3.8 Summary: Dielectrics

The dielectric constant ϵ_r "somehow" describes the interaction of dielectric (i.e. more or less insulating) materials and electrical fields; e.g. via the equations ⇒

- $\underline{D}$ is the **electrical displacement** or **electrical flux density**, sort of replacing $\underline{E}$ in the Maxwell equations whenever materials are encountered.
- C is the capacity of a parallel plate capacitor (plate area A, distance d) that is "filled" with a dielectric with ϵ_r
- n is the index of refraction; a quantity that "somehow" describes how electromagnetic fields with extremely high frequency interact with matter.
  in this equaiton it is assumed that the material has no magnetic properties at the frequency of light.

$$\underline{D} = \epsilon_0 \cdot \epsilon_r \cdot \underline{E}$$

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

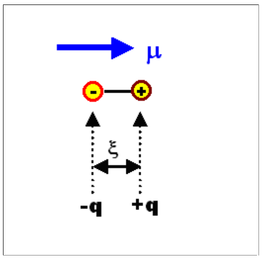
$$n = (\epsilon_r)^{1/2}$$

Electrical fields inside dielectrics polarize the material, meaning that the vector sum of electrical dipoles inside the material is no longer zero.

- The decisive quantities are the dipole moment $\underline{\mu}$, a vector, and the Polarization P, a vector, too.
- Note: The dipole moment vector points from the negative to the positive charge - contrary to the electrical field vector!
- The dipoles to be polarized are either already present in the material (e.g. in $\mathbf{H_2O}$ or in ionic crystals) or are induced by the electrical field (e.g. in single atoms or covalently bonded crystals like **Si**)
- The dimension of the polarization $\underline{P}$ is **[C/cm^2]** and is indeed identical to the net charge found on unit area ion the surface of a polarized dielectric.

$$\underline{\mu} = q \cdot \underline{\xi}$$

$$\underline{P} = \frac{\Sigma \underline{\mu}}{V}$$



The equivalent of "Ohm's law", linking current density to field strength in conductors is the Polarization law:

- The decisive material parameter is χ ("kee"), the **dielectric susceptibility**
- The "classical" flux density D and the Polarization are linked as shown. In essence, $\underline{P}$ only considers what happens in the material, while D looks at the total effect: material plus the field that induces the polarization.

$$\underline{P} = \epsilon_0 \cdot \chi \cdot \underline{E}$$

$$\epsilon_r = 1 + \chi$$

$$\underline{D} = \underline{D}_0 + \underline{P} = \epsilon_0 \cdot \underline{E} + \underline{P}$$

Polarization by necessity moves masses (electrons and / or atoms) around, this will not happen arbitrarily fast.

- ϵ_r or χ thus must be functions of the frequency of the applied electrical field, and we want to consider the whole frequency range from **RF** via **HF** to light and beyond.

$\epsilon_r(\omega)$ is called the "**dielectric function**" of the material.

The tasks are:

- Identify and (quantitatively) describe the major mechanisms of polarization.
- Justify the assumed linear relationship between P and χ.
- Derive the dielectric function for a given material.

(Dielectric) polarization mechanisms in dielectrics are all mechanisms that

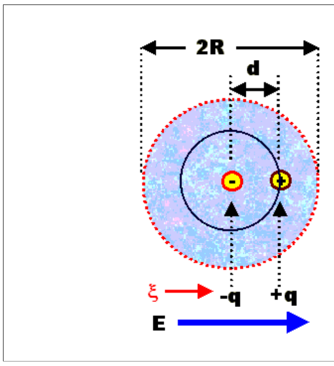
1. Induce dipoles at all (always with $\boldsymbol{\mu}$ in field direction)
   ⇒ Electronic polarization.
2. Induce dipoles already present in the material to "point" to some extent in field direction.
   ⇒ Interface polarization.
   ⇒ Ionic polarization.
   ⇒ Orientation polarization.

Quantitative considerations of polarization mechanisms yield

- **Justification (and limits) to the $\underline{P} \propto \underline{E}$ "law"**
- **Values for χ**
- **$\chi = \chi(\omega)$**
- **$\chi = \chi$(structure)**

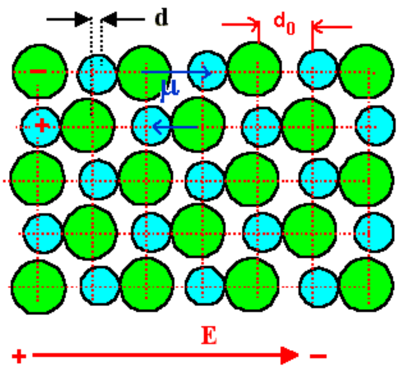
Electronic polarization describes the separation of the centers of "gravity" of the electron charges in orbitals and the positive charge in the nucleus and the dipoles formed this way. it is always present

- It is a very weak effect in (more or less isolated) atoms or ions with spherical symmetry (and easily calculated).
- It can be a strong effect in e.g. covalently bonded materials like **Si** (and not so easily calculated) or generally, in solids.



