. Only in *liquids*; can be large. Not important.	$\epsilon_r \approx 2 \ldots 100$	$\mu_r \approx 1{,}0001$	Average small orientation of existing dipoles free to rotate in *solids*. Always small; not important. Extreme case: *Ferromagnetism*.

Ionic polarization			No direct counterpart
Net dipole moment from distribution of charges. Important.	$\epsilon_r \approx 2 \dots 100$		
Ferroelectricity Natural dipoles defined by crystallography are lined up. Important.	$\epsilon_r > 1000$	$\mu_r > 1000$	*Ferromagnetism* Natural magnetic moments are lined up in any directions (with crystal directions preferred). ***Extremely*** important.

Multiple Choice Test zu

4.1.2 Origin of Magnetic Dipoles

Start Multiple Choice

Multiple Choice Test zu

4.1.3 Classification of Magnetic Materials

Start Multiple Choice

Multiple Choice Test zu

4.1.4 Definitions and General Relations - Summary

Start Multiple Choice

Multiple Choice Test zu

4.3.3 Magnetic Domains

Start Multiple Choice

Multiple Choice Test zu

4.3.4 Domain Movement

Start Multiple Choice

Multiple Choice Test zu

4.3.5 Losses and Frequency Behaviour

Start Multiple Choice

Multiple Choice Test zu

4.3.7 Ferromagnetism - Summary

Start Multiple Choice

Multiple Choice Test zu

4.4.1 Application of Magnetic Materials

Start Multiple Choice

Multiple Choice Test zu

4.5.1 Magnetic Materials - Summary

Start Multiple Choice

Exercise 4.3.1 Maximal Magnetization

What is the ultimate magnetization we can reasonably expect for a permanent magnet?

- Consider reasonable magnetic moments of atoms in combination with reasonable densities
- Compare to the graph given in the backbone.

Illustration

Link to the solution

Exercise 4.3-2: Magnetic Moments of Fe, Ni, Co

Given the type of the lattice, the lattice constants of **Fe**, **Ni**, **Co** (look it up!), and the magnetization curves in chapter 4.3-2, the question is:

- How large are the magnetic moments of these atoms in terms of a Bohr magneton?

Link to the solution

Illustration

No Solution to Exercise 4.3-1

Do it yourself!

Illustration

Solution to Exercise 4.3-2

▶ Given the type of lattice, the lattice constants of **Fe**, **Ni**, **Co** (look it up!), and the magnetization curves in chapter 4.3-2: How large are the magnetic moments of these atoms in terms of a Bohr magneton?

▶ Simple - but still a bit tricky.

Illustration

🔵 First we get the basic data:

- Lattice **Fe**: **bcc**; lattice constant **a = 2.86 Å**; atomic density $\rho_A(Fe)$ = 2/0.286³ atoms/nm³ = 85.5 atoms/nm³
- Lattice **Nifcc**; lattice constant **a = 3.52 Å**; atomic density $\rho_A(Ni)$ = 4/0.352³ atoms/nm³ = 91.7 atoms/nm³
- Lattice **Co**: **bcc**; lattice constant **a = 2.51 Å, c = 4.0 7Å**; atomic density $\rho_A(Co)$ = 2/[½ · c · a² · 3½ atoms/nm³ = 90.1 atoms/nm³

🔵 Then we realize that the curves in chapter 4.3-2 give the maximum magnetization, i.e. the magnetization state for all magnetic moments perfectly aligned. From the figure we can deduce the following numerical values for the saturation magnetization m_{Sat}:

- $m_{Sat}(Fe) = 17 \cdot 10^5$ **A/m**
- $m_{Sat}(Fe) = 5 \cdot 10^5$ **A/m**
- $m_{Sat}(Fe) = 14 \cdot 10^5$ **A/m**

🔵 However, the units shown are **A/m**, which are not what we would expect. Obviously we must convert this to - well, what exactly?

▶ If we look at a Bohr magneton, m_{Bohr}, we have

$$m_{Bohr} \; = \; 9.27 \cdot 10^{-24} \; Am^2$$

🔵 Obviously, the unit we need is **Am²**. We obtain that by multiplying the **A/m** by **m³**, which makes clear that the m_{Sat} numbers given are per **m³** - as they should be!

▶ The magnetic moments m_A per atom are thus

$$m_A \; = \; \frac{m_{Sat}}{\rho_A}$$

What we obtain is

$$m_A(Fe) \; = \; \frac{17 \cdot 10^5 \; A/m}{85.5 \; atoms/nm^3} \; = \; \frac{17 \cdot 10^5 \; A \cdot 10^{-27} \; m^3}{85.5} \cdot \frac{}{m} \; = \; 1.98 \cdot 10^{-23} \; A/m^2 \; = \; 2.14 \; m_B$$

$$m_A(Ni) \; = \; 5.45 \cdot 10^{-24} \; A/m^2 \; = \; 0.588 \; m_B$$

$$m_A(Co) \; = \; 1.55 \cdot 10^{-23} \; A/m^2 \; = \; 1.67 \; m_B$$

▶ Now that is an interesting result! It's satisfying because we actually get sensible numbers close to a Bohr magneton, and it's challenging because those numbers are not very close to **1**, **2**, or possibly **3**.

🔵 For example, how can a **Ni** atom have a magnetic moment of **0.588 m_B**, and a **Fe** atom one of **2.14 m_B**, considering that the spins of the electrons carry exactly **1 m_B**?

▶ There are two possibilities for this apparent discrepancy:

1. Our calculation is somehow a bit wrong
2. There are some effects not yet discussed that change the magnetic moment an atom in a crystal lattice carries around with itself somewhat.

🔵 The first possibility can be ruled out, because in standard textbooks, e.g. in the "*Kittel*" we find the following values for m_A

- $m_A(Fe) = 2.22 \; m_B$
-

- $m_A(Ni) = 0.606\ m_B$
- $m_A(Co) = 1.72\ m_B$

Not identical, but close enough. In fact, looking more closely, the Kittel values are for **T = 0 K**, whereas our values are for room temperature **T = 300 K** and thus should be a bit smaller.

Obviously, this leaves us with some effects not yet discussed. What these effects could be, we can only guess at. Here is a short list:

- There might be some interaction between the spins of the electrons and the "orbits" of the electrons that modifies the magnetic moment
- The free electrons of the electron gas in our metal also "feel" the ordered spins of the atoms and react to some extent by adjusting their spins.

This can lead to quite sizable effects. Dysprosium (**Dy**), for example, a rare earth metal, is a ferromagnet below its Curie temperature of **88 K** and its atoms than carry an $m_A(Dy) = 10.2 m_B$.

Magnetic Moments of Atoms

Illustration

▶ If we talk about the properties of atoms, we *must* use quantum mechanics. If you are familiar with the mathematical formalism of operators, eigenstates etc., its straight forward (but still complicated). If you don't feel so hot about this, it is almost hopeless.

● But not quite. All one has to know or accept is that even in quantum mechanics there is such a thing as momentum, and in particular **angular momentum**. True, the angular momentums resulting from electrons "orbiting" the nucleus in a certain orbital are quantized, and their projection onto some direction is quantized, too, but nevertheless we can assign a total angular momentum **_J_** to a given atom in a given state, which then is always tied in with some quantum number **_J_** (notice: no underlining) going with **_J_**.

● Usually with "a given state" we mean the ground state of that atom, but it could have an excited state or it could even be ionized - and this might change its total angular momentum **_J_**.

▶ There are always two components to the total angular momentum:

  1. The total orbital angular momentum **_L_** (correlated to some quantum number **_L_**) resulting, if you like, from summing up (with quantum mechanical rules) the angular momentums resulting from the electrons "orbiting" the nucleus.
  2. The total spin angular momentum **_S_** (correlated to some quantum number **_S_**; use the (German) link for an example) resulting from summing up (with quantum mechanical rules) the intrinsic angular momentums of the electrons that are coupled to their spin.

▶ If we have determined **_L_** and **_S_** (and I'm not saying that this is trivial, just that it is doable), we obtain for the magnetic moment of an isolated atom the following rather simple formula:

$$\mu_{atom} \ = \ - \ g \cdot \mu_B \cdot J$$

▶ The interesting quantity is **_g_**, the **g**-factor or **Landé**-factor; it is given by

$$g \ = \ 1 \ + \ \frac{J(J+1) + S(S+1) - L(L+1)}{2J(J+1)}$$

● OK, not overly helpful at first sight, but nevertheless quite useful. We could start to calculate magnetic moments of isolated atoms - but that is not too exciting for technical purposes, where we rarely use the magnetic properties of dilute gases. We could also, however, use this as a base to wonder about the magnetic moments of *ions*, as we find them e.g., in crystal lattices including metals (ions in the "electron gas"!). Now that would be useful.

▶ If we do this as best as possible for some interesting crystals like **Fe**, **Ni**, **Co** or some of their compounds, we find that the theoretical results are often quite close to the measured values, but sometimes they are spectacularly wrong.

● That simply means that the bonding between atoms, which we haven't considered yet, might come into the act, too, heavily modifying the magnetic properties of isolated atoms or simple ions.

● Slowly things start to look complicated. And we aren't even near to explaining ferromagnetism - a very specific interaction of the magnetic moments of neighboring atoms.

● So relax, lean back, and just accept that atoms might have some specific magnetic moment, that might depend on how they are incorporated into some solid, but that it is always in the order of a Bohr magneton. if you do that, you can go right on to chapter 4.1.3.

Domain Structures

Here are some domain structures as found in the Web. These pictures are scientific citations and thus do not infringe on Copyrights.

Unfortunately, some of these pictures do not obey the first law of scientific picture publishing, which is:

You must always have a scale on your micrographs!

Illustration
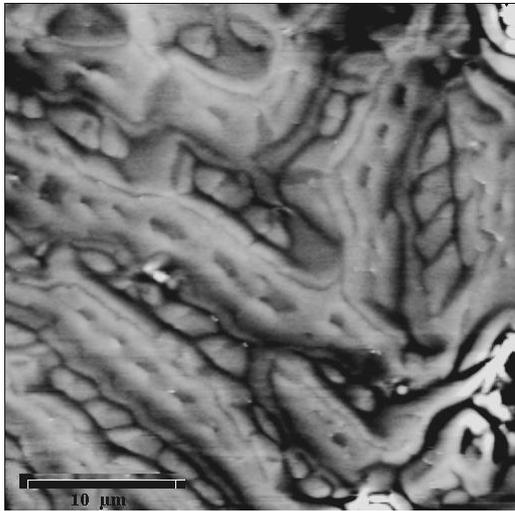
Domain structure of native *magnetite* (obtained by
"magnetic force microscope imaging"). It is quite complicated.
Source: http://premare.imr.tohoku.ac.jp/
SDurbinWWW/magndomn.html.

