Dielectric Solids / Insulators

Part 1: general review

- **Introduction into the physics of dielectrics.**
- **ii. Electric dipole - definition.**
- **a) Permanent dipole moment,**
- **b) Induced dipole moment.**
- **iii. Polarization and dielectric constant.**
- **iv. Types of polarization**
- **a) electron polarization,**
- **b) atomic polarization,**
- **c) orientation polarization,**
- **d) ionic polarization.**

Ancient times

1745 first capasitor constructed by Cunaeus and Musschenbroek
And is known under name of Leyden jar

1837 Faraday studied the insulation material, which he called the ***dielectric***

Middle of 1860s Maxwell’s unified theory of electromagnetic phenomena

$$\varepsilon = n^2$$

1887 Hertz

1847 Mossotti

1897 Drude

1879 Clausius

Lorentz-Lorentz

1912 Debye

Internal field

Dipole moment

Maxwell Equations and Polarization

СГС	СИ
$\operatorname{rot} \boldsymbol{H} = \frac{4\pi}{c}\boldsymbol{j} + \frac{1}{c}\frac{\partial}{\partial t}(\boldsymbol{E} + 4\pi\boldsymbol{P});$	$\operatorname{rot} \boldsymbol{H} = \boldsymbol{j} + \frac{\partial}{\partial t}(\varepsilon_0\boldsymbol{E} + \boldsymbol{P});$
$\operatorname{rot} \boldsymbol{E} = -\frac{1}{c}\frac{\partial \boldsymbol{B}}{\partial t};$	$\operatorname{rot} \boldsymbol{E} = -\frac{\partial \boldsymbol{B}}{\partial t};$
$\operatorname{div}(\boldsymbol{E} + 4\pi\boldsymbol{P}) = 4\pi\rho;$	$\operatorname{div}(\varepsilon_0\boldsymbol{E} + \boldsymbol{P}) = \rho;$
$\operatorname{div} \boldsymbol{B} = 0;$	$\operatorname{div} \boldsymbol{B} = 0.$

The polarization P is defined as the dipole moment per unit volume, averaged over the volume of a cell. The total dipole moment is defined as

$$\boldsymbol{d} = \sum_i e_i \boldsymbol{r}_i$$

If the net charge of the system is zero, the electric moment is independent of the choice of the origin.

Each microscopic dipole ***p*** creates the electric field

$$(\text{СГС}) \quad \boldsymbol{E}(\boldsymbol{r}) = \frac{3(\boldsymbol{p}\cdot\boldsymbol{r})\,\boldsymbol{r} - r^2\boldsymbol{p}}{r^5}; \qquad (\text{СИ}) \quad \boldsymbol{E}(\boldsymbol{r}) = \frac{3(\boldsymbol{p}\cdot\boldsymbol{r})\,\boldsymbol{r} - r^2\boldsymbol{p}}{4\pi\varepsilon_0 r^5}$$

The vector fields *E* and *D*.

The polarization proportional to the field strength. The proportional factor χ *is called the* ***dielectric susceptibility.***

$$\boldsymbol{D} = \boldsymbol{E} + 4\pi \boldsymbol{P} = (1 + 4\pi\chi)\boldsymbol{E} = \varepsilon \boldsymbol{E} \qquad (1.19)$$

in which ε is called the ***dielectric permittivity***. It is also called the dielectric constant, because it is independent of the field strength. It is, however, dependent on the frequency of applied field, the temperature, the density (or the pressure) and the chemical composition of the system.

For very high field intensities the proportionality no longer holds.→**Dielectric saturation and non-linear dielectric effects.**

$$\boldsymbol{P} = \chi \boldsymbol{E} \qquad (1.21)$$

For non-isotropic dielectrics, like most solids, liquid crystals, the scalar susceptibility must be replaced by a tensor.

Hence, the permittivity **ε** must be also be replaced by a tensor:

$$D_x = \varepsilon_{11}E_x + \varepsilon_{12}E_y + \varepsilon_{13}E_z$$

$$D_y = \varepsilon_{21}E_x + \varepsilon_{22}E_y + \varepsilon_{23}E_z \qquad (1.22)$$

$$D_z = \varepsilon_{31}E_x + \varepsilon_{32}E_y + \varepsilon_{33}E_z$$

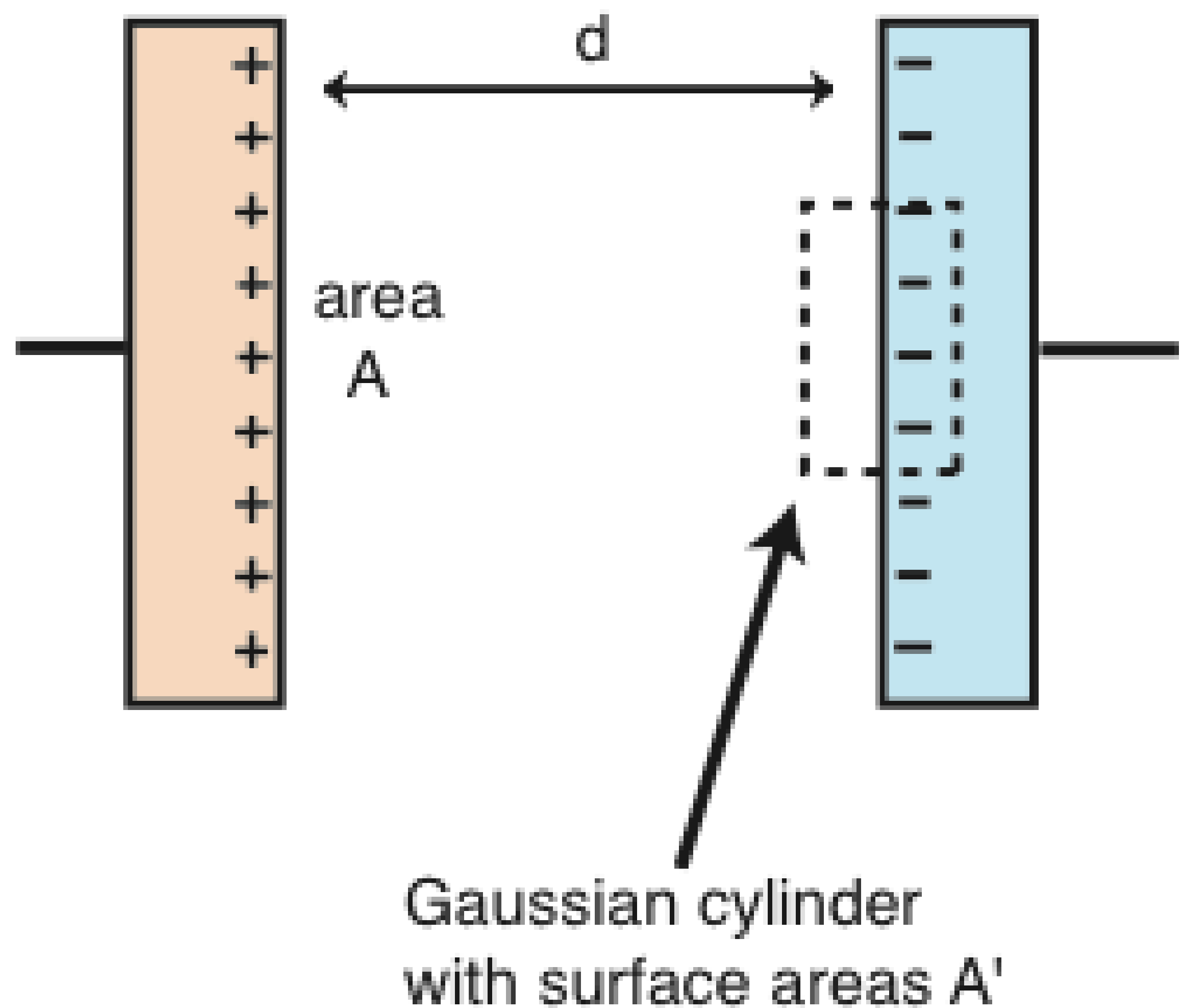
How to measure the dielectric susceptibility?

Plane-plate capacitor

$$\oint \boldsymbol{\mathcal{E}} d\mathbf{A} = \oint \mathcal{E}_{\perp} dA = \frac{Q_{encl}}{\epsilon_0}$$

$$\mathcal{E} A' = \frac{\sigma A'}{\epsilon_0}$$

$$\mathcal{E} = \frac{\sigma}{\epsilon_0}$$



$$C = Q\frac{1}{U} = \sigma A \frac{1}{\mathcal{E} d}$$

$$= \sigma A \frac{\epsilon_0}{\sigma d} = \frac{A\epsilon_0}{d}$$

- High capacitance can be achieved by large A or small d.
- Both approaches give rise to several problems.