Ionic polarization describes the net effect of changing the distance between neighboring ions in an ionic crystal like **NaCl** (or in crystals with some ionic component like **SiO$_2$**) by the electric field

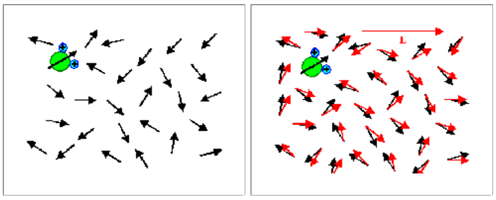
- Polarization is linked to bonding strength, i.e. Young's modulus **Y**. The effect is smaller for "stiff" materials, i.e. **P ∝ 1/Y**



Orientation polarization results from minimizing the free enthalpy of an ensemble of (molecular) dipoles that can move and rotate freely, i.e. polar liquids.

- It is possible to calculate the effect, the result invokes the Langevin function

$$L(\beta) = \coth(\beta) - \frac{1}{\beta}$$



Without field **With field**

- In a good approximation the polarization is given by ⇒

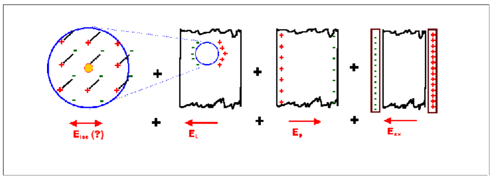
$$\langle P \rangle = \frac{N \cdot \mu^2 \cdot E}{3kT}$$

The induced dipole moment **μ** in all mechanisms is proportional to the field (for reasonable field strengths) at the location of the atoms / molecules considered.

$$\underline{\mu} = \alpha \cdot E_{loc}$$

- The proportionality constant is called polarizability α; it is a microscopic quantity describing what atoms or molecules "do" in a field.
- The local field, however, is not identical to the macroscopic or external field, but can be obtained from this by the Lorentz approach
- For isotropic materials (e.g. cubic crystals) one obtains

$$E_L = \frac{P}{3\epsilon_0}$$

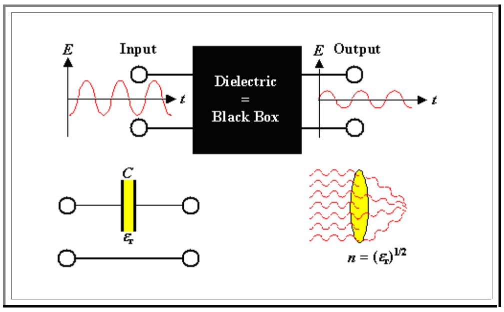


$$E_{loc} = E_{ex} + E_{pol} + E_L + E_{near}$$

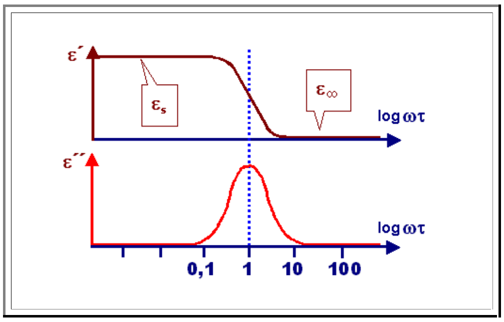
- Knowing the local field, it is now possible to relate the microscopic quantity α to the macroscopic quantity ε or ϵ_r via the Clausius - Mosotti equations ⇒
  - While this is not overly important in the engineering practice, it is a momentous achievement. With the Clausius - Mosotti equations and what went into them, it was possible for the first time to understand most electronic and optical properties of dielectrics in terms of their constituents (=atoms) and their structure (bonding, crystal lattices etc.)
  - Quite a bit of the formalism used can be carried over to other systems with dipoles involved, in particular magnetism=behavior of magnetic dipoles in magnetic fields.

$$\frac{N \cdot \alpha}{3\,\epsilon_0} = \frac{\epsilon_r - 1}{\epsilon_r + 2} = \frac{\chi}{\chi + 3}$$