A very nice picture of the domain structure of **Fe + 3% Si**.
(From a paper entitled: Interaction Between domain walls and
structural defects as a background for magnetic inspection
of steel structures" by E.S. **Gorkunov**, Yu.N. **Dragoshansky**
(from the Proceedings of the 15th World Conference on
Nondestructive Testing Roma (Italy) 15-21 October 2000))

A labyrinth of magnetic domain as seen in an amorphous membrane of **Gd-Co**.
Historical picture from unclear source.
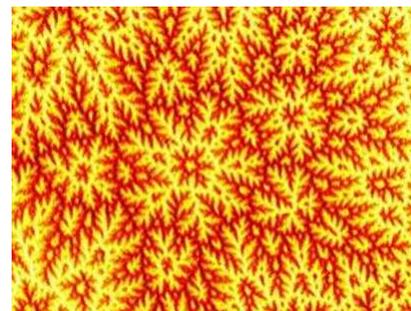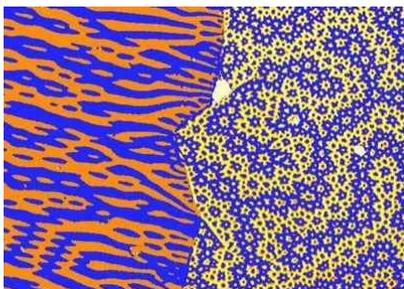
Domains in **NdFeB** material. The domain character in this
highly anisotropic material depends on the orientation of the easy
axis of magnetization relative to the surface. In the grain on the right
the axis is oriented perpendicularly, resulting in fine branched domains,
while the grain on the left has a lower degree of
misorientation relative to the surface.
From *A. Hubert and R. Schäfer, Magnetic Domains.*
The Analysis of Magnetic Microstructures, Springer,
Berlin-Heidelberg-New York, 1998. With friendly
permission of R. Schäfer.

Domain branching observed at the surface of a **Co** crystal
with strong out-of-plane anisotropy.
Same source as to the left.

Newton vs. Huygens

Advanced

�! As we learned in High school, **Isaac Newton** (1643 - 1727), the science hero of the 17th century, propagated the view that *light consists of small particles or corpuscles*.

  ● He based his book „Opticks or a treatise of the reflections, refractions, inflections and colours of light" on this point of view, and since he didn't do so badly, it was far from obvious that he should be wrong.

  ● For example, he deduced that white light consists of of colored light (corpuscles of different sizes) that get separated in a prism or generally in glass. Prior to his insight, everybody believed that glass somehow changed the light. Based on this he not only explained the nature of a rainbow but also concluded that a telescope based on mirrors should be superior to one with lenses because of their "chromatic aberration" (he did not use this term, of course). He even built a prototype of a mirror based telescope but, bad luck, it wasn't better than the lens telescopes of his times because his mirror suffered from spherical aberration.

  ● He knew that his corpuscle model could not (easily) explain some known effects around interference or polarization tied to birefringence (first described in 1669 by **Erasmus Bartholin**) but so what. There was a lot of other stuff in the 17th century that had not yet been satisfactorily explained.

▸ **Huygens** (1629-1695), a Dutch mathematician, physicist and so on, formulated the **Huygens principle**, nowadays better known as **Huygens–Fresnel principle**, and generally argued that light consists of waves.

  ● **Augustin-Jean Fresnel** (1788 – 827), was a French engineer who contributed significantly to the establishment of the theory of wave optics long after Huygens, so from my point if view it is OK to just call it Huygens principle.

  ● Huygens experimented with Icelandic crystals (calcite) that showed double refraction (birefringence) and explained it with his wave theory and polarized light. Based on his insights he also constructed and made better lenses and thus microscopes, telescopes and so on. Moreover, he made seminal contributions to mechanics and was instrumental in early probability theory.

  ● He fought Newton tooth and nail about the nature of light. He lost the fight. Newton appealed to the "Royal Society", the topmost authority in those bygone times, and **1715** it ruled that Newton's point of view was the correct one. This was not as stupid as it appears now. Huygens, as we know now, was right but could not really prove his assertions then. For that another **75** years needed to pass.

▸ Enter **Thomas Young** (1773 - 1829). While he started as a physician, he mutated and became a true physicist early in life and proved beyond doubt that *light is a wave*.

  ● Somewhat ironically, it weren't only the seminal **double slit interference experiments** done around 1802 but also the explanation of "**Newton rings**" that convinced all and sundry that light is a wave and *not* a particle.

  ● Young did not just establish the wave nature of light but contributed to many other aspects of physics or, as we would call it now, materials science. "**Young's modulus**", for example, is named after him for good reasons. Moreover, he was also instrumental in deciphering hieroglyphic and other forgotten scripts.

▸ So Newton was wrong - or was he? Enter **Albert Einstein** (1879 - 1955). In **1905**, the "annus mirabilis", he postulated the **photon**, a kind of light *particle*, to explain the photo electric effect (that should get him his one Nobel prize in 1921). He also published the special theory of relativity in this year and the explanation of Brownian motion, i.e.. the atomic theory of diffusion. By the way, he received his Ph.D. (Dr. degree) a year later in **1906**.

  ● So light is now a particle once more? Of course meanwhile we know better. We know since **Louis-Victor Pierre Raymond duc de Broglie** (1892 - 1987) established in **1924** that particles are also waves, that there is no such thing as a pure wave or a pure particle.

  ● There are only "things" described by a *wave function* that comes out as a solution of the Schrödinger equation (or the more general equations of quantum (field) theory). There are no problems anymore, except that explaining that to somebody not used to quantum theory is like explaining color to the blind, symphonies to the deaf, reason to a lawyer, conservation laws to an economist or truth to a theologian. It's tough.

  ● We also know now how we might simplify and approximate the problem at hand by looking at the "thing" either as a pure particle or a pure wave.

Interference Paradox

▶ Consider two Laser beams ideally described by $\underline{E} = \underline{E_0}\exp(\underline{kx} - \omega t)$ but with phase differences of **180°** or π.

   ● With some device (semitransparent mirror, prisms, ...) we get both light beams to travel along the same **x-**direction as shown below. They must now cancel each other completely. There is no light anymore along the x-direction!
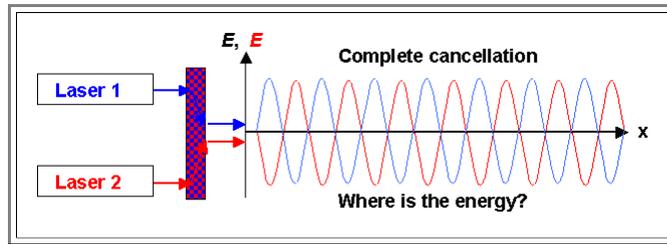

   ● We have a big paradox:

   > **Where is the energy contained in the two Laser beams**
   > **that are still emitted by the running Lasers?**

▶ If you find the situation a bit artificial and not related to practical live consider this question:

   ● There are earphones already on the market where an acoustic signal generated "live" and exactly in antiphase to some signal measured - e.g. the noise in an airplane - cancels that signal and thus you do not hear the noise anymore. Similar but not the same because the acoustic energy contained in the cabin noise is still mostly there.

   ● So how about large-scale development efforts to cancel the noise in modern cars by generating "anti noise" and beaming it into the inside by loudspeakers. The noise generated by the engine and whatever else contains energy, and so does the anti-noise generated by the speaker system. But if the system works it is now quiet and the acoustic energy has "disappeared". Since energy cannot disappear, the question is: where is it?

▶ Let's inch towards the answer. Despite some claims to the opposite, there is no easy answer. Consult this link, for example.

   ● Let's look at a *real* situation where the paradox appreears to some extent: **antireflection coatings** as shown below.
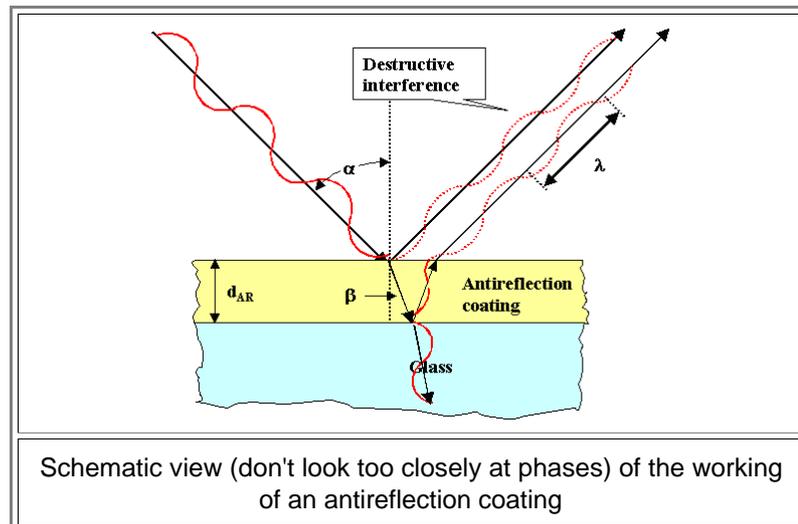
Schematic view (don't look too closely at phases) of the working
of an antireflection coating

   ● By putting a dielectric layer with the right index of refraction **n** - thickness **d_{AR}** combination on top of, e.g., a piece of glass, the two reflected beams - one at the **AR** coating - air interface, one from the **AR** coating - glass interface - exactly cancel each other. There is thus no reflected beam; it isn't called antireflection coating for nothing.

   ● Where is now the energy no longer contained in the non-existent reflected beam? In the transmitted beam, of course - where else? That's why you see better through lenses with an antireflection coating: more light reaches your eye.

▶ Clear - but note that we have not really *proved* that statement!

   ● The interference paradox essentially *challenges* the validity of the energy conservation law. The argumentation above, however, is based on energy conservation being always valid.

- Nevertheless, the statement that the energy cancelled by destructive interference is now somewhere else is generally true because it can be *proved* that energy conservation still obtains!

In the top picture the crucial part is the "*some device (semitransparent mirror, prisms, ...)*" brings the beams together.

- There is *no* device that can do that without reflecting some of the intensity. If you get the case of fully destructive interference to the right, you will have to produce a lot of reflection to the left. In other constructions you might even influence what the light sources do, up to inducing self-destruction of the Lasers (e.g. by pointing two Lasers against each other).

But again; it is one thing to make these statements and another thing to prove them by calculating the various intensities. If you want to dig deeper, consider the following case.

- Two simple dipole antennas emitting radio waves are put close together (distance much smaller than the wavelength). You feed both antennas with the same signal but with an adjustable phase difference. This is technically easy to do.