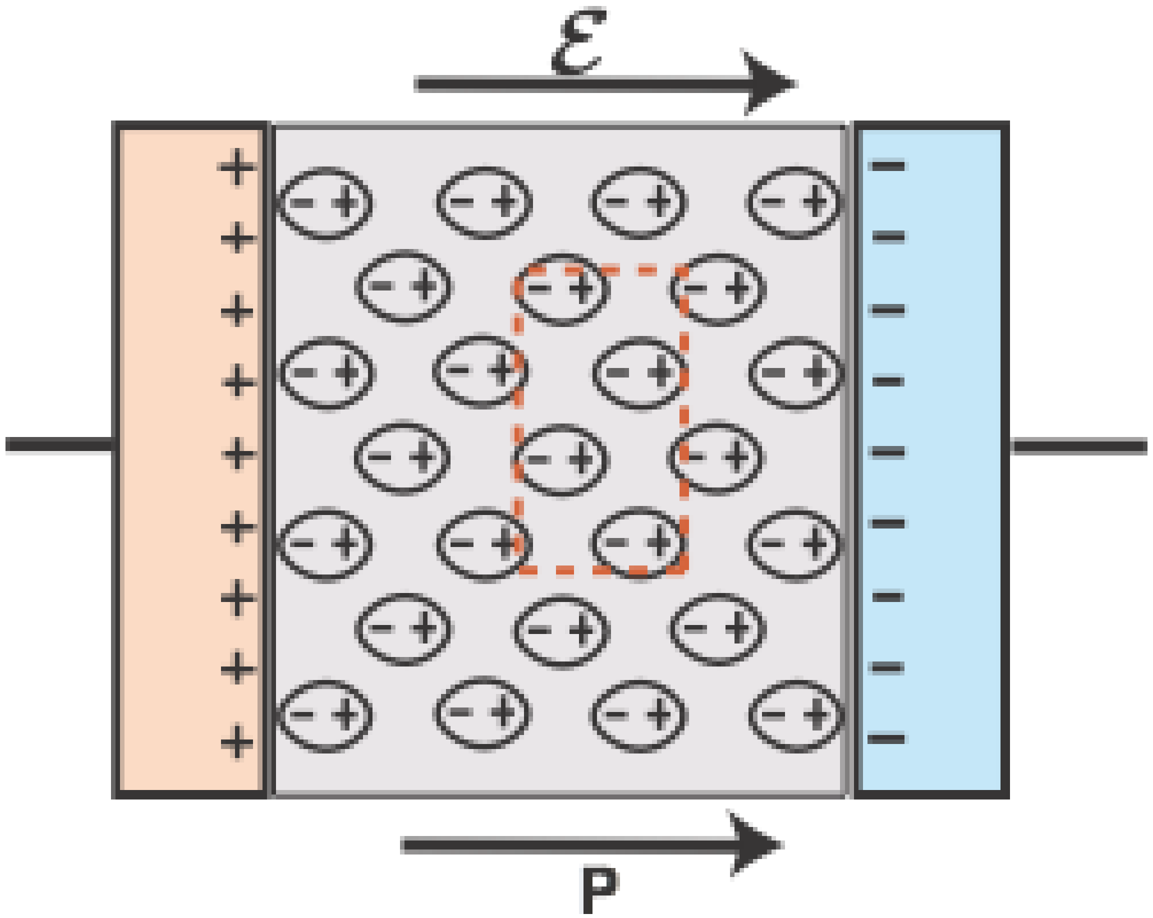
Plane-plate capacitor with dielectric

polarizable units:

$$p = q\delta$$

for the solid

$$P = \frac{N}{V} q\delta$$



- For any macroscopic Gaussian surface inside the dielectric, the incoming and outgoing electric field is identical (because the total average charge is 0).
- The only place where something macroscopically relevant happens are the surfaces of the dielectric.

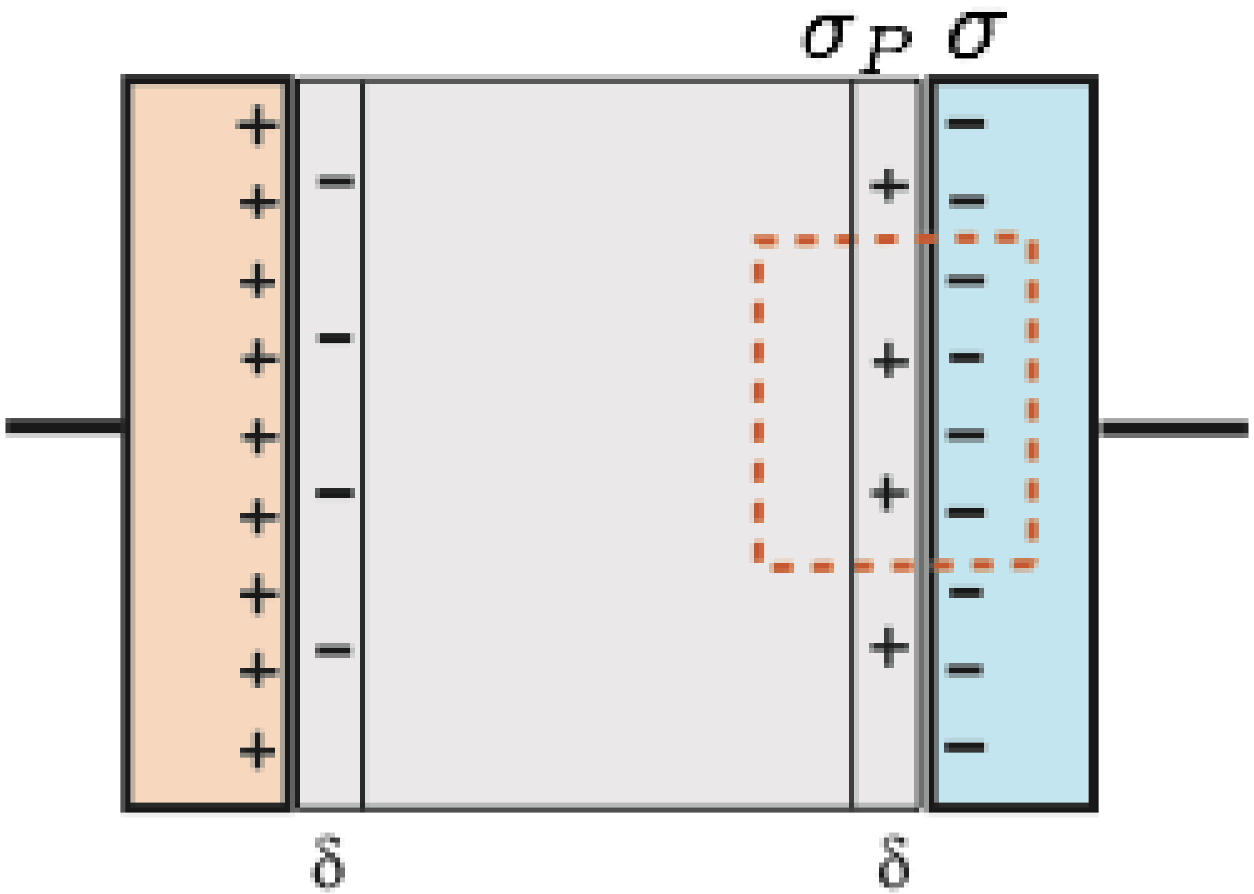
Plane-plate capacitor with dielectric

$$Q_P = A\frac{N}{V}q\delta$$

$$\sigma_P = \frac{N}{V}\delta q = P$$

$$\mathcal{E} = \frac{\sigma - \sigma_P}{\epsilon_0} = \frac{1}{\epsilon_0}(\sigma - P)$$

$$P = \epsilon_0 \chi_e \mathcal{E}$$



$$\mathcal{E} = \frac{\sigma}{\epsilon_0(1+\chi_e)} = \frac{\sigma}{\epsilon_0\epsilon}$$

$\varepsilon = 1 + \chi_e$

capacitance increase by a factor of ε

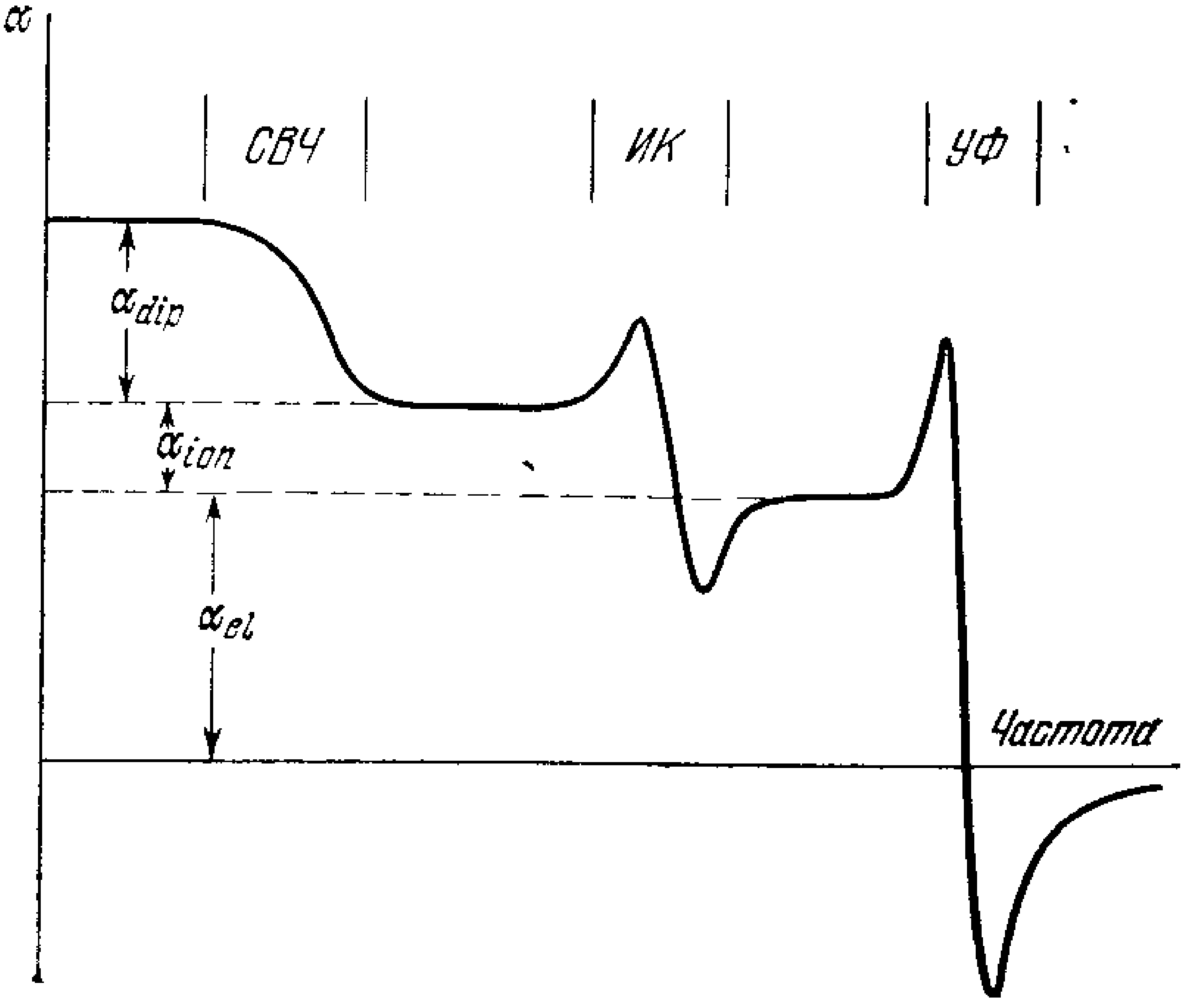
$$C = \frac{A\epsilon_0(1+\chi_e)}{d} = \frac{\varepsilon\varepsilon_0 A}{d}$$