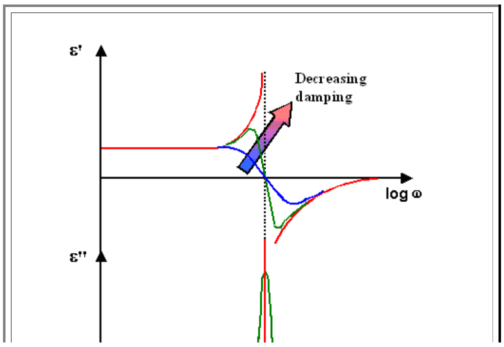
- Alternating electrical fields induce alternating forces for dielectric dipoles. Since in all polarization mechanisms the dipole response to a field involves the movement of masses, inertia will prevent arbitrarily fast movements.
  - Above certain limiting frequencies of the electrical field, the polarization mechanisms will "die out", i.e. not respond to the fields anymore.
  - This might happen at rather high (=optical) frequencies, limiting the index of refraction $n = (\epsilon_r)^{1/2}$



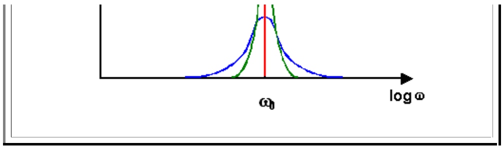
- The (only) two physical mechanisms governing the movement of charged masses experiencing alternating fields are relaxation and resonance.
- *Relaxation* describes the decay of excited states to the ground state; it describes, e.g., what happens for orientation polarization after the field has been switched off.
  - From the "easy to conceive" time behavior we deduce the frequency behavior by a Fourier transformation
  - The dielectric function describing relaxation has a typical frequency dependence in its real and imaginary part ⇒



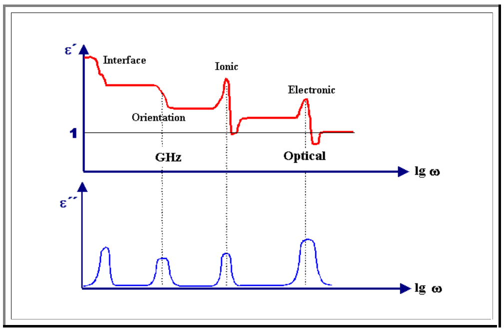
- Resonance describes anything that can be modeled as a mass on a spring - i.e. electronic polarization and ionic polarization.
  - The decisive quantity is the (undamped) resonance frequency $\omega_0 = (k_S / m)^{1/2}$ and the "friction" or damping constant k_F
  - The "spring" constant is directly given by the restoring forces between charges, i.e. Coulombs law, or (same thing) the bonding. In the case of bonding (ionic polarization) the spring constant is also easily expressed in terms of Young's modulus ***Y***. The masses are electron or atom masses for electronic or ionic polarization, respectively.



- The damping constant describes the time for funneling off ("dispersing") the energy contained in one oscillating mass to the whole crystal lattice. Since this will only take a few oscillations, damping is generally large.
- The dielectric function describing relaxation has a typical frequency dependence in its real and imaginary part ⇒
  The green curve would be about right for crystals.



- The complete frequency dependence of the dielectric behavior of a material, i.e. its dielectric function, contains all mechanisms "operating" in that material.
  - As a rule of thumb, the critical frequencies for relaxation mechanisms are in the **GHz** region, electronic polarization still "works" at optical (**10^{15} Hz**) frequencies (and thus is mainly responsible for the index of refraction).
  - Ionic polarization has resonance frequencies in between.
  - Interface polarization may "die out" already a low frequencies.
- A widely used diagram with all mechanisms shows this, but keep in mind that there is no real material with all 4 major mechanisms strongly present!
  ⇒



- A general mathematical theorem asserts that the real and imaginary part of the dielectric function cannot be completely independent
  - If you know the complete frequency dependence of either the real or the imaginary part, you can calculate the complete frequency dependence of the other.
  - This is done via the Kramers-Kronig relations; very useful and important equations in material practice.
    ⇒

$$\epsilon'(\omega) = \frac{-2\,\omega}{\pi} \int_0^\infty \frac{\omega^* \cdot \epsilon''(\omega^*)}{\omega^{*2} - \omega^2} \cdot d\omega^*$$

$$\epsilon''(\omega) = \frac{2\,\omega}{\pi} \int_0^\infty \frac{\epsilon'(\omega^*)}{\omega^{*2} - \omega^2} \cdot d\omega^*$$