- For a phase difference of π the emitted waves would cancel. The situation is exactly the same as shown above except that it could be done easily. The problem is that we have no mirrors or gadgets now that can take the "blame" as in the example above. This case, however, can be calculated in detail.

- What one finds out by going through the proper equations is that antennas do not just emit, they also "receive". There is always some coupling expressed in some *impedance* that is not constant but depends on what the two antennas do. Important terms like *near-field* and *far-field* come into their own, and in the end - well, read the article yourself!

Questions and Answers about Details of Light Waves

Here is the relevant picture and the questions going with it from subchapter 5.1.4:

$$E_y(t) = E_{y0} \cdot \exp\{i(kx - \omega t)\}$$
$$E_z(t) = H_{z0} \cdot \exp\{i(kx - \omega t)\}$$
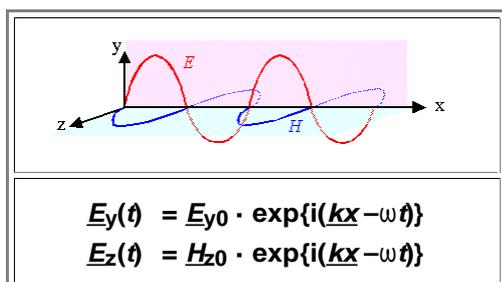
1. Is the electrical and magnetic field really in phase as shown above?
2. Can polarization be described by a vector? Could I just use a unit vector in E_0-direction?
3. How do I describe polarization in the particle picture?
4. How large is the electrical field E_0 in a typical light wave. How large (roughly) is it for one photon of given energy?
5. Let's assume you know the electrical field E_0: how large is the magnetic field H_0 going with it?

Let's consider some answers

1. Is the electrical and magnetic field really in phase as shown in the drawing above?

Yes it is - all serious sources agree even so the reasons given are mostly not obvious. The real question, of course, is: *why* should this be a question at all?

- Solving the Maxwell equations quite generally for the "wave" case, simply gives solutions with no phase differences of the form:

$$E(r,t); \; H(r,t) = E_0; \; H_0 \cdot \exp\{i(kr - \omega t)\}$$

True enough. But this simple solution describes an *infinitely* extended electromagnetic plane wave—something that *does not exist*. So let's look what happens for *finite* waves that have a beginning at some point in space.

- Not so easy for light. The generation of a photon is always a quantum mechanical effect not covered by the Maxwell equations. However, the equation above is valid for *all* electromagnetic waves. It is also valid, e.g. for the radio waves produced by a simple *dipole antenna* and this is covered by the Maxwell equations. We thus can look at the generation of a radio wave instead of a light wave; something easier to conceive than the generation of a light wave by the transition of an electron from one energy level to another one.
- The figure below shows the principle. An AC current is fed to a dipole, it drives charges to the two ends. Maximum current flows when there are no charges at the dipole ends, we then have maximum magnetic fields and no electric field
- The charges transported to the end of the dipole cause an electrical field that opposes current flow. Eventually, at maximum charge and thus electrical field, current flow is zero and there is no magnetic field.
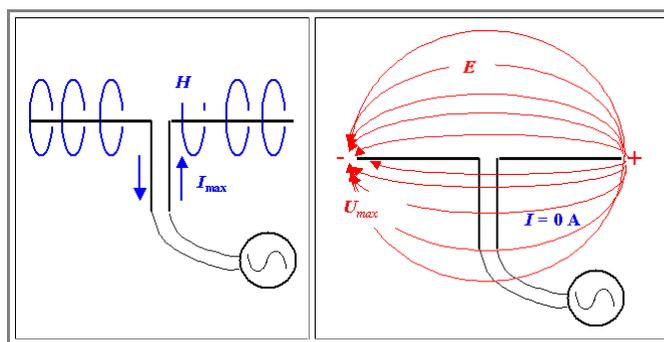
- The unavoidable conclusion is that at the place where we *make* the wave - and it doesn't matter what kind of wavelength you envision - the electrical field and the magnetic field are **90°** *out of phase*!

Now we have a problem: far away from the "light source" the two fields are *in* phase but where we make them they are *out* of phase!

- The problem is solved when one looks at the full set of equations (not easy). Far away from the dipole, in the **far field**, we "see" a point source that emits a spherical wave and there is no phase difference, indeed. Close to the dipole (measured in units of the wavelength), in the **near field**, we do *not* see a point source but a complex geometry as sketched above. The fields in the near field do not have spherical symmetry and phases right at the dipole are different by **90°**, indeed.
- In mathematical terms, we superimpose a complicated near field term with a general $1/r^n$ dependence **(n > 1** on a simple spherical wave. The near-field term dominates close to the antenna. Since it decreases faster than the spherical wave term, for large distances we can neglect the near-field term and are left with a spherical wave that appears to be a plane wave if you only look in parts of space.

You don't need to know this but you should be aware that as soon as you leave the ideal realm of the simple plane wave without a beginning and an end, things tend to get *much more* complicated. But things also tend to be *much more* like what we actually know.

2. Can polarization be described by a vector? Could I just use a unit vector in E_0-direction?

Yes, you can describe polarization by vector. But beware! Polarization in general is more tricky than you might think and a simple vector is not always enough to describe it mathematically. (Remember the problems encountered in using a polar vector for describing rotations?). You will need a tensor / matrix if you go about it systematically.

That was more or less a quote from here.

3. How do I describe polarization in the particle picture?

You don't. You look at the *spin* of the particle instead.

Read more about it here.

4. How large is the electrical field E_0 in a typical light wave. How large (roughly) is it for one photon of given energy?

The first question can be answered without too much trouble; the second question is tricky.

Look at the exercise to these (and other) questions. Try to do it. Then look a the solution.

5. Let's assume you know the electrical field E_0: how large is the magnetic field H_0 going with it?

Here is the relevant equation.

Edwin Herbert Land and Polaroid

Edwin Herbert Land (* 7. May **1909** in Bridgeport, Connecticut, USA; † 1. March **1991** in Cambridge, USA) founded the **Polaroid Corporation** in **1937**, a company known to almost everybody before the advent of digital cameras around 2000. A Polaroid camera (introduced Christmas 1948) could produce a paper picture minutes after it was taken.

More important to us here, he also invented the first polarizing foil. For that he relied on a discovery made earlier by the British toxicologist **William Bird Herapath**. One of his assistants (for reasons not quite clear to me) added some Iodine (**J**) to **dog piss** around **1850** and produced needle-shaped greenish crystals. Two of those crystals crossing each other at a certain angle appeared black, however. Of course we understand immediately that this is simply a "crossed polarizer" effect . Back in **1850** this was understood, too, but considered remarkable. The crystals were properly named *Herapathite* and identified as Iodine-Chininsulfate (the dogs were fed Chinin before they were allowed to go to the bathroom)

Land managed to incorporate **Herapathite crystal** (made without the help of dogs, I hope) into plastic foils, and by stretching the whole thing to align them.

Since it is known *now* that Iodine additions to some polymers turn them into *conducting* polymers, some confusion arose if the polarizing mechanism depends on conducting nanorods in Lang's foils. Well, most likely not. Lang's polarizers depend on the second of our two principles.

Todays simple linear polarizing foils probably do not employ Herapathite any more. It is surprisingly difficult to find out exactly how they are made and work, however.

Anyway, the punch line is that it took about **150** years to unravel the crystal structure of Herapathite. The deed was done by chemists of the University of Seattle, details can be found in: Science 12 June 2009: Vol. 324, p. 1407 ; authors Bart Kahr, John Freudenthal, Shane Phillips and Werner Kaminsky. Here is a picture from this reference (Copyright Bart Kahr)

The crystal structure of herapathite. Iodine atoms are purple spheres. The absorbing axis is vertical. Solvent molecules and sulfate ions have been removed for clarity.
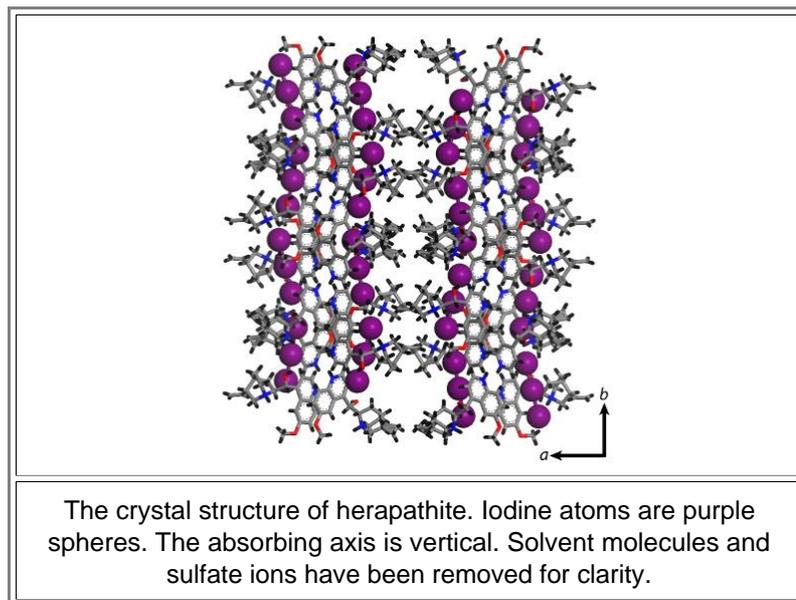
Well, you can almost feel that this crystal must somehow polarize light. And, maybe, those Iodine atom chains do produce some conductivity? The *question* then is if a nanorod conductor grid would still work on molecular dimensions far smaller than the wavelength?

Relax. If you look at the complex index of refraction, you first realize that the conductivity σ is part of it. Secondly, you realize that a herapathite crystal cannot possibly by isotropic but must carry an ϵ and thus also *n tensor* around with it - the question is moot. It's all contained in the complex index of refraction!

There is much to be learned from that story:

One can become rich and famous by exploiting a material properties that are not really understood. That's what (sometimes) distinguishes pragmatic engineers from hard-core scientists.

There is a lot of stuff out there that is far more complex than our ubiquitous **fcc** crystals but is useful and money-making.

Next time you step into dog shit: don't curse but consider if it might be useful for something. As always, it's advisable to motivate graduate students to do the dirty work!

Advanced

Types of Luminescence

Advanced

▶ In alphabetical order we have:

▶ **Bioluminescence**, i.e. luminescence generated by a living organism.

● The light generating molecules become excited by a chemical reaction; bioluminescence is thus related to *chemiluminescence*. Some biological entities like bugs, e.g. *fireflies*, denizens of the deep like anglerfish, some mushrooms and even bacteria can control this reaction. They produce the chemicals *luciferin* (a pigment) and *luciferase* (an enzyme). The luciferin reacts with oxygen to create light. The luciferase acts as a catalyst to speed up the reaction.