so the E-field decreases by a factor of ε

The dielectric constant

material	dielectric constant ε
vacuum	1
air	1.000576 (283 K, 1013 hPa)
rubber	2.5 - 3.5
SiO_2	3.9
glass	5-10
NaCl	6.1
ethanol	25.8
water	81.1
strontium titanate	350

Frequency dependence of dielectric susceptibility



Types of polarization

For isotropic systems and leaner fields in the case of static electric fields

$$P = \frac{\varepsilon - 1}{4\pi} E$$

The applied electric field gives rise to a dipole density

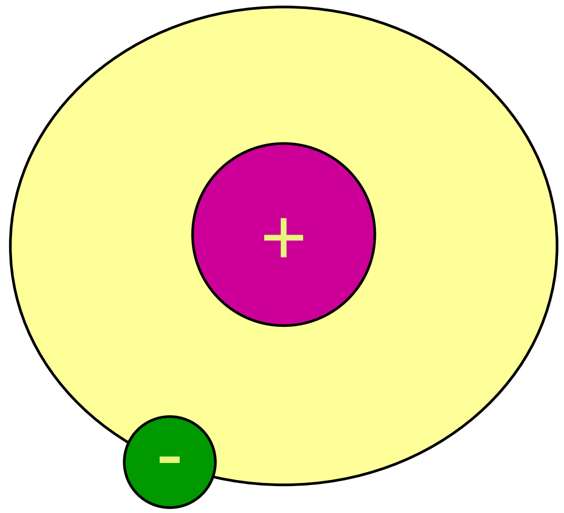
There can be two sources of this induced dipole moment:

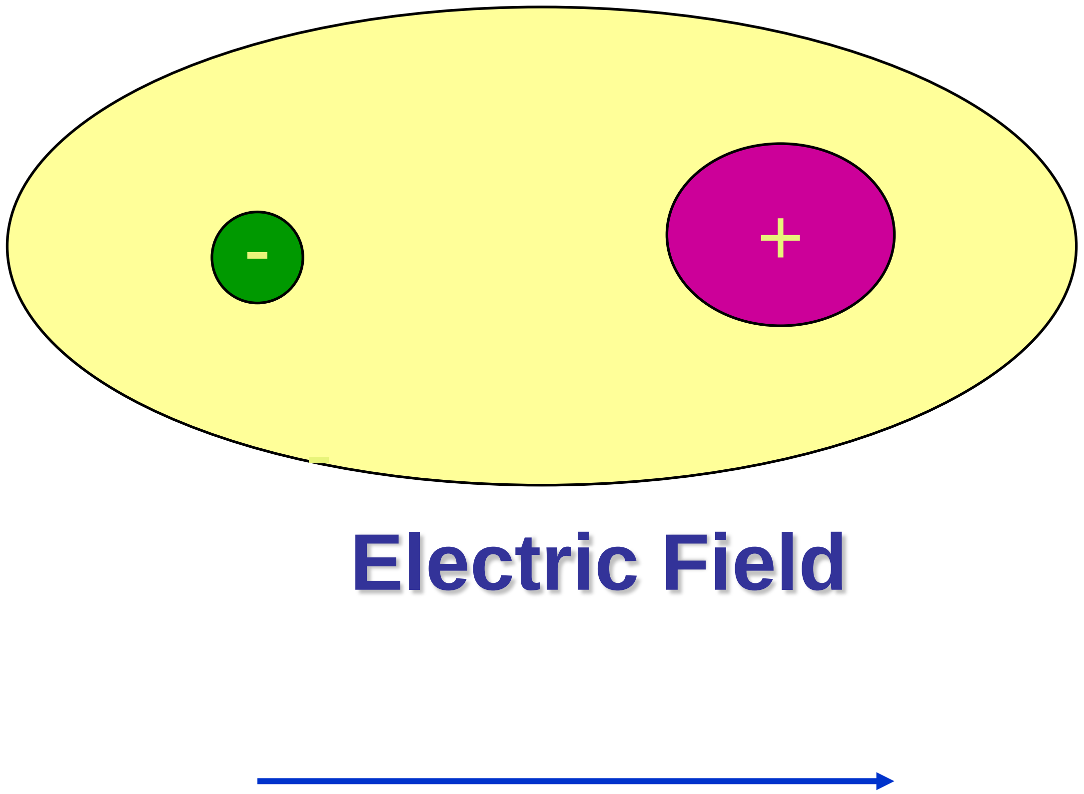
Deformation polarization

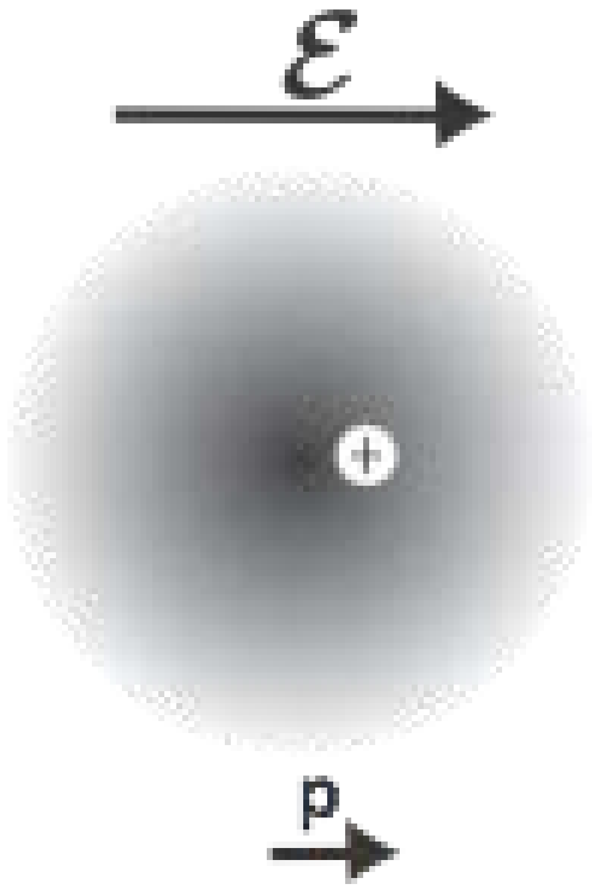
a. **Electron polarization** - the displacement of nuclear and electrons in the atom under the influence of external electric field. As electrons are very light they have a rapid response to the field changes; they may even follow the field at optical frequencies.

b. **Atomic polarization** - the displacement of atoms or atom groups in the molecule under the influence of external electric field.