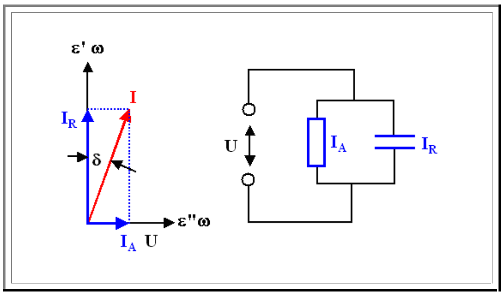
- The frequency dependent current density ***j*** flowing through a dielectric is easily obtained. ⇒
  - The in-phase part generates active power and thus heats up the dielectric, the out-of-phase part just produces reactive power
  - The power losses caused by a dielectric are thus directly proportional to the imaginary component of the dielectric function

$$j(\omega) = \frac{dD}{dt} = \epsilon(\omega) \cdot \frac{dE}{dt} = \underbrace{\omega \cdot \epsilon'' \cdot E(\omega)}_{\text{in phase}} + \underbrace{i \cdot \omega \cdot \epsilon' \cdot E(\omega)}_{\text{out of phase}}$$

$$L_A = \text{power turned into heat} = \omega \cdot |\epsilon''| \cdot E^2$$

- The relation between active and reactive power is called "tangens Delta" (**tg(δ)**); this is clear by looking at the usual pointer diagram of the current

$$\frac{L_A}{L_R} := \text{tg}\,\delta = \frac{I_A}{I_R} = \frac{\epsilon''}{\epsilon'}$$



  - The pointer diagram for an *ideal* dielectric **$\sigma(\omega=0)=0$**can always be obtained form an (ideal) resistor ***R***(ω) in parallel to an (ideal) capacitor ***C***(ω).
  - ***R***(ω) expresses the apparent conductivity **$\sigma_{DK}(\omega)$** of the dielectric, it follows that

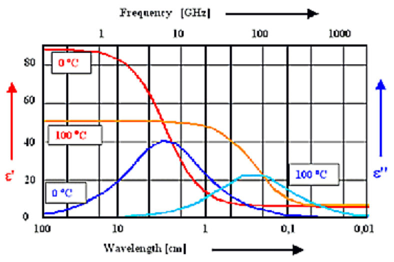
$$\boxed{\sigma_{DK}(\omega) \; = \; \omega \cdot \epsilon''(\omega)}$$

- For a *real* dielectric with a non-vanishing conductivity at zero (or small) frequencies, we now just add another resistor in parallel. This allows to express *all* conductivity effects of a real dielectric in the imaginary part of its (usually measured) dielectric function via

$$\boxed{\epsilon'' = \frac{\sigma_{total}}{\omega}}$$

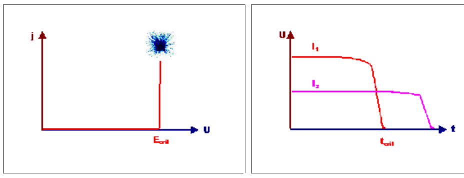
  - We have no *all* materials covered with respect to their dielectric behavior - in principle even metals, but then resorting to a dielectric function would be overkill.

- A good example for using the dielectric function is "dirty" water with a not-too-small (ionic) conductivity, commonly encountered in food.



  - The polarization mechanism is orientation polarization, we expect large imaginary parts of the dielectric function in the **GHz** region.
  - It follows that food can be heated by microwave (ovens)!

- The first law of materials science obtains: At field strengths larger than some critical value, dielectrics will experience (destructive) electrical breakdown
  - This might happen suddenly (then calls break-down) , with a bang and smoke, or
  - it may take time - months or years - then called failure.
  - Critical field strength may vary from **< 100 kV/cm** to **> 10 MV / cm**.



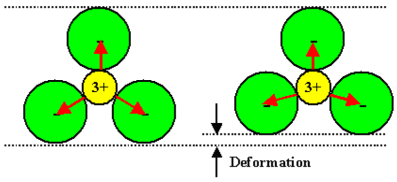
- Highest field strengths in practical applications do not necessarily occur at high voltages, but e.g. in integrated circuits for very thin (a few **nm**) dielectric layers
  - Properties of thin films may be quite different (better!) than bulk properties!

Example 1: TV set, **20 kV** cable, thickness of insulation=**2 mm.** ⇒ ***E*=100 kV/cm**
Example 2: Gate dielectric in transistor, **3.3 nm** thick, **3.3 V** operating voltage. ⇒ ***E*=10 MV/cm**

- Electrical breakdown is a major source for failure of electronic products (i.e. one of the reasons why things go "kaputt" (=broke)), but there is no simple mechanism following some straight-forward theory. We have:
  - *Thermal breakdown*; due to small (field dependent) currents flowing through "weak" parts of the dielectric.
  - *Avalanche breakdown* due to occasional free electrons being accelerated in the field; eventually gaining enough energy to ionize atoms, producing more free electrons in a runaway avalanche.
  - *Local discharge* producing micro-plasmas in small cavities, leading to slow erosion of the material.