Firefly attracting females with lit up behind (Source Wikipedia)	Mushroom; glowing just for fun? (Source amazingdata.com)
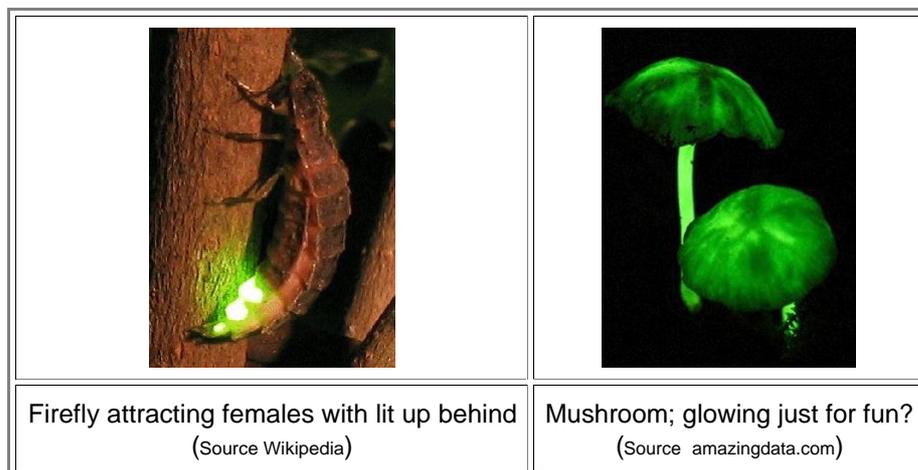
▶ **Chemiluminescence** (or "chemoluminescence") results from some (actually amazingly few) chemical or electrochemical reactions.

● The energy needed comes from the reaction enthalpy. The reaction produces some new molecule that can have its electrons in an exited state right after it was formed. Decay to a ground state may then produce visible light (the exception) or release the energy in some other way (the rule).

● The flash of light you see when some dynamite explodes is not chemiluminescence even so the energy comes from a chemical reaction but simply black body radiation or **incandescence** from things getting very hot very quickly.

▶ **Crystalloluminescence** is occasionally produced during crystallization

● It's another variant of chemiluminescence because the energy comes essentially from bonding between atoms.

▶ **Electroluminescence** generates light in response to an electric current passing through some material

● In essence, electroluminescence results radiative recombination of electrons and holes; typically (but not exclusively) in semiconductors. We have treated that extensively before. It is the basis for LED's and semiconductor Lasers and thus of prime importance in the context of light sources.

● Recently electroluminescence is also used for characterizing solar cell. Feed a large current into a *good* solar cell in the dark and your IR camera will see (weak) electroluminescence even so **Si** is an indirect semiconductor. The reason is simple: Good solar cells, by definition, are **Si** devices where all regular recombination channels have been "closed off", i.e. made inefficient, otherwise the solar cell cannot be good. Radiant recombination then "wins" and is raised to a level where it can be detected The following picture shows an example.

Electroluminescence from solar cell	**Photoluminescence from solar cell**
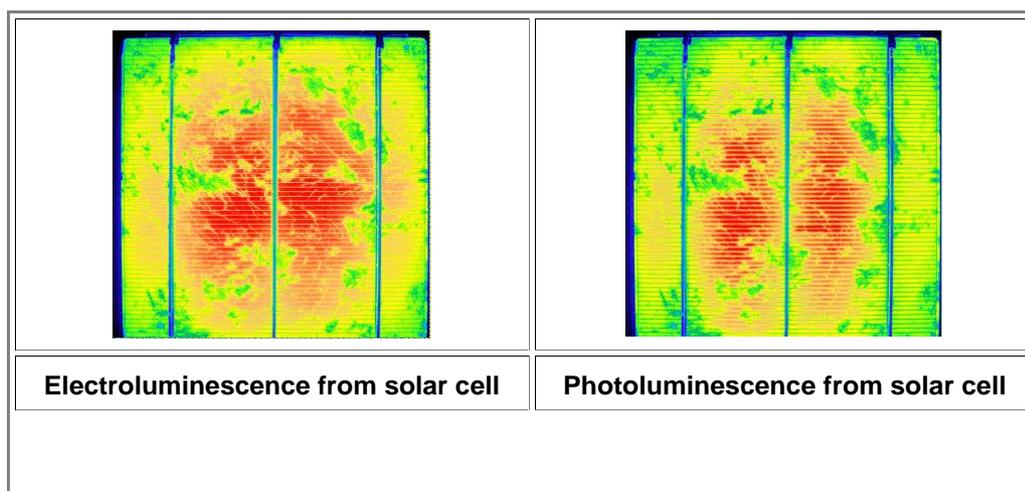
> Colors code intensity. The pictures look almost identical but differences not only exist but contain a lot of specific information about this solar cell.

Cathodoluminescence occurs when an electron beam impacts on a luminescent material such as a "phosphor"

- For almost **100** years cathodoluminescence was used for making displays, your classical *cathode ray tube* or TV tube that was recently replaced by flat screen displays like LCD's.
- We still need cathodoluminescence for electron microscope (*TEM* type) screens for obvious reasons. But we can also look at the cathodoluminescence that specimen produce in the electron beam of an *SEM*; then we use it as an analytical tool. The "phosphors" tend to be large bandgap semiconductors line **ZnO**, again for (hopefully) obvious reasons; if color is needed like for an (old fashioned) TV, more involved different materials emitting red, green, and blue are necessary.

Mechanoluminescence, resulting from any mechanical action on a solid, can be subdivided into:

- **Triboluminescence** (one of my favorites). Take a lump of sugar, go into a dark room, wait a while so your eyes adapt, and than violently crush that sugar between your teeth (keeping your lips open, so you can see your teeth and the sugar in a mirror). Blue flashes of light will be generated! Triboluminescence happens quite a lot, it is just not seen at daylight conditions because it is typically weak. It happens when bonds in a material are broken because that material is scratched, crushed, or rubbed. The effect is not really understood; separation and reunification of electrical charges seems to play a role; and there might simply be sparking in large electric fields.
- **Fractoluminescence**, pretty much the same thing as triboluminescence.
- **Piezoluminescence**, is produced by the action of pressure on, well, piezoelectric materials. It's different from the above because you do not need to break bonds but just some elastic deformation.

Photoluminescence is caused by moving electrons to energetically higher levels through the absorption of photons.

- It's easily done in semiconductors with photons of energy larger than the bandgap, radiating recombination channels than produce bandgap light. The solar cell picture above gives an example. It was irradiated with very intense red light; the luminescence occurs in the IR.

Radioluminescence is generated when some materials are exposed to ionizing radiation like α, β or γ rays.

- It was used, even so that is hard to believe nowadays, to make watch dials glow in the around 1960. A mixture of radium and copper-doped zinc sulfide was used to paint the dials, giving a greenish glow. Radioluminescence is also used for detecting ionizing radiation, especially γ rays, by analyzing the light flashed generated when a γ quant is absorbed in certain crystals.

Sonoluminescence is the emission of short bursts of light from imploding bubbles in a liquid when excited by sound.

- It had been known for some time but produced a lot of excitement in 1989 when stable single-bubbles could be produced that emit intense light in very short bursts. The mechanism is not really clear at present and rather outlandish explanations (e.g. an analogy to radiation from black holes or nuclear fusion taking place)) have been proposed by well know scientists. It appears likely, however, that the bubbles "just" produce an extremely hot plasma (up to 20.000 K) for very short times.

Thermoluminescence, describes the phenomenon that certain crystalline materials emit light when heated that is *not* black body radiation or incandescence

- What happens is that previously absorbed energy from, e.g., electromagnetic or ionizing radiation was stored (meaning the excited electrons just stay on upper energy levels), typically at defects. It is released in the form of light if some thermal energy allows the excited electrons to overcome the energy barrier that kept then "up".
- Thermoluminescence is an important method for dating some archeological artifacts. Ceramic parts being buried receive some ionizing dose from radioactive elements in the soil or from cosmic rays that is proportional to their age - and so is the intensity of the luminescence produced upon heating.

History of the Laser

▶ Lasers are one big success story - and an embodiment of **Feynmans** famous sentence:

- *"There are certain situations in which the peculiarities of quantum mechanics can come out in a special way on a large scale".*
- It is *not* necessary to to emphasize how important Lasers are to all of us - to the scientist, the patient in a hospital, the consumer listening to her discs, the supermarket cashier, the geometer - and just about everybody else. It should be quite clear.
- It is, however, *quite* necessary to emphasize that Lasers (and, of course, all of solid state electronics), are purely *quantum mechanical devices*, because this is simply not known to the "people in the street" (including those in suits; and this says something about the state of general eduction in this country).

▶ Here are a few milestones in the development of the Laser.

▶ The first major date is **1916**, when Albert **Einstein** introduced the concept of *stimulated emission*.

▶ It took till **1953** to demonstrate stimulated emission experimentally. This was achieved by **Gordon**, **Zeiger** and **Townes**.

- The researchers used the two lowest vibrational energy levels of ammonia molecules and obtained a very narrow emission line at **12.6 mm**, i.e. in the "micro"wave region.
- This is where the name "*Maser*" comes from.
- Follow-up on the "Maser" finally led to Nobel prizes shared between *Townes* and the Russians **Basov** and **Prokhorov** in **1964**.

▶ Meanwhile, however, **Maiman** produced the first *optical Maser*, as the Laser was originally called in **1960**.

- The light came from Cr^{3+} ions fixed in an Al_2O_3 crystal - a **ruby** in other words, at a wavelength of **694,3 nm**.
- Pumping took place with an intense light source, and the Laser only emitted a short pulse.

▶ **1962** the first semiconductor Laser was produced, by *N.G. Basov*.

Advanced (vertical side text)

Einstein and the Photoelectric Effect

Hit any materials *hard enough* with some light and you will kick out some electrons. That phenomena is known as the *photoelectric effect*, and electrons emitted in this manner may be referred to as "photoelectrons".

- The photoelectric effect was first observed by **Heinrich Hertz** in **1887**; the phenomenon was also known as the "**Hertz effect**" then.

- The strange thing was that *"hard enough"* did not mean, as one would have expected, *plenty of light* or, more precisely, large amplitudes of the light waves. Instead it meant *high enough frequency*. No amount of light with a frequency just a little bit too small could produce any photoelectrons, while light with a frequency just above a critical values did - even at low intensities. It was just *how many* electrons were released per second that depended on the intensity but not *if* electrons were kicked out.

- There is simply no way to understand this observation employing only "wave" optics. You need the photon concept.