Deformation (electronic) polarization







for one atom $\mathbf{p} = \alpha\boldsymbol{\mathcal{E}}$

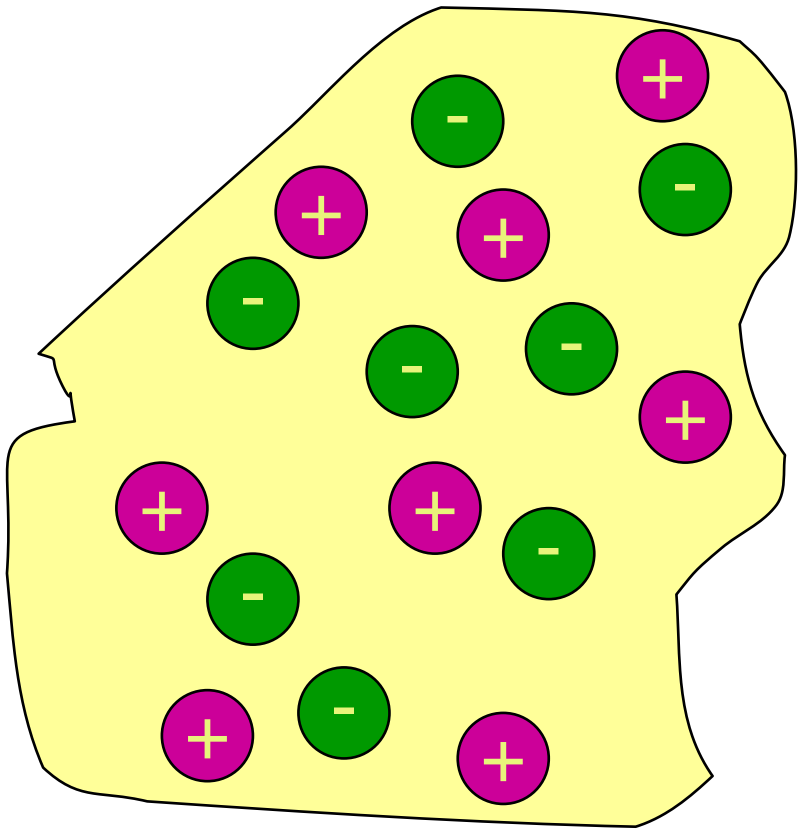
for the solid $\mathbf{P} = \frac{N}{V} q\boldsymbol{\delta} = \frac{N}{V}\mathbf{p}$

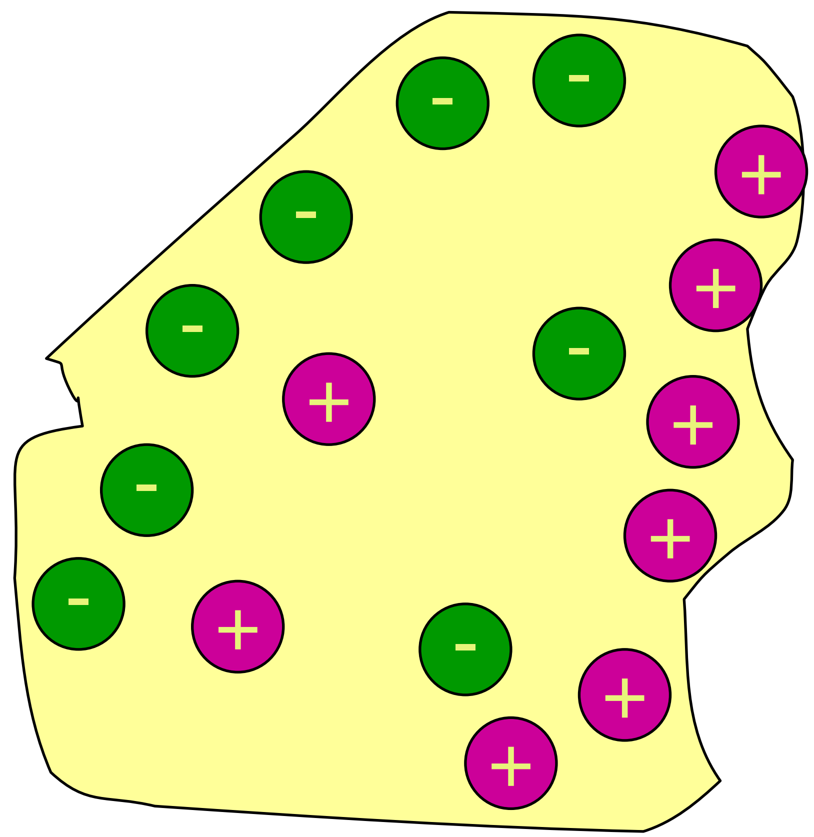
Electronic polarization is very fast (short relaxation time τ)

Ionic Polarization

In ionic lattice, the positive ions are displaced in the direction of an applied field while the negative ions are displaced in the opposite direction, giving a resultant (*apparent*) dipole moment to the whole body.

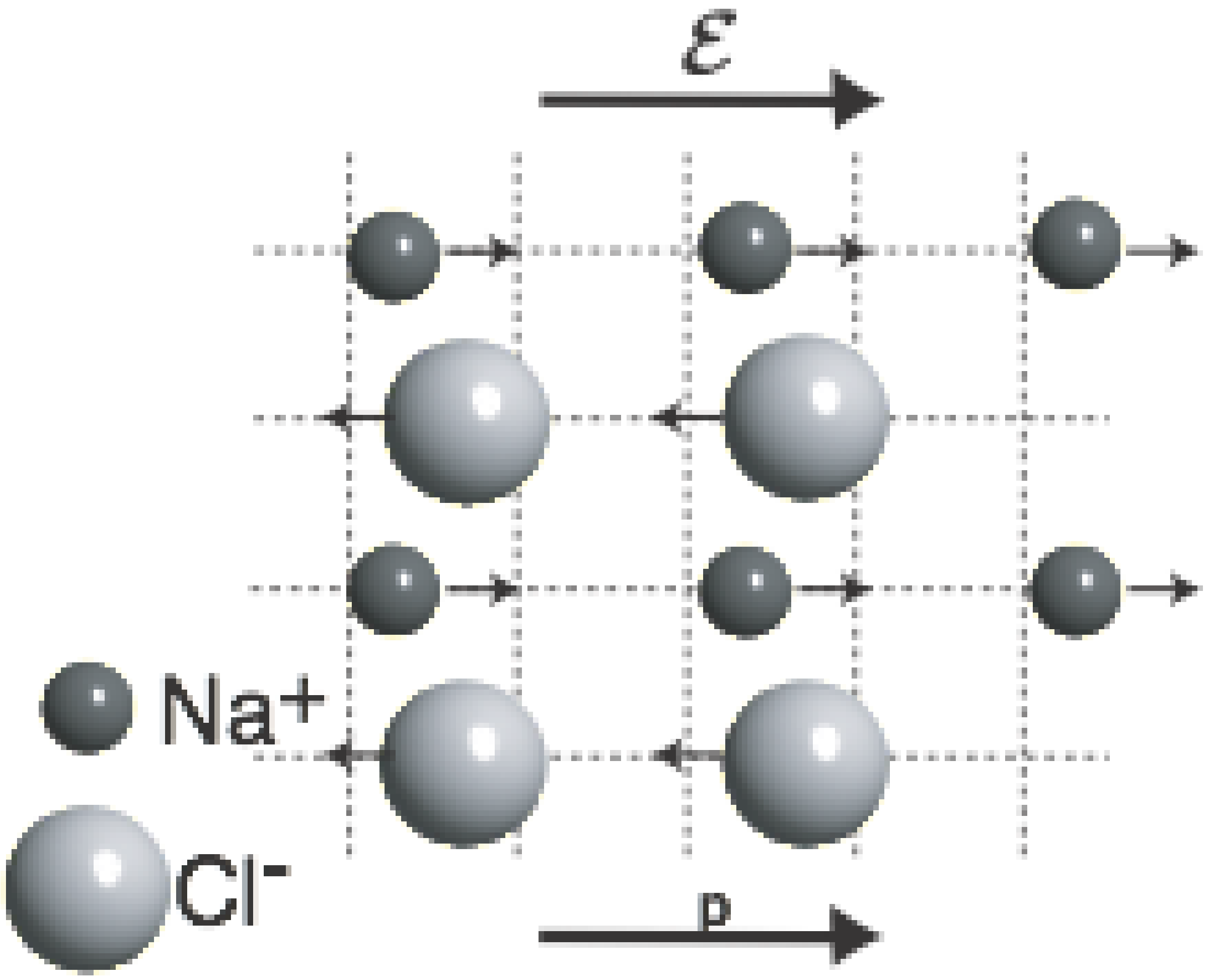
Ions are much heavier than electrons, and need longer relaxation time.