  - *Electrolytic breakdown* due to some ionic micro conduction leading to structural changes by, e.g., metal deposition.

- Polarization ***P*** of a dielectric material can also be induced by mechanical deformation ***e*** or by other means.
  - *Piezo electric materials* are anisotropic crystals meeting certain symmetry conditions like crystalline quartz (**SiO_2**): the effect is linear.
  - The effect also works in reverse: Electrical fields induce mechanical deformation
  - Piezo electric materials have many uses, most prominent are quartz oscillators and, recently, fuel injectors for Diesel engines.

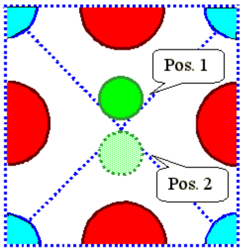


P = const. · e

- *Electrostriction* also couples polarization and mechanical deformation, but in a quadratic way and only in the direction "electrical fields induce (very small) deformations".
  - The effect has little uses so far; it can be used to control very small movements, e.g. for manipulations in the **nm** region. Since it is coupled to electronic polarization, many materials show this effect.

$$e = \frac{\Delta l}{l} = \text{const} \cdot E^2$$

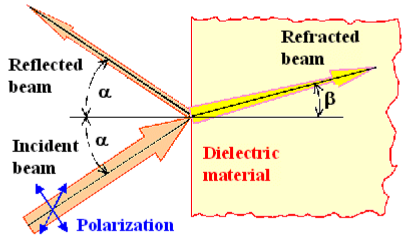
- *Ferro electric materials* posses a permanent dipole moment in any elementary cell that, moreover, are all aligned (below a critical temperature).
  - There are strong parallels to ferromagnetic materials (hence the strange name).
  - Ferroelectric materials have large or even very large (**$\epsilon_r > 1.000$**) dielectric constants and thus are to be found inside capacitors with high capacities (but not-so-good high frequency performance)



$BaTiO_3$ unit cell

- *Pyro electricity* couples polarization to temperature changes; *electrets* are materials with permanent polarization, ... There are more "curiosities" along these lines, some of which have been made useful recently, or might be made useful - as material science and engineering progresses.

- The basic questions one would like to answer with respect to the optical behaviour of materials and with respect to the simple situation as illustrated are:
  1. How large is the fraction ***R*** that is reflected? **1 – *R*** then will be going in the material.
  2. How large is the angle β, i.e. how large is the refraction of the material?
  3. How is the light in the material absorbed, i.e. how large is the absorption coefficient?
  - Of course, we want to know that as a function of the wave length λ or the frequency **ν=c/λ**, the angle α, and the two basic directions of the polarization (



- All the information listed above is contained in the complex index of refraction ***n**** as given ⇒

$n=(\epsilon_r)^{1/2}$	Basic definition of "normal" index of refraction ***n***
$n^* = n + i \cdot \kappa$	Terms used for complex index of refraction ***n**** ***n***=real part κ=imaginary part
$n^{*2}=(n + i\kappa)^2 = \epsilon' + i \cdot \epsilon''$	Straight forward definition of ***n****

- Working out the details gives the basic result that
  - Knowing ***n***=real part allows to answer question **1** and **2** from above via "Fresnel laws" (and "Snellius' law", a much simpler special version).
  - Knowing κ=imaginary part allows to answer question **3** ⇒

$$E_x = \underbrace{\exp - \frac{\omega \cdot \kappa \cdot x}{c}}_{\text{Amplitude: Exponential decay with } \kappa} \cdot \underbrace{\exp[\, i \cdot (k_x \cdot x - \omega \cdot t)]}_{\text{"Running" part of the wave}}$$

- Knowing the dielectric function of a dielectric material (with the imaginary part expressed as conductivity σ_{DK}), we have (simple) optics completely covered!
  - If we would look at the tensor properties of ε, we would also have crystal optics (=anisotropic behaviour; things like birefringence) covered.
  - We must, however, dig deeper for e.g. non-linear optics ("red in - green (double frequency) out"), or new disciplines like quantum optics.

$$n^2 = \frac{1}{2}\left(\epsilon' + \left(\epsilon'^{\,2} + \frac{\sigma_{DK}{}^2}{4\epsilon_0{}^2\omega^2} \right)^{½} \right)$$

$$\kappa^2 = \frac{1}{2}\left(-\,\epsilon' + \left(\epsilon'^{\,2} + \frac{\sigma_{DK}{}^2}{4\epsilon_0{}^2\omega^2} \right)^{½} \right)$$

Questionaire

Multiple Choice questions to all of 3