Much later (in **1921**) the **Compton effect** once more demonstrated that light with high frequencies (also called **X**-rays or γ radiation) shows distinct particle properties when encountering atoms.

- The Hertz effect had to wait for **18** years before an explanation was found in **1905** by Albert**Einstein**. He solved the apparent paradox by introducing what we now call the "**photon**", a discrete quanta of light, somewhat particle-like, instead of a continuous wave.

- Einstein based his approach on **Max Planck's** theory of black-body radiation. He postulated that the energy in each quantum of light was equal to the frequency multiplied by a constant, later called Planck's constant. A photon above a threshold frequency then has the required energy to eject a single electron, creating the observed effect

Multiple Choice Test zu

5.1.1 Basic Optics

Start Multiple Choice

Multiple Choice Test zu

5.1.4 Energy Flow, Poynting Vector and Polarization

Start Multiple Choice

Multiple Choice Test zu

5.1 Basic Optics

Start Multiple Choice

Multiple Choice Test zu

5.2.1 Interaction between Light and Matter

Start Multiple Choice

Multiple Choice Test zu

5.2.2 Fresnel Equations

Start Multiple Choice

Multiple Choice Test zu

5.2.3 The Complex Index of Refraction

Start Multiple Choice

Exercise 5.1.1 Derivation of Snellius Law

Consider the situation as given in the figure.
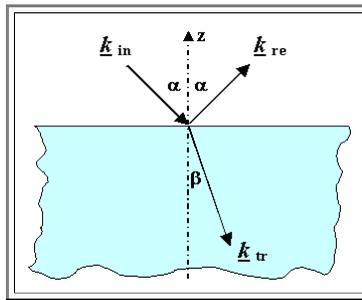
- Assume that the light consists of a stream of photons, all with the same energy **h**ν and with momentums given by $\hbar\,\underline{k}$.
- Assume a certain flux of photons (= number per second and cm^2) given by I_{in}, I_{ref}, and I_{tr}. Also assume that you have "mirror" reflection, i.e. both angles are identical (= α)

Show that you obtain $I_{tr} = I_{in} - I_{ref}$ and Snellius law (**sin**α**/sin**β = **n**) from energy and momentum conservation.

Link to the solution

Exercise 5.1.2 Energy, Field Strength and Photons

You have a **LED** as a light source that emits a monochromatic light beam with wave length (in air) of λ **= 500 nm**. The light is generated in a very small volume ("point source") and spreads out in a cone that illuminates a circle with radius **1 cm** at a distance of **10 cm** on some white paper. The **LED** has an over-all or plug efficiency of **50 %** and is driven at **2V** with **20 A**.

Here are the questions:

- How much power in **W/m²** flows into the paper?
- How does that number compare with the light power coming from the sun at "AM 1" conditions (High noon, equation, no clouds)? You're supposed to know this basic number in some "simple number approximation".
- How many photons per second must hit the piece of paper, if we discuss the energy flux now in the particle picture?
- What kind od field strength would we have on the paper? Consider first that the light beam is fully coherent, next that the photons are completely uncorrelated.

If we now follow the light beam back to its source, we can obtain a few more insights:

- What does the number of photons produced per second tell you about recombination rates, carrier densities, and current densities in the semiconductor?

Link to the solution

Exercise 5.1.3 Polarization

A light beam with intensity I_0 passes through *one* ideal polarizer.

1. How does the intensity relate to the electrical field strength?
2. The incoming ("input") light beam is unpolarized. How large is the intensity at the output?
3. Does this intensity change if you rotate the polarizer around the axis coinciding with the propagation direction of the light = optical axis?
4. The incoming light beam is **100 %** linearly polarized. How large is the intensity on the output as a function of the angle between polarization direction of the light and polarizing direction of the polarizer.

A light beam with intensity I_0 first passes through one ideal polarizer, and then through a *second* one. Both polarizers can be rotated freely around the optical axis.

1. The light beam is unpolarized. How large is the intensity on the output if both ideal polarizers are in parallel?
2. The light beam is unpolarized. How large is the intensity on the output if the ideal polarizers are "crossed", i.e. their polarization directions are at right angles?
3. The light beam is **100 %** linearly polarized. How large is the intensity of the output as a function of the variable angle α between the two polarizing directions of the polarizers and the fixed angle β between the polarization direction of the light and the first polarizer it encounters? Note that in this case you rotate the *second* polarizer.
4. Does the result for the question above change if you rotate the *first* polarizer and keep the second one at the fixed angle β?
5. Is for all of the above the direction of the light paths always reversible as stated before?

Now consider a system with *two* fixed *crossed* polarizers and a *third* one that can be rotated *in between* the two crossed ones.

1. The incoming light beam is unpolarized. How large is the intensity of the output as a function of the variable angle α between the first (fixed) and the third polarizer that can be rotated?
2. The incoming light beam is **100 %** linearly polarized. How large is the intensity on the output as a function of the variable angle α between the first (fixed) and the third polarizer (can be rotated) considering that the angle β between the incoming light polarization and the polarization direction of the first polarizer is fixed at a value β?

Good schematic drawings with proper values at the axes are sufficient

Link to the solution

Exercise 5.2.1 Fresnel Cofficients

Consider an unpolarized light beam hitting the surface of an isotropic glass with **n = 1,5** at right angles (α = **0°**).
Hint: to avoid **0/0** situations consider small α and β with **cos**α, β **= 1**.

- Derive the simplified Fresnel equations <u>as given in the script</u> for α **= 0°**

- How much of the light will be reflected?

- What is the phase relation between incoming, reflected and transmitted light?

- How does the beam leave the crystal (Intensity and polarization)

- Now consider these questions for some polarization of the incoming light.

Link to the solution

Exercise 5.2.2 Fresnel Equations and LEDs

Consider a simple light emitting diode, working as shown schematically. All the light is generated in a small volume as indicated, and we assume that the semiconductor is fully transparent (which is not really true). The index of refraction of semiconductors is rather large; you may take it to be **n = 3**
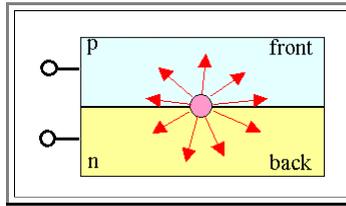
- The simple question is: How much (in **%**) of the light generated is transmitted through the front (upper) surface?
- Suggest measures to improve that percentage.

Link to the solution

Exercise 5.2.3 Attenuation of Light

Starting <u>from</u>

$$E_x = \exp-\frac{\omega \cdot \kappa \cdot x}{c} \cdot \exp[\,i \cdot (k_x \cdot x - \omega \cdot t)]$$

Decreasing **Plane wave**
amplitude

- Give maximal values for κ (damping constant, attenuation index, extinction coefficient) if a penetration depth of **1m**, **100 m 10^4 m** is specified for the light intensity.
- Calculate what that would mean in terms of *only* ϵ'' or *only* ϵ''.
- Discuss the results with respect to the complex index of refractions of **Si** and the dielectric function of **GaAs** as given in this <u>link</u> for frequencies above and below the band gap (after you located the band gap by straight thinking).

Link to the <u>solution</u>

Exercise 5.2.4 Fresnel Equations and Polarization

Consider to use the Brewster angle for obtaining polarized light.

Design a polarizer from some common optical materials that works in this way . Discuss its performance.

Hint 1: Redraw the <u>graphs for the Fresnel equations</u> in chapter 2.2.2 for the transmitted beam.
Hint 2. Consider to use your design for, e.g., polarizing sun glasses.

Illustration

Link to the **solution**

Exercise 5.2.5 Rayleigh Scattering

Illustration

1. Generate some numbers for *scattering cross sections* using the equations given.

Look, e.g., at "air" molecules including some water vapor or ozone as scatterers, and wave lengths from the **IR** to the **UV**.

2. Derive or justify the equation $l_{sc} = 1/n\sigma$. Show that for air we get $l_{sc} (=) 160 \cdot \lambda^4$ if we give l in **km** and λ in **µm**.

Hint 1: Consider the particle to be a cube with σ being the area of a face. All light will be scattered if the total area of those cubes projected on a surface perpendicular to the light beam covers that area completely. λ_{sc} then is the length of a cube that contains enough particle to meet that condition.
Hint 2: The volume of an air "molecule" can be estimated from the fact the *liquid* air has about the same density as water.

3. Generate some numbers for penetration depths in air. How thick does an ozone (O_3) layer with a density $n_{Oz} = 8\ ml/m^3$ have to be to absorb most of the incoming ultraviolet radiation (especially "**UV-B**"; $\lambda \approx 300\ nm$)

Link to the solution

Solution to Exercise 5.1-1: Derivation of Snellius Law

Show that you obtain $l_{tr} = l_{in} - l_{ref}$ and Snellius law ($\sin\alpha/\sin\beta = n$) from energy and momentum conservation

Illustration
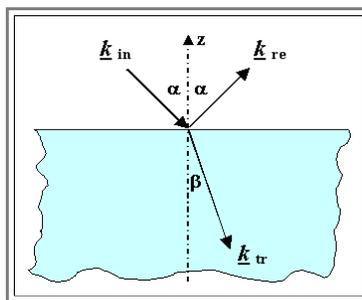
Solution:

- The intensity I of the beams is given by their power (energy /t) which is given by the nunber of photons/s in the beams: E_{in}, E_{re}, E_{tr}. Everythin always per cm^2 but that is not important for what follows.
- *Energy conservation* demands

$$E_{in} = E_{re} + E_{tr}$$

$$E_{tr} = E_{in} - E_{re}$$

$$l_{tr} = l_{in} - l_{re}$$

Looking at the **x**-component of the momentum **p** and considering that the wavelength in the material is λ/n we have

$$|p_{z,\,in}| = l_{in}\hbar k_{in} \cdot \sin\alpha = \frac{l_{in}\hbar \cdot 2\pi \cdot \sin\alpha}{\lambda}$$

$$|p_{z,\,re}| = l_{re}\hbar k_{re} \cdot \sin\alpha = \frac{l_{re}\hbar \cdot 2\pi \cdot \sin\alpha}{\lambda}$$

$$|p_{z,\,tr}| \quad l_{tr}\hbar k_{tr} \cdot \sin\beta = \frac{l_{tr}\hbar \cdot 2\pi \cdot \sin\beta \cdot n}{\lambda}$$

- *Momentum conservation* demands that $p_{z,\,in} + p_{z,\,tr} - p_{z,\,re} = 0$, or

$$l_{in}\sin\alpha + l_{tr}\sin\beta \cdot n - l_{re}\sin\alpha = 0$$

- Substituting $l_{re} = l_{in} - l_{tr}$ leads straight ot

$$n = \frac{\sin\alpha}{\sin\beta}$$

Solution to Exercise 5.1-2 Energy, Field strength and Photons

▶ You have a **LED** as a light source that emits a monochromatic light beam with wave length (in air) of λ = **500 nm**. The light is generated in a very small volume ("point source") and spreads out in a cone that illuminates a circle with radius **1 cm** at a distance of **10 cm** on some white paper. The **LED** has an over-all or plug efficiency of **50 %** and is driven at **2V** with **20 A**.