Electric field

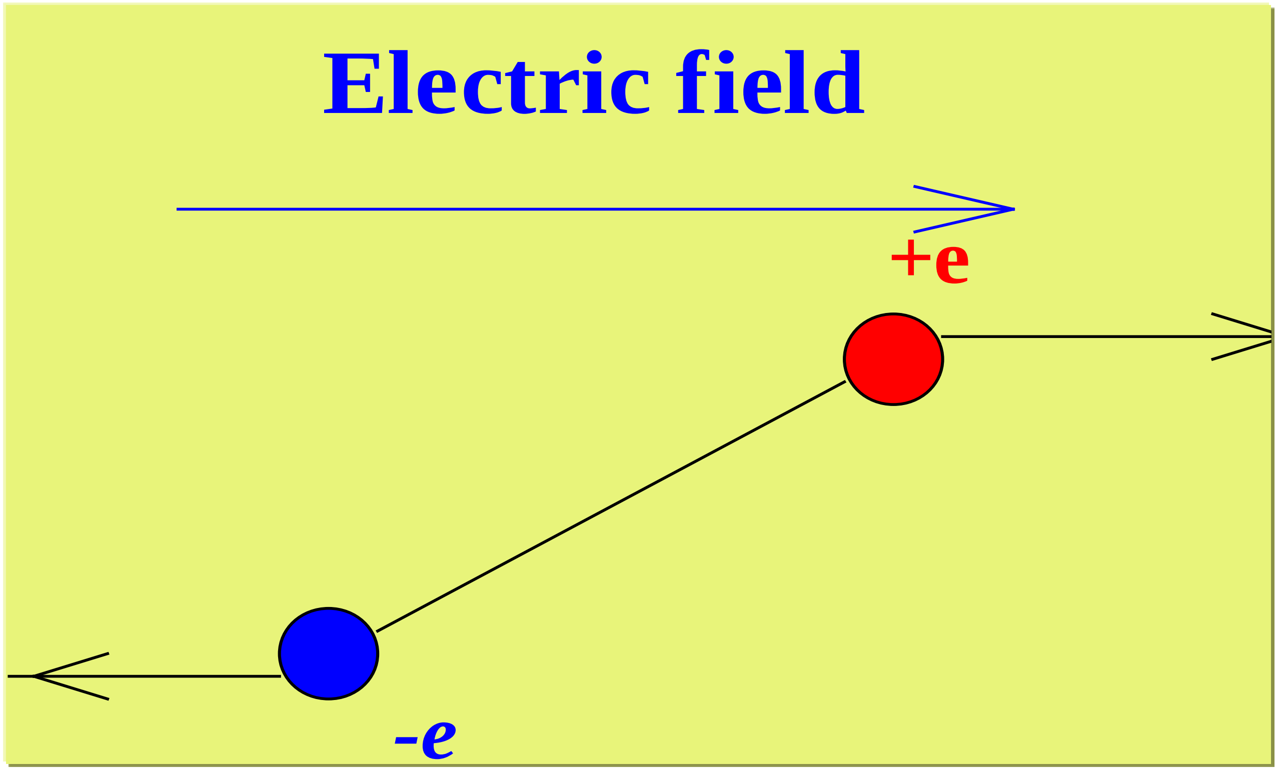
Microscopic origin: ionic polarization

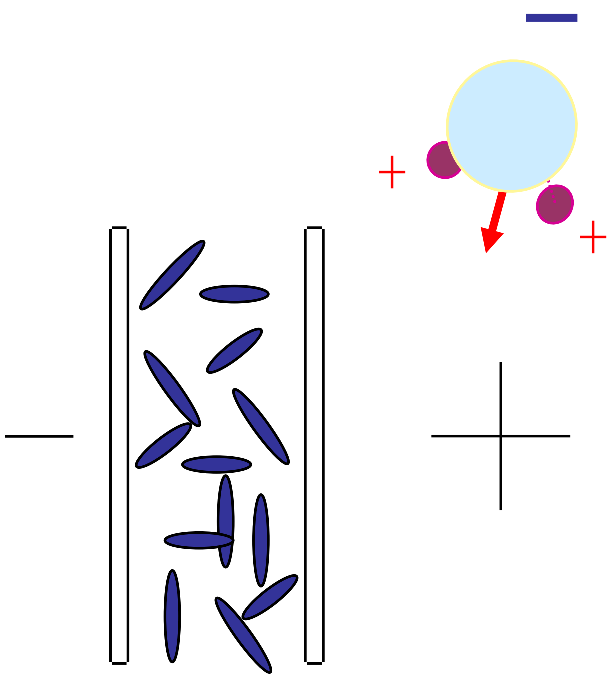


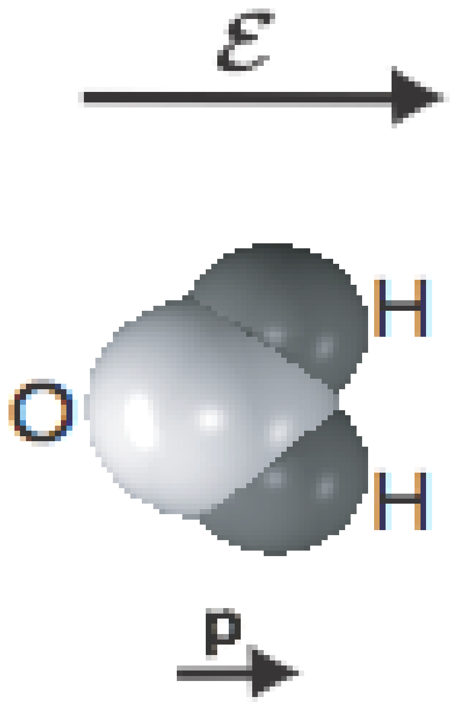
$$\mathbf{P} = \frac{N}{V} q\boldsymbol{\delta} = \frac{N}{V}\mathbf{p}$$

Orientation polarization:

The electric field tends to direct the permanent dipoles.







$$\mathbf{P} = \frac{N}{V} q\delta = \frac{N}{V}\mathbf{p}$$

Ions are much heavier than electrons, and their motion needs longer relaxation time.

Ориентационная поляризуемость (расчет)

Потенциальная энергия U молекулы с постоянным моментом p в поле E есть

$$U = -\mathbf{p}\cdot\mathbf{E} = -pE\cos\theta,$$

Величина поляризации

$$P = Np\,\langle\cos\theta\rangle,$$

Согласно закону распределения Больцмана

$$\langle\cos\theta\rangle = \left(\int e^{-\beta U}\cos\theta\, d\Omega\right)\cdot\left(\int e^{-\beta U}\, d\Omega\right)^{-1},$$

$$\langle\cos\theta\rangle = \frac{\int\limits_0^{\pi} 2\pi\sin\theta\cos\theta\exp(\beta pE\cos\theta)\,d\theta}{\int\limits_0^{\pi} 2\pi\sin\theta\exp(\beta pE\cos\theta)\,d\theta},\qquad d\Omega = \sin\theta\, d\varphi\, d\theta.$$

$$\langle\cos\theta\rangle = \left(\int\limits_{-1}^{+1} e^{sx}s\,ds\right)\cdot\left(\int\limits_{-1}^{+1} e^{sx}\,ds\right)^{-1} = \frac{d}{dx}\ln\int\limits_{-1}^{+1} e^{sx}\,ds =$$

$$= \frac{d}{dx}\ln\left(e^{x}-e^{-x}\right) - \frac{d}{dx}\ln x = \operatorname{cth} x - \frac{1}{x} \equiv L(x).$$

обозначения: $s \equiv \cos\theta,\quad x \equiv pE/k_BT,$

функция Ланжевена L(x).

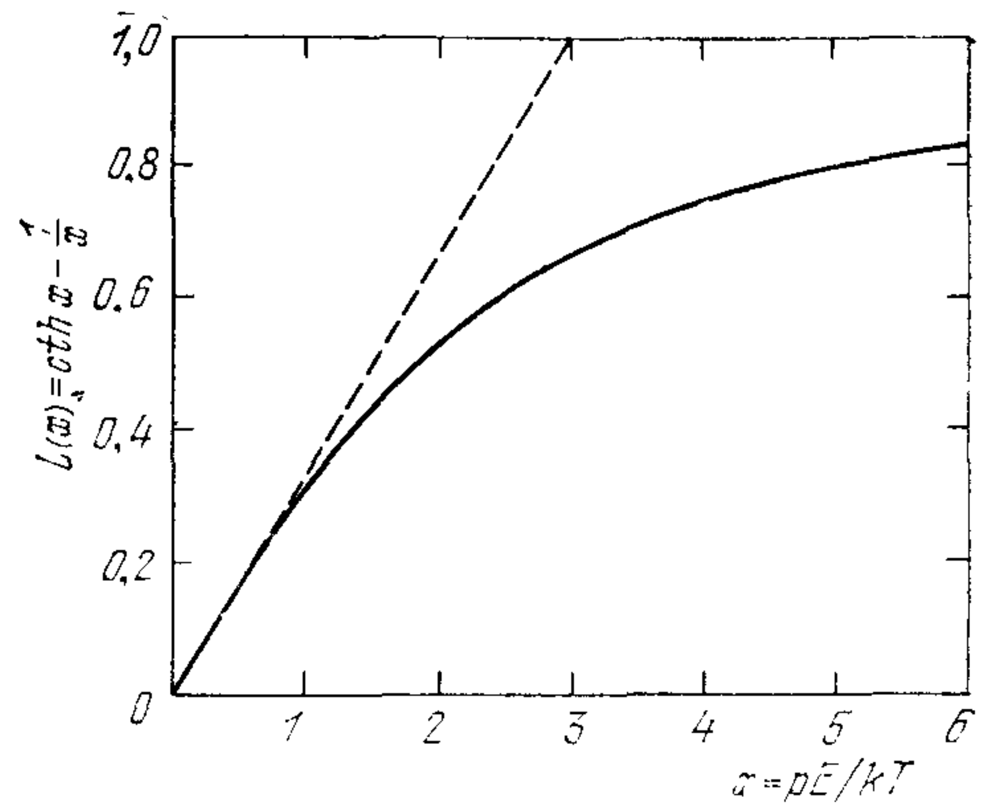
Orientation polarization (limiting cases)

At x<<1 $\operatorname{cth} x = \frac{1}{x} + \frac{x}{3} - \frac{x^3}{45} + \ldots; \quad L(x) \approx \frac{x}{3} = \frac{pE}{3k_B T}$

and polarization $P = Np \langle \cos\theta \rangle = \frac{Np^2E}{3k_BT}$.

At x>>1 polarization saturates to a finite value $P = Np$

Рис. 13.15. График функции Ланжевена $L(x)$, где $x = pE/k_BT$. Наклон кривой в начале координат показан пунктирной прямой. Величина поляризации, составляющая 80% от значения, отвечающего насыщению, соответствует $pE/k_BT = 5$.



Frequency dependence - Debye approximation: $\alpha(\omega) = \frac{\alpha_0}{1 - i\omega\tau}$,

where in liquids the relaxation time is determined by viscosity: $\tau = \frac{4\pi\eta a^3}{k_BT}$

For water this gives $\tau = 10^{-11}$c

Polar and Non-polar Dielectrics

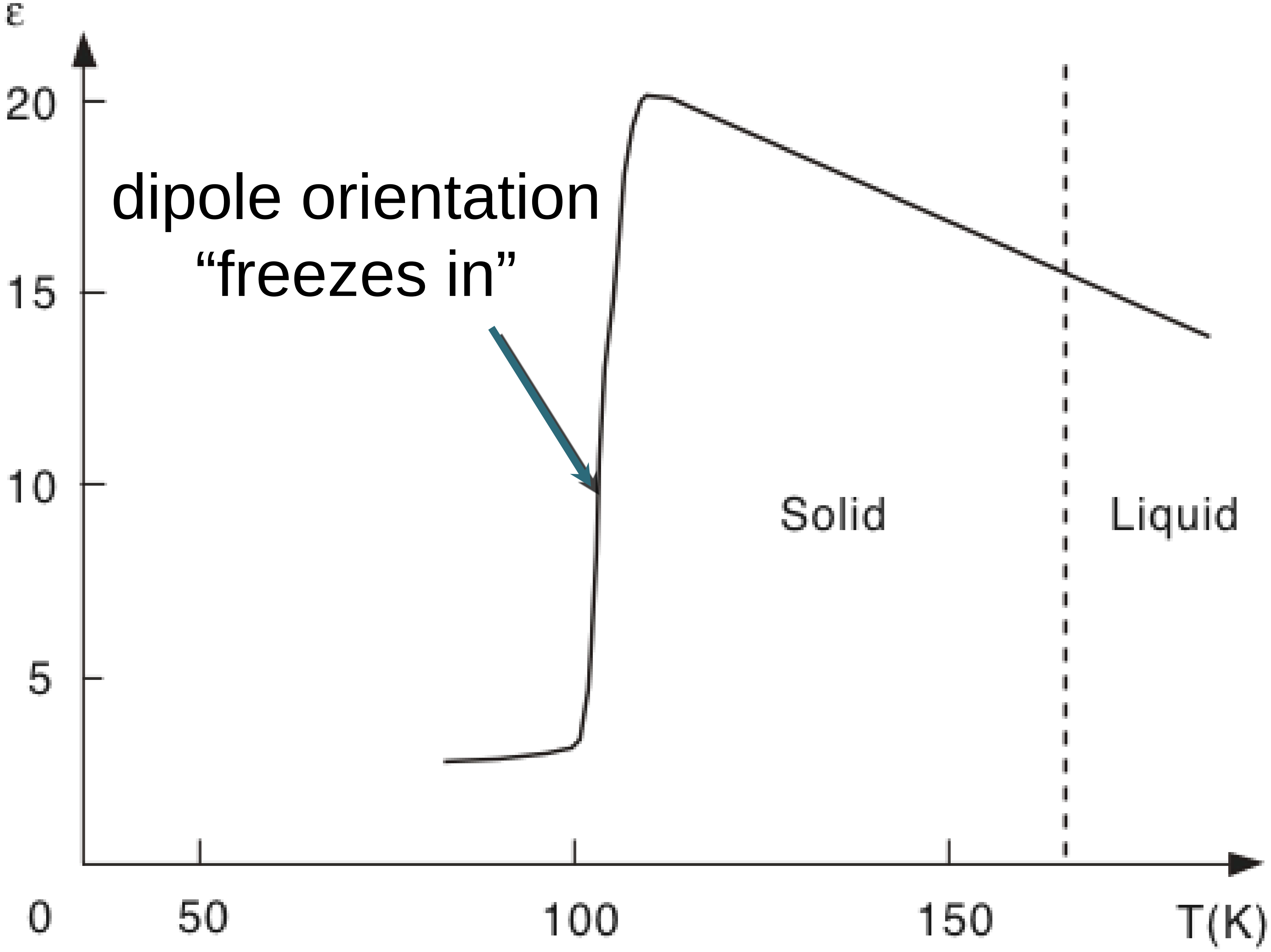
To investigate the dependence of the polarization on molecular quantities it is convenient to assume the polarization ***P*** to be divided into two parts: the induced polarization $\boldsymbol{P}_{\alpha}$ caused by the translation effects, and the dipole polarization $\boldsymbol{P}_{\mu}$ caused by the orientation of the permanent dipoles.

$$\frac{\varepsilon - 1}{4\pi}\boldsymbol{E} = \boldsymbol{P}_{\alpha} + \boldsymbol{P}_{\mu}$$

A ***non-polar dielectric*** *is one whose molecules possess no permanent dipole moment.*

A ***polar dielectric*** *is one in which the individual molecules possess a dipole moment even in the absence of any applied field, i.e. the center of positive charge is displaced from the center of negative charge.*

Example: Hydrogen chloride

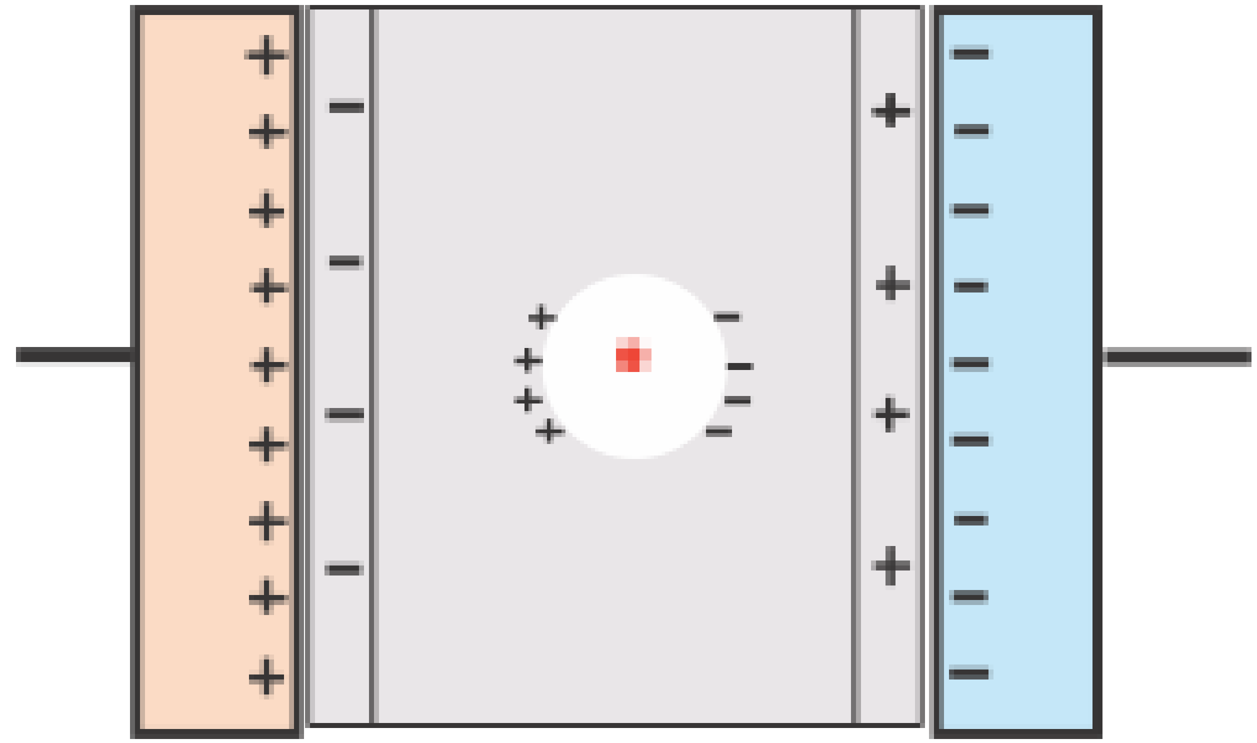


Local field slides

One can calculate polarization of a molecule in external electric field.
But what is the actual electric field, which this molecule feels?

This question is not simple, and depends on the sample shape.

The local field at a point in the dielectric



field by external charges on plates $\mathbf{E}_0$

field by surface charges depolarization field $\mathbf{E}_1$

average macroscopic field $\mathbf{E} = \mathbf{E}_0 + \mathbf{E}_1$

field from the surface dipoles of a spherical cavity large against microscopic dimensions $\mathbf{E}_2$

field from inside this cavity $\mathbf{E}_3$

total local field $\mathbf{E}_{loc} = \mathbf{E}_0 + \mathbf{E}_1 + \mathbf{E}_2 + \mathbf{E}_3 = \mathbf{E} + \mathbf{E}_2 + \mathbf{E}_3$

Depolarization field E_1

If P_x, P_y, P_z are the components of the polarization P referred to the principal axes, then the components of the depolarization field are written

$$\text{(CGS)} \quad E_{1x} = -N_x P_x \; ; \qquad E_{1y} = -N_y P_y \; ; \qquad E_{1z} = -N_z P_z \; ;$$

$$\text{(SI)} \quad E_{1x} = -\frac{N_x P_x}{\epsilon_0} \; ; \qquad E_{1y} = -\frac{N_y P_y}{\epsilon_0} \; ; \qquad E_{1z} = -\frac{N_z P_z}{\epsilon_0} \; ,$$