> **Question 1:** How much power in **W/m^2** flows into the paper?

Total power = UI = **40 W**
Light power = **50 %** of total power = **20 W**
Light flux = 20 W / πr^2 = **6,37 W/cm^2**
With **eV** instead of **Ws = J** and **1 J = 1 Ws = 6,24 · 10^{18} eV** we have
Light flux = **3,97 · 10^{19} eV / s · cm^2**.

> **Question 2:** How does that number compare with the light power coming form the sun at "AM 1" conditions (High noon, equation, no clouds)? You're supposed to know this basic number in some "simple number approximation".

▶ The sun at a cloudless day at high noon at the equator delivers about **1 kW/m^2 = 1000 / 10000 W/cm^2 = 0,1 W/cm^2**
Our LED thus delivers a very high (and unrealistic) intensity of **63,7** times more than the sun.

> **Question 3:** How many photons per second must hit the piece of paper if we discuss the energy flux now in the particle picture?

▶ A wavelength of **500 nm** corresponds to a photon with energy $h\nu$ = hc/λ = {(4,1356 · 10^{-15}) · (3 · 10^{17})} / 500 eVs · nms^{-1} · nm^{-1} = **2,48 eV**. The necessary **3,97 · 10^{19} eV/scm^2** thus corresponds to **3,97 · 10^{19} / 2,48 = 1,60 · 10^{19} photons/scm^2** Since we need to illuminate an area of **3,14 cm^2**, we need **5,03 · 10^{19} photons/s**

> **Question 4:** What kind of field strength would we have on the paper? Consider first that the light beam is fully coherent, next that the photons are completely uncorrelated.

▶ The energy flux in the light beam is given by
$\langle S \rangle$ = $\frac{1}{2}E_0H_0$ = $(E_0)^2/(Z_W)$ = **6,37 W/cm^2**

> For the electrical field strength in a fully coherent wave we have
> E_0 = $[Z_W \cdot 6,37 \text{ VW/Acm}^2]^{1/2}$ = $[377 \cdot 6,37 \text{ V}^2/\text{cm}^2]^{1/2}$ = **49 V/cm**
> That is a rather low field strength.

> A completely incoherent light consists of waves with all kinds of phases and all kinds of directions of the electrical field vectors. The total field strength then is a vector sum that tends to average to zero.
> We might assume that the number of independent "waves" equal the number of photons. That gives the field strength per wave = photon to E_{Ph} = 49 / 5,03 · 10^{19} V/cm = **9,74 · 10^{-19} V/cm**. That is, of course, a rather meaningless number.

> If we consider that a photon delivers an energy of **2 eV** to an area of about **1 µm^2** within **1 ns**, we would get $E_{Ph} \approx$ **3,5 V/cm**, which is more like it but still more or less nonsense.

> How about assuming that the *energy* W_{Ph} of a photon (= **2,5 eV**, for example) is contained in a volume of λ^3 (1 µm)^3, for example). We then have roughly W_{Ph} = $(\frac{1}{2}\epsilon_0 \cdot E^2)/\lambda^3$ from the relation between energy *density* and field strength E.
> Going through the numbers we obtain $E_{Ph} \approx$ **3.000 V/cm**. That is a number one could live with.

> **Question 5:** What does the number of photons produced per second tell you about recombination rates, carrier densities, and current densities in the semiconductor?

▶ We need at least a recombination rate of R = **5,03 · 10^{19} s^{-1}** between electrons and holes that produces light. If we loose some of the light, the rate must be higher. The recombination ot the carriers take place in a device volume V_{Dev} given by lateral area F of the device times length l_{Rec} of the recombination zone; V_{Dev} = $F \cdot l_{Rec}$.

> We can always express the specific recombination rate per **cm^{-3}** by R = 5,03 · 10^{19}/s · $F \cdot l_{Rec}$ = n/τ with n = surplus carrier density, τ = carrier life time $\approx$ **1 ns**.

> The necessary carrier density that must be supplied by the current is thus n = $R\tau / F \cdot l_{Rec}$. If we assume F = 10^{-4} cm^2, τ = 10^{-9} s; we have n = **5,03 · 10^{18} m^{-3}** which looks reasonable.

▶ The total current I was **20 A**. The current *density* j for a device with cross-sectional area F of **10^{-4} cm^{2}cm^2** is
j = **2 · 10^5 A/cm^2** which is a bit on the high side..

● The number N_e of electrons (or holes "on the other side") that we inject is N_e = 20 (C/s) / 1,6 · 10^{-19} C = 1,25 · 10^{20} s^{-1}. If half of this electrons recombine and produce light (we assumed an efficiency of 50 %), we have 6,25 · 10^{19} electrons per second available for this, a number that matches quite *fortuitously* with the required 5,03 · 10^{19} s^{-1}. Or maybe, it's not that *accidental*?

Solution to Exercise 5.1-3 Polarization

1. question:: A light beam with intensity I_0 passes through *one* ideal polarizer.

1. How does the intensity relate to the electrical field strength?

Intensity neasures the energy or better *power flux* contained in the light. it is propotional to the square of the electrical field strength

2. The incoming ("input") light beam is unpolarized. How large is the intensity at the output?

It's obviously $I_0/2$. Considering this picture we can decompose the light beam in two fully polarized beams, each having the intensity $I_0/2$. The polarizer takes out one of the beams and $I_0/2$ remains.

3. Does this intensity change if you rotate the polarizer around the axis coinciding with the propagation direction of the light = optical axis?

No.

4. The incoming light beam is **100 %** linearly polarized. How large is the intensity on the output as a function of the angle between polarization direction of the light and polarizing direction of the polarizer.

The intensity must betwen **100 %** and **0 %** of the incoming intensity for an angle of $\alpha = $ **0°** and **90°** , respectively.
For an arbitrary angle α we have a field strength $E(\alpha) = E_0 \cdot \cos\alpha$; the transmitted intensity then scales with $(\cos\alpha)^2$ between the extremes.

2. question: A light beam with intensity I_0 first passes through one ideal polarizer, and then through a *second* one. Both polarizers can be rotated freely around the optical axis.

1. The light beam is unpolarized. How large is the intensity on the output if both ideal polarizers are in parallel?

It's still $I_0/2$ because two polarizers in parallel behave just like one.

2. The light beam is unpolarized. How large is the intensity on the output if the ideal polarizers are "crossed", i.e. their polarization directions are at right angles?

The intensity is zero.

3. The light beam is **100 %** linearly polarized. How large is the intensity of the output as a function of the variable angle α between the two polarizing directions of the polarizers and the fixed angle β between the polarization direction of the light and the first polarizer it encounters? Note that in this case you rotate the *second* polarizer.

After passing through the first polarizer, the intensity is $I_0 \cdot (\cos\beta)^2$. After passing through the second polarizer we have $I = I_0 \cdot (\cos\beta)^2 \cdot (\cos\alpha)^2$

4. Does the result for the question above change if you rotate the *first* polarizer and keep the second one at the fixed angle β?

No.

5. Is for all of the above the direction of the light paths always reversible as stated before?

Tricky. Just reversing arrowheads obviously doesn't work.
You can't get a higher intensity from a lower one as you would if you just reverse the sign of the Poyntig vector as shown below.
Using a mirror symmetry works but this trival.

Starting situation.

Reversing vector signs does not work.

Mirroring works.
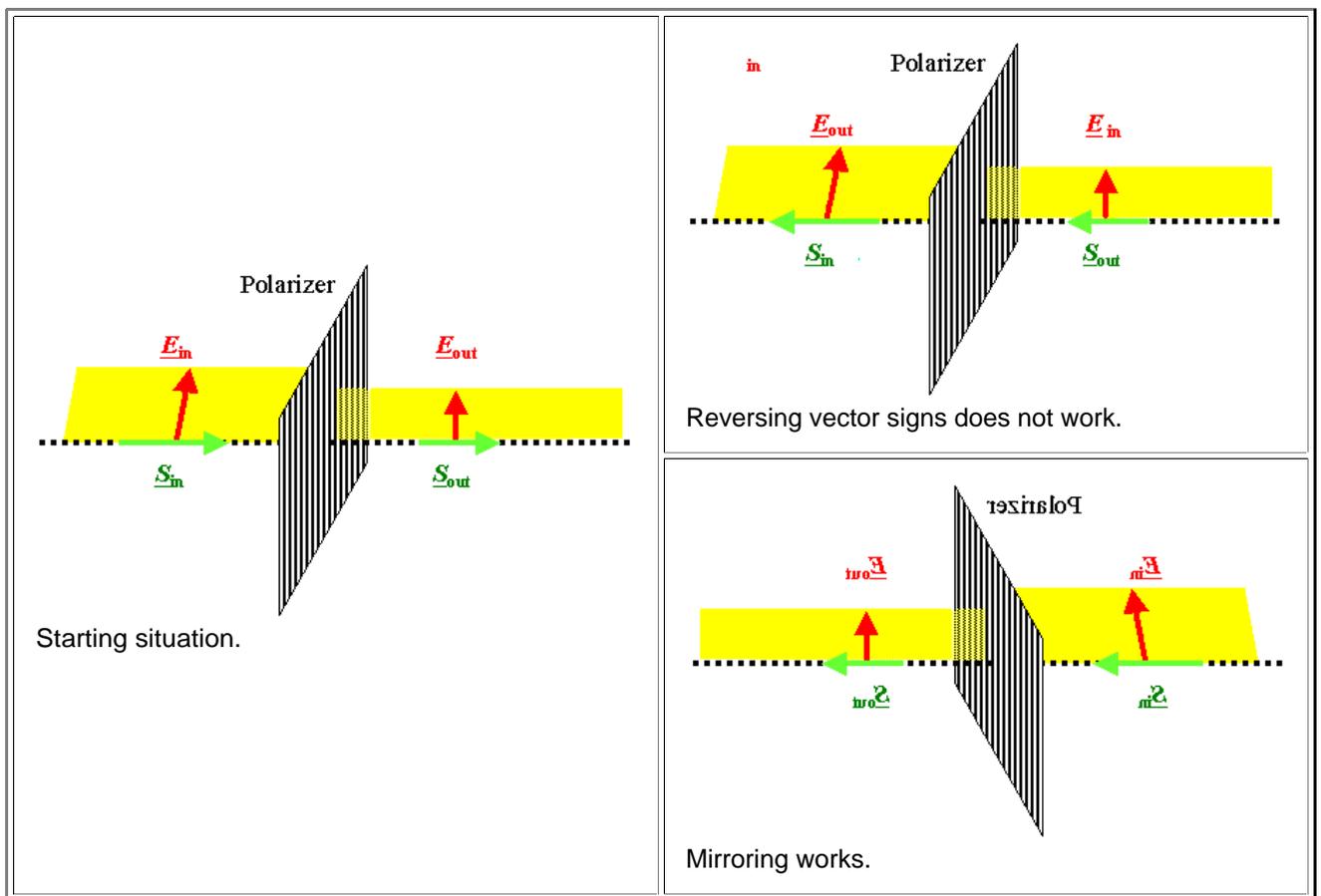
3. question: Now consider a system with *two* fixed *crossed* polarizers and a *third* one that can be rotated *in between* the two crossed ones.