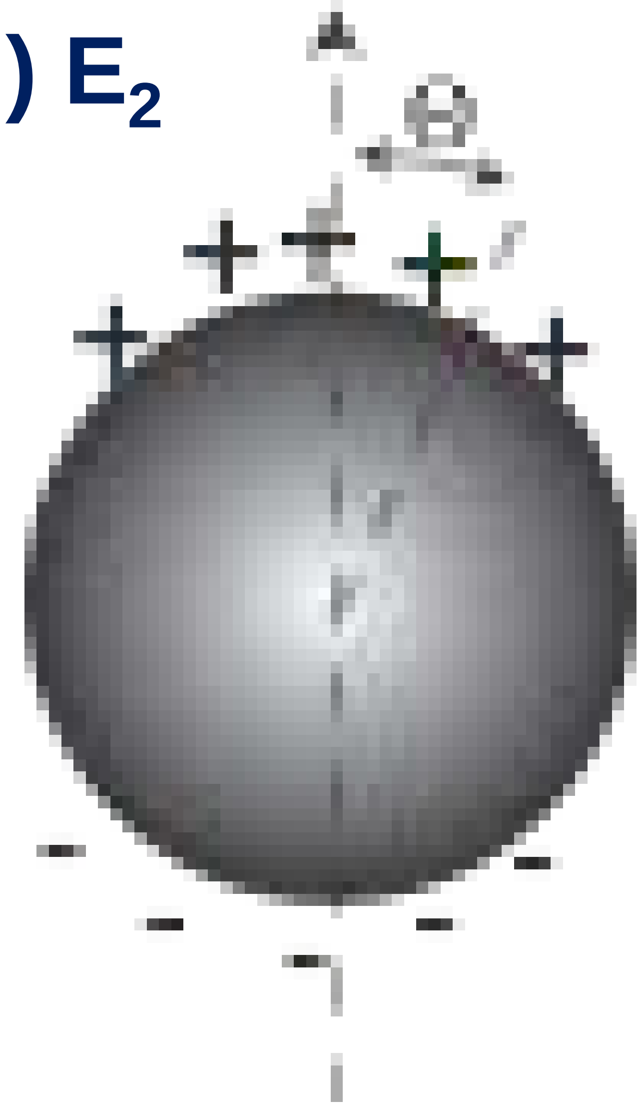
In limiting cases N has the values:

Shape	Axis	N (CGS)	N (SI)
Sphere	any	$4\pi/3$	1/3
Thin slab	normal	4π	1
Thin slab	in plane	0	0
Long circular cylinder	longitudinal	0	0
Long circular cylinder	transverse	2π	1/2

The local field at a point in the dielectric (2)

Calculation of the cavity field (Lorentz Field) E_2

(z is direction between plates)



$$\mathbf{E}_2 = \int \frac{1}{4\pi\epsilon_0}\frac{\sigma}{r^2}\hat{\mathbf{r}}dS$$

in z direction

$$E_2 = \int \frac{1}{4\pi\epsilon_0}\frac{\sigma}{r^2}\cos\Theta dS$$

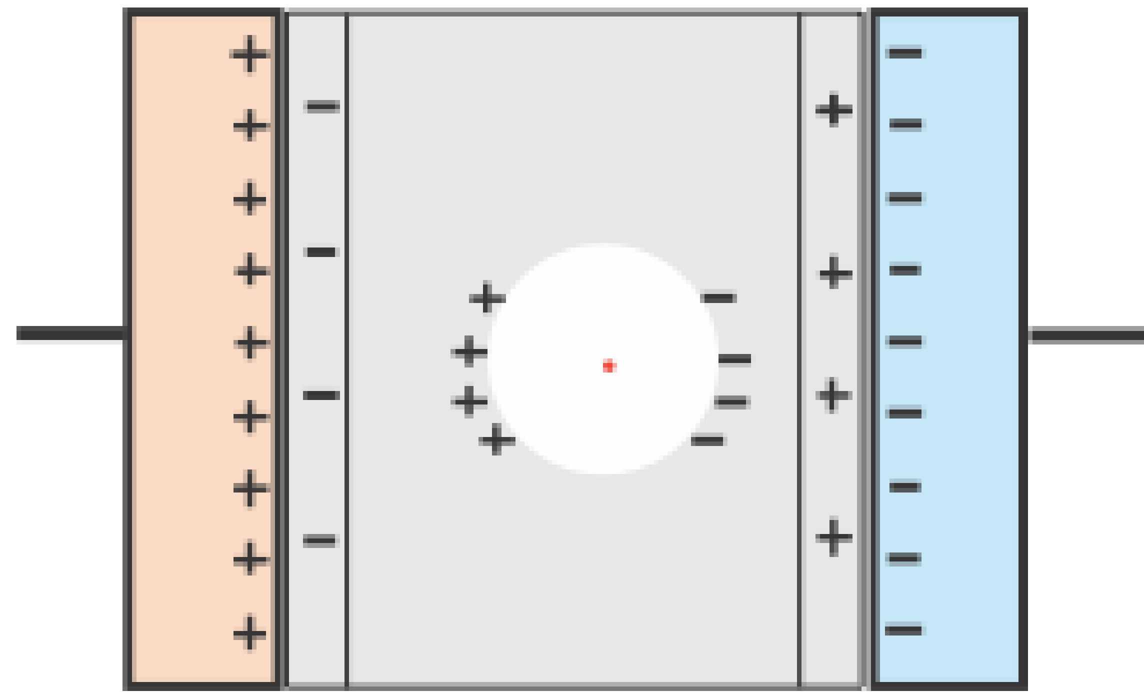
surface charge density on sphere $\sigma = P\cos\Theta$

$$E_2 = \int \frac{1}{4\pi\epsilon_0}\frac{P\cos\Theta}{r^2}\cos\Theta dS = \int_0^{2\pi}\int_0^{\pi}\frac{1}{4\pi\epsilon_0}\frac{P\cos\Theta}{r^2}\cos\Theta r^2\sin\Theta d\phi d\Theta = \frac{1}{3\epsilon_0}P$$

(СГС) $$\boldsymbol{E}_2 = \int_0^{\pi}(a^{-2})(2\pi a\sin\theta)(a\,d\theta)(\boldsymbol{P}\cos\theta)(\cos\theta) = \frac{4\pi}{3}\boldsymbol{P};$$

The local field at a point in the dielectric (3)

calculation of the field inside the cavity for a cubic lattice



field of a dipole (along z)

$$\mathbf{E}(\mathbf{r}) = \frac{3(\mathbf{p}\cdot\mathbf{r})\mathbf{r} - r^2\mathbf{p}}{4\pi\epsilon_0 r^5}$$

$$E_z(r) = p\frac{3z^2 - r^2}{4\pi\epsilon_0 r^5}$$

field at centre for all dipoles in cavity

$$E_z(r) = p\sum_i \frac{3z_i^2 - r_i^2}{4\pi\epsilon_0 r_i^5} = p\sum_i \frac{2z_i^2 - x_i^2 - y_i^2}{4\pi\epsilon_0 r_i^5} = 0 \quad !$$

$$\sum_i \frac{z_i^2}{r_i^5} = \sum_i \frac{x_i^2}{r_i^5} = \sum_i \frac{y_i^2}{r_i^5}$$

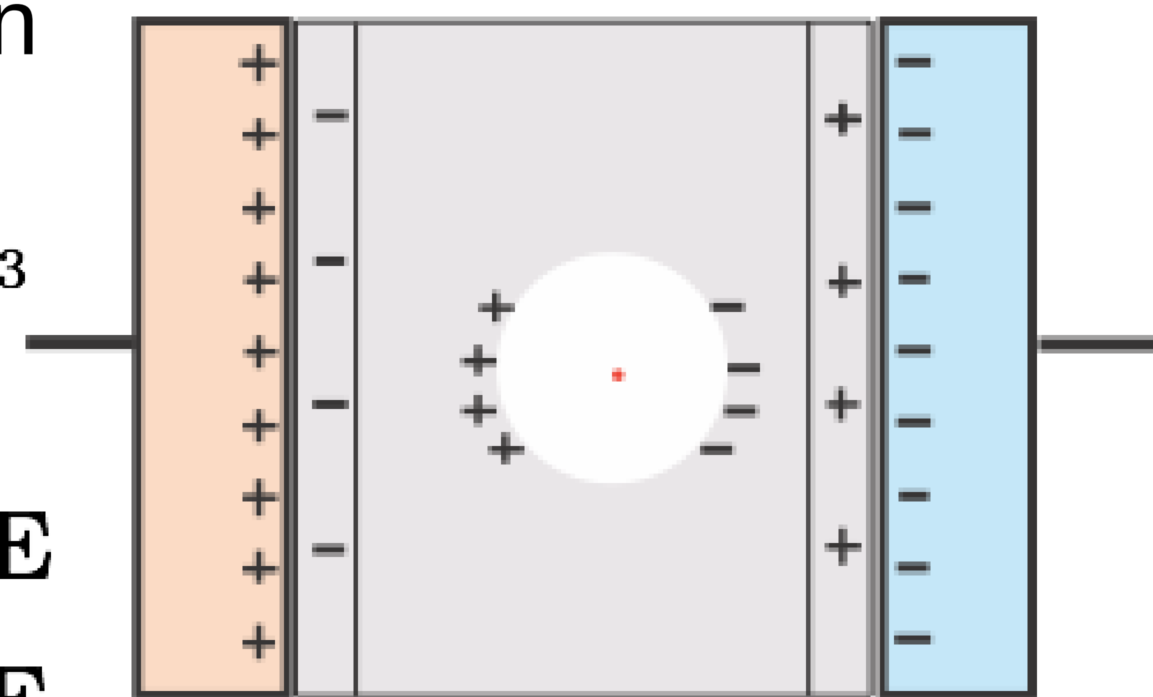
The local field at a point in the dielectric

calculation of the total local field in cubic surrounding

$$\mathbf{E}_{loc} = \mathbf{E}_0 + \mathbf{E}_1 + \mathbf{E}_2 + \mathbf{E}_3 = \mathbf{E} + \mathbf{E}_2 + \mathbf{E}_3$$