1. The incoming light beam is unpolarized. How large is the intensity of the output as a function of the variable angle α between the first (fixed) and the third polarizer that can be rotated?

After the first polarizer, the intensity is $I_0/2$; it decreases with $(\cos\alpha)^2$ behind the third polarizer that can be rotated . The second (fixed and crossed with respect to the first one) polarizer transmits components with a $(\sin\alpha)^2$ dependence (make a simple drawing and do the geometry!) so all together we have for the output

$$I(\alpha) = \frac{I_0}{2} \cdot (\cos\alpha)^2 \cdot (\sin\alpha)^2$$

$I(\alpha = 0°) = 0$
$I(\alpha = 45°)$ = maximal value = $(I_0/2) \cdot 0,25$
$I(\alpha = 90°) = 0$

2. The incoming light beam is **100 %** linearly polarized. How large is the intensity on the output as a function of the variable angle α between the first (fixed) and the third polarizer (can be rotated) considering that the angle β between the incoming light polarization and the polarization direction of the first polarizer is fixed at a value β?

As above except that the intensity after the first polarizer is now $I_0 \cdot (\cos\beta)^2$

Solution to Exercise 5.2-1: Fresnel Coefficients

Consider an unpolarized light beam hitting the surface of an isotropic glass with **n = 1,5** at right angles (α = 0°).

Derive the simplified Fresnel equations as given in the script for α = 0°

Setting the cosines to **1** in the **TE** or **TM** case gives

TE case	TM case
$E_{ref} = E_{in} \cdot \dfrac{\sin\beta - \sin\alpha}{\sin\beta + \sin\alpha}$	$E_{ref} = E_{in} \cdot \dfrac{\sin\beta - \sin\alpha}{\sin\beta + \sin\alpha}$
Division by $\sin\beta$; $\sin\alpha/\sin\beta = n$	
TE and TM	
$E_{ref} = - E_{in} \cdot \dfrac{n - 1}{n + 1}$ *q.e.d*	

- There is thus no difference between the **TE** and **TM** case.

How much of the light will be reflected?

We can use the simple equations for perpendicular incidence from above, re-written for intensities:

$$\frac{I_{ref}}{I_{in}} = \left(\frac{n-1}{n+1}\right)^2$$

- The intensity of the reflected light is thus

$$I_{ref} = I_{in} \left(\frac{n-1}{n+1}\right)^2$$

$$= I_{in} \left(\frac{0{,}5}{2{,}5}\right)^2$$

$$= 0{,}04 \; I_{in}$$

- The reflected intensity is thus **4 %** of the incoming intensity.

What is the phase relation between incoming, reflected and transmitted light?

To answer that question we must look at the field strength. There is a *minus sign* and the the phase of the reflected beam thus is phase-shifted by **180 ° = π**

How does the beam leave the crystal (Intensity and polarization)?

For the transmitted beam we have the simple relation $I_{tr} = I_{in} − I_{re}$. The intensity of transmitted beam thus is **96 %** of the incoming intensity for an optical material with $n = 1,5$.

- At the "exit" from the $n = 1,5$ optically dense material to the $n = 1$ less dense material α and β interchange their role or $\sinβ/\sinα = n = 1,5$ now. Taking this into account we get the same equations for the perpendicular incidence as above but without the *"−" (minus) sign* for the field strengths. This means that **96 % of 96 % (= 92,16 %)** of the incoming beam exits the optical material.

- How about phases? Looking at the original Fresnel equations for the electrical field strength we see that in both the **TE** and **TM** case there is no sign and therefore phase jump for the *transmitted* wave for all angles (since α, β **<= 90 º** in all cases). For the reflected wave at the optically less dense medium (the wave reflected back into the interior of the optical material) there isn't a phase change either because the minus sign is no longer there.

Now consider these questions for some polarization of the incoming light.

No difference since we have the same equations for both the **TE** and **TM** case.

# Solution to Exercise 5.2-2: Fresnel Equations and LEDs

Illustration

Consider a simple light emitting diode schematically working as shown. All light is generated in a small volume as indicates an we assume that the semiconductor is fully transparent (which is not really true). The index of refraction of semiconductors is rather large; you may take it to be **n=3**
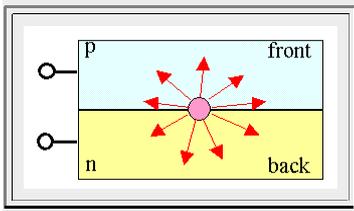
The simple question is: How much (in **%**) of the light generated is transmitted through the front (upper) surface?

First, it is important to make a drawing of the situation with respect to reflected and transmitted light:
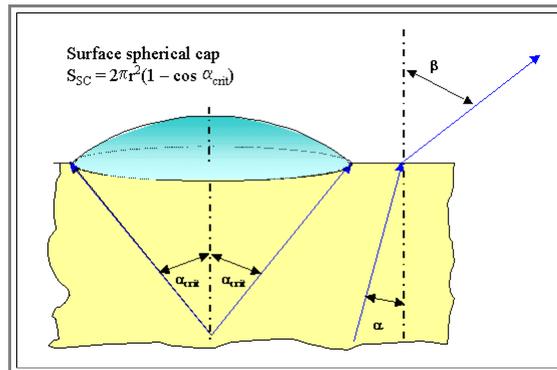
- Light hitting the surface with an angle larger than α_{crit} will suffer total reflection and remains inside the semiconductor where it is eventually absorbed. Light emitted "downwards might get out of the semiconductor but is absorbed in the housing.

- It follows that only light paths' inside the cone with opening angle **2α_{crit}** will get out to where we need them. Steric analysis gives the surface of the spherical cap belonging to the **2α_{crit}** cone to $S_{SC}=2\pi r^2 \cdot (1 - \cos\alpha_{crit})$.

- The percentage of the light intensity I_{out} coming out relative to the light intensity I_{total} emitted into the full sphere with surface **4πr^2** is thus

$$\frac{I_{out}}{I_{total}} = \frac{2\pi r^2 \cdot [1 - \cos(\alpha_{crit})]}{4\pi r^2} = \frac{1 - \cos(\alpha_{crit})}{2}$$

Now we need to determine α_{crit}. Looking a the picture (and reversing the arrows) we write Snellius' law for total reflection as $\sin\beta=n \cdot \sin\alpha_{crit}=1$. It follows that $\alpha_{crit}=n^{-1} \cdot \arcsin\beta$.

- For **n=3** this gives us **19,47 °**. Insertion gives I_{out}/I_{total}=**0,0286**

- Only **2.86 %** of the radiation produced is useful**!!!!!** We have a severe problem here!

Suggest measures to improve that percentage.

The *first* thing to do is to add a reflector at the bottom. That doubles the efficiency.
Second thing to do is to put a material with an **n** between that of air and the semiconductor on top. This increases α_{crit} and the beneficial effect is clear from the picture .
Third thing to do is to shape you semiconductor in such a way that reflected light will get out after a second internal reflection. An inverted pyramid is a good shape for this (can you see why?).
Fourth.....
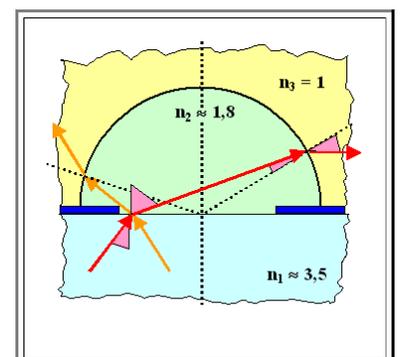
You get, maybe, the idea, that **LEDs** with an overall efficiency (electrical energy in / light energy out) of **50 %** are not made "just so" but contain a lot of engineering.

Solution to 5.2-3: Attenuation of Light

Illustration

$$E_x = \exp{-\frac{\omega \cdot \kappa \cdot x}{c}} \cdot \exp[i \cdot (k_x \cdot x - \omega \cdot t)]$$

Decreasing amplitude   **Plane wave**

Starting from the equation at right

Give maximal values for κ (damping constant, attenuation index, extinction coefficient) if a penetration depth of **1m**, **100 m** **10^4 m** is specified for the light intensity.

The *intensity* **I** is proportional to E^2 and thus decreases with $I = I_0 \exp - \{(2\omega \cdot \kappa \cdot x)/c\}$.

- We have $\ln\{I/I_0\} = -(2\omega \cdot \kappa \cdot x)/c$, or $\kappa = -\{c/2x\omega\}\ln\{I/I_0\}$.
  If we assume that $I/I_0 = 1/e$ as a measure of still sufficient intensity, we have $\ln(I/I_0) = -1$ and thus obtain $\kappa = (1/x) \cdot (c/2\omega)$.
- Taking $\omega = 10^{16}$ s^{-1} we have $c/2\omega = 3 \cdot 10^8$ ms^{-1} / $2 \cdot 10^{16}$ s^{-1} = $1,5 \cdot 10^{-8}$ m. We arrive at the following table for $\kappa = 1,5 \cdot 10^{-8}/x$ for **x** given in meter (m).

x	κ
1 m	$1,5 \cdot 10^{-8}$
100 m	$1,5 \cdot 10^{-10}$
10^4 m	$1,5 \cdot 10^{-12}$

Obviously the imaginary part of the complex index of refraction needs to be rather small if we talk about "optics". If it would be **1,5**, i.e. about the same as the real part, the penetration depth would be 10^{-8} **m = 10 nm**—we have a rather opaque material in this case.

Calculate what that would mean in terms of *only* ϵ'' or *only* ϵ''.

From the definition of the complex index of refraction we have $2\kappa^2 = (\epsilon'^{\,2} + \epsilon''^{\,2})^{1/2} - \epsilon'$.

- For small ϵ'' we can develop the square root into a series and get $(\epsilon'^{\,2} + \epsilon''^2)^{1/2} \approx \epsilon' + \epsilon''/2\epsilon'$.
- This leads to $\epsilon'' = 4\kappa^2 \cdot \epsilon'$. For a reasonable $\epsilon' = 2$ (giving **n = 1,4**) we have $\epsilon'' = 1,8 \cdot 10^{-15}$; $1,8 \cdot 10^{-29}$, $1,8 \cdot 10^{-23}$ for the three κ values from above.

To relate κ to the static conductivity σ_{static} we use the equation $\sigma_{DK}/2\epsilon_0\omega = n\kappa$, which gives

- $\sigma_{DK} = 2n\kappa\epsilon_0\omega = \kappa \cdot 2,8 \cdot 10^{16} \cdot 8,854 \cdot 10^{-12}$ s^{-1}A·s·V^{-1}m^{-1} = $\kappa \cdot 2,48 \cdot 10^5$ $(\Omega m)^{-1}$
- Plugging in the numbers for κ we get

κ	σ_{DK} [Ωm^{-1}]	$\rho_{DK} = 1/\sigma_{DK}$ [Ω**cm**]
$1,5 \cdot 10^{-8}$	$3.72 \cdot 10^{-3}$	$2,69 \cdot 10^4$
$1,5 \cdot 10^{-10}$	$3.72 \cdot 10^{-5}$	$2,69 \cdot 10^6$
$1,5 \cdot 10^{-12}$	$3.72 \cdot 10^{-7}$	$2,69 \cdot 10^8$

- For large penetration depth we need pretty good DC insulators. For **100 km = 10^5 m**, something a fibre optic cable should do, we have about **3 GΩcm**, a number that is not too large for good insulators like glass. Of course, the static resistivity is not the only reason for absorption.

Discuss the results with respect to the complex index of refractions of **Si** and the dielectric function of **GaAs** as given in this link for frequencies above and below the band gap (after you located the band gap by straight thinking)

First we look at the GaAS curves with a linear scale.

- For energies below the bandgap, GaAs is transparent and both κ and ϵ'' should be zero. That's the case for energies **< 1.4 eV** as easily seen in the *linear* GaAs diagrams with the **eV** scale. The correct value is **1,42 eV**, so optical measurements do provide easy access to bandgaps.

Or do they?

- The log scale picture for Si is better suited to look for precise numbers. First, we need to convert wavelengths to **eV** via $E = h\nu = hc/\lambda$. A big drop in κ for Si occurs around **400 nm** , corresponding to $(4,1356 \cdot 10^{-15}$ **eVs** $\cdot 3 \cdot 10^8$ **ms**$^{-1})/400 \cdot 10^{-9}$ **m = 3,1 eV** **????**

- Aha! We are far off the proper value of **1,1 eV**. Obviously the proper wavelength must be about twice as large, **847 nm** to be exact. That is still in the infrared as is should be since **Si** wafers are not transparent to any visible wavelength.

- What we learn is that the bandgap does show up very clearly in optical measurement (look at the linear scales!) but that precision measurements might be more tricky than naively expected.

Solution to 5.2-4: Fresnel Equations and Polarization

Consider to use the Brewster angle for obtaining polarized light.
Design a polarizer from some common optical materials that works in this way . Discuss its performance.
Hint 1: Redraw the graphs for the Fresnel equations in chapter 2.2.2 for the transmitted beam.
Consider to use your design for, e.g., polarizing sun glasses.

Illustration

Here is the redrawn graph:
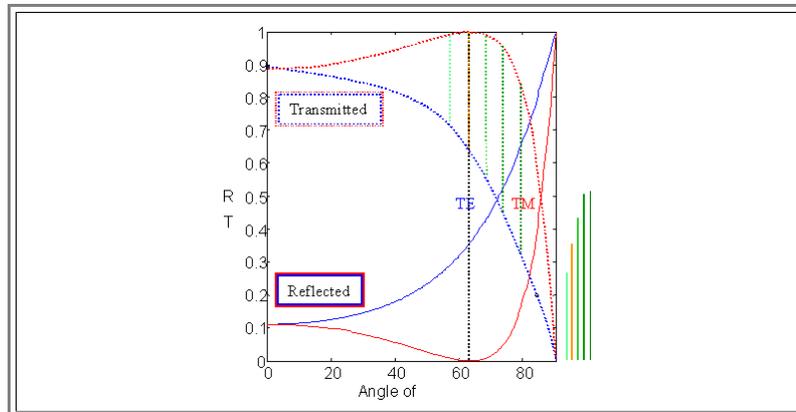
- If we hit the surface of our ***n = 2*** material under the **Brewster angle** (about **63$^{\mathbf{o}}$**; otherwise calculate it (with some effort) from the Fresnel equations for ***E*$_{\mathbf{ref}}$ (TM) = 0**), there will be no reflection for the **TM** polarization. Reflected light thus will be fully **TE** polarized.

- That implies that *all* of the reflected light is *TE polarized*. The intensity relation between **TE** and **TM** for the *reflected* light is (nominally) something : nothing or just very large. The intensity difference is just **TE**

- The intensity difference between **TE** and **TM** for the *transmitted* light is no longer zero as for the incident light, but **TM - TE > 1**. The length of the green-yellow bars above indicates this. They are shown on the right in their length relation and one realizes that a maximum **TM - TE** occurs at angles somewhat larger than the Brewster angle.

This gives us an idea for a polarizer design:
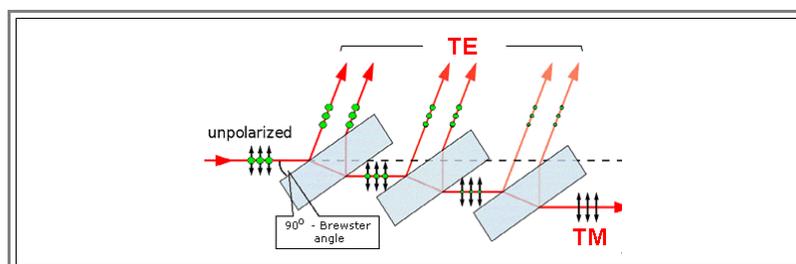

Looks ***awkward*** because it is awkward.

- Why don't we operate in reflections? Because it is not very practical. There is very shallow incidence, and since light beams not coming form Lasers are never exactly parallel or monochromatic, there is always some "noise" in the degree of polarization. The intensity is also quite low because most of the incoming light is transmitted. Switching several Brewster polarizers in series as shown would be better (but not good). However, the beams reflected form several "mirrors" will not form a good image.

- So we look at the transmitted beam. more than three plates would then be needed to produce a decent polarization in transmission. Of course, if you intend to work in transmission, you would go off the Brewster angle a bit to optimize the **TE – TM** difference.

As far as polarizing sun glasses are concerned: forget any "Brewster" construction for obvious reasons.

- So what are Brewster polarizers good for? Well, consider that you need to polarize **far UV** light or some other weird but sometimes necessary wavelength. Than Brewster polarizers might be your *only* option!

Solution to Exercise 5.2-3: Rayleight Scattering

Sorry. No solution offered here
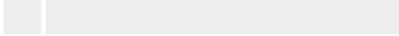
Illustration

Complex Index of Refraction of Silicon and GaAs

Here is the complex index of referaction of *Silicon* (from Handbook of Optical Constants of Solids (E.D. Palik))
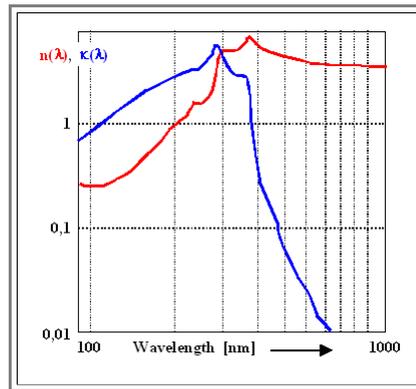
- Note that the imaginary part κ increases as soon as the wavelength is small enough for band-to-band absorption processes; i.e. $h \cdot \nu > E_G$ applied (with E_G = band gap).

Here is the dielectric function and the complex index of refraction for GaAs.

- Note that several groups actually *calculated* those curves and that they match rather nicely with the measured values.

GaAs: Real and imaginary part of ε

GaAs: Real (n) and imaginary (κ) part of the index of refraction

Source: A B Djurisic and E H Li
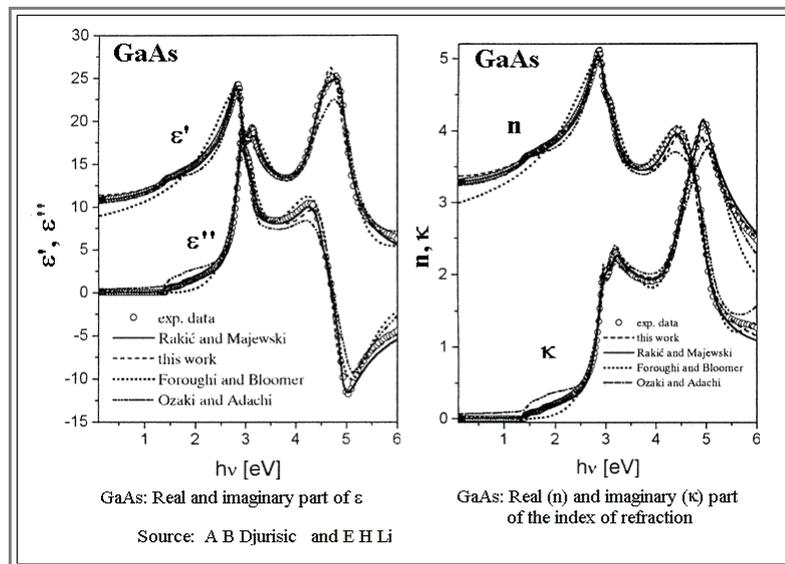
Polarizing IR and UV Light

Here's a good book dealing (in parts) with the topic.

Illustration
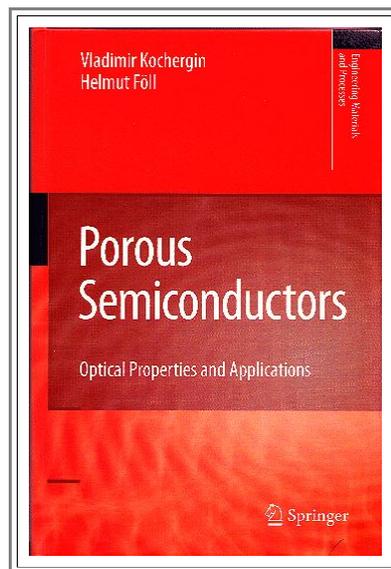
Just kidding. Or may be not?
Anyway, I just never got around to write this module in the proper way. And the book does contain some information to the topic