$$= \mathbf{E} + \frac{1}{3\epsilon_0}\mathbf{P}$$

(SI) $\mathbf{P} = (\epsilon - 1)\epsilon_0 \mathbf{E}$



it follows that (SI) $\mathbf{E}_{\rm loc} = \frac{1}{3}(\epsilon + 2)\mathbf{E}$

$$\mathcal{E}_{\rm loc} = \frac{1}{3}(\epsilon + 2)\mathcal{E}$$

$$\mathbf{P} = \frac{N}{V}\alpha\mathcal{E}_{\rm loc} = \frac{N\alpha}{3V}(\epsilon + 2)\mathcal{E}$$

$$\mathbf{P} = (\epsilon - 1)\epsilon_0\mathcal{E}$$

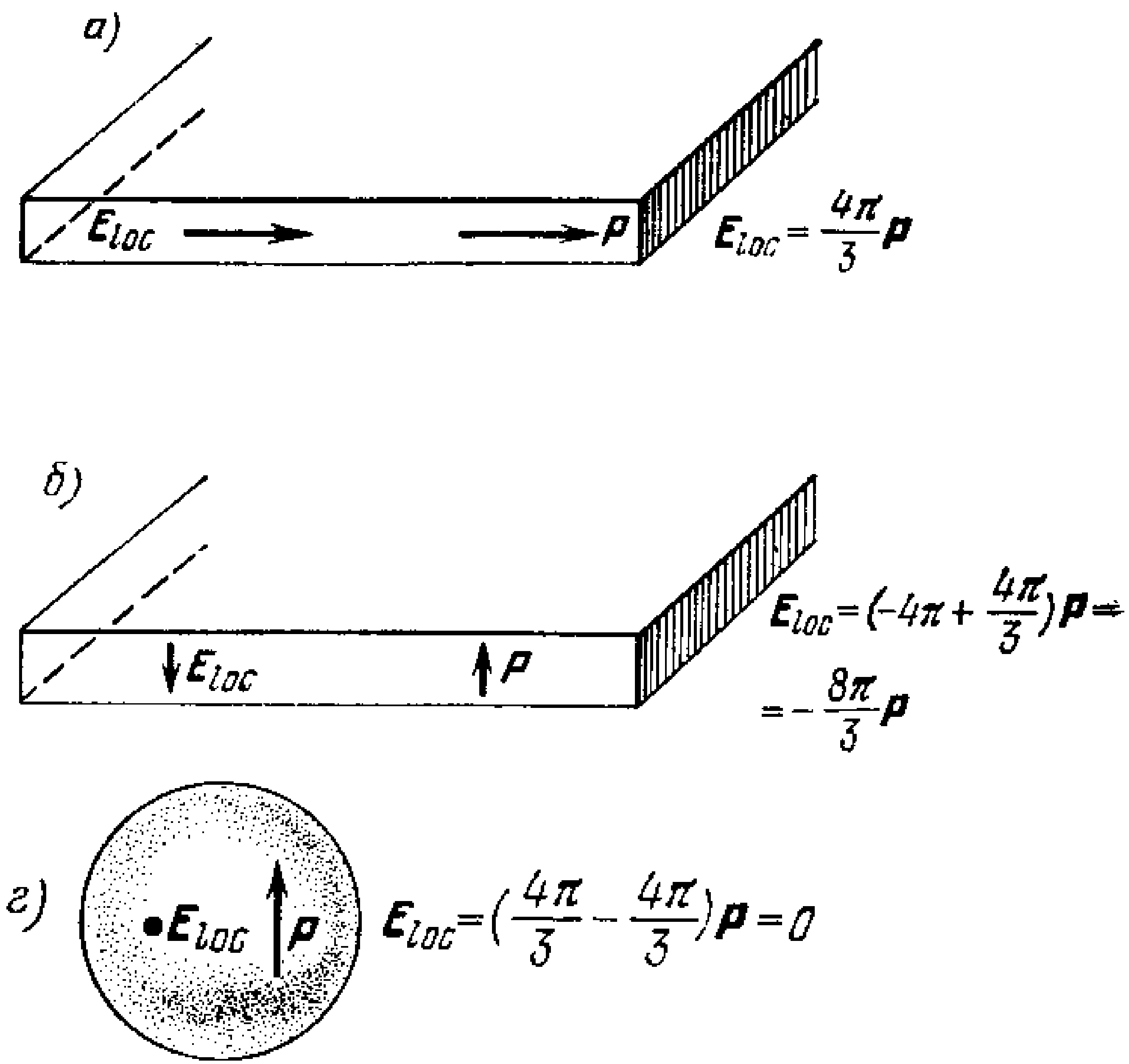
Clausius-Mossotti relation

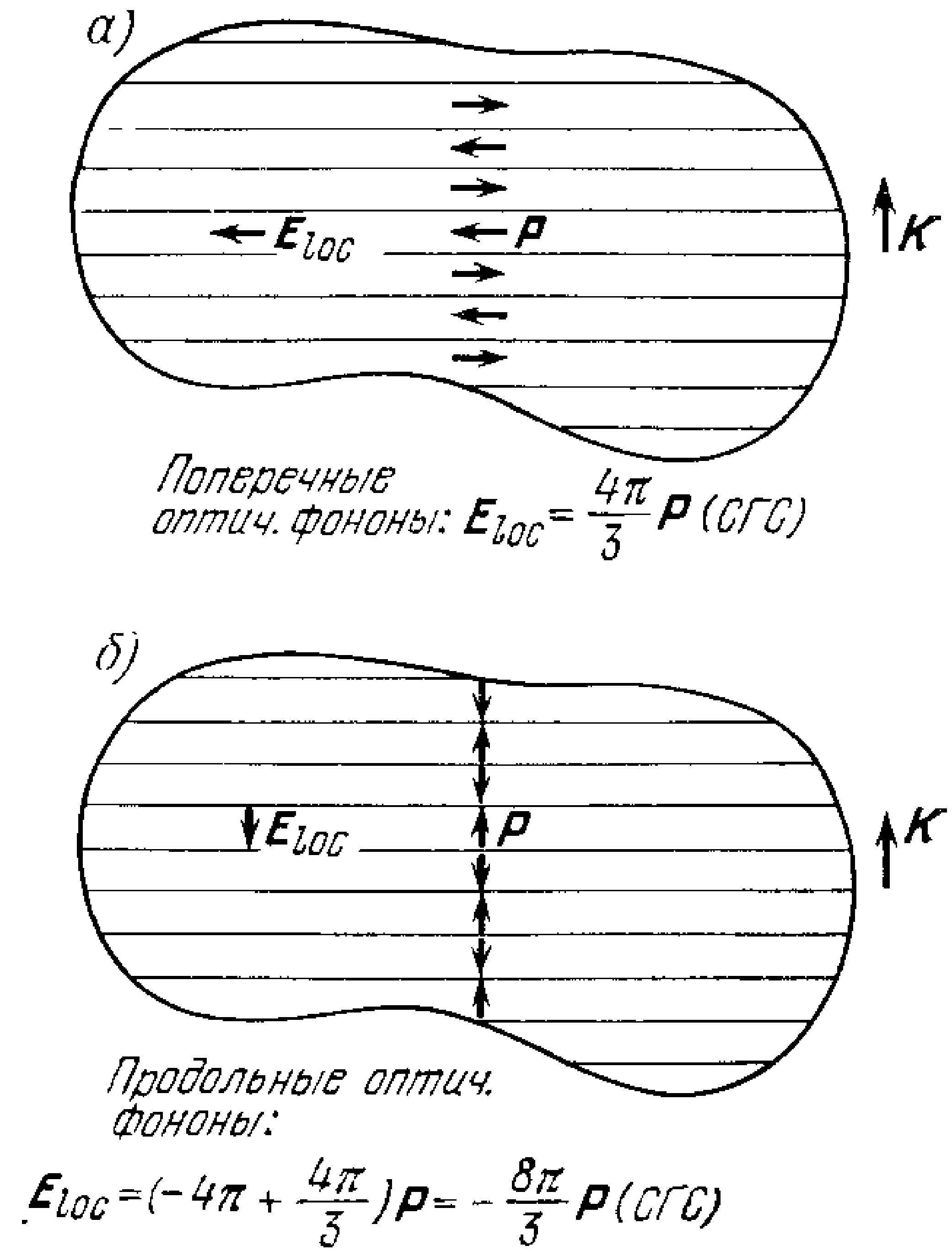
$$\alpha = \frac{\epsilon - 1}{\epsilon + 2}\frac{3\epsilon_0 V}{N}$$

Polarization α_j of individual molecules is related to dielectric constant as

(СГС) $\frac{\varepsilon - 1}{\varepsilon + 2} = \frac{4\pi}{3}\sum N_j\alpha_j$; (СИ) $\frac{\varepsilon - 1}{\varepsilon + 2} = \frac{1}{3\varepsilon_0}\sum N_j\alpha_j$.

Local field for various sample shapes





(Чтобы получить выражение для E_{loc} в системе СИ, надо умножить P на $1/4\pi\varepsilon_0$.)

Характерное расположение локального электрического поля и поляризации P обычно способствует распространению поперечных и препятствует распространению продольных оптических фононов. Поэтому $\omega_L > \omega_T$.

The dielectric constant

material	dielectric constant ε
vacuum	1
air	1.000576 (283 K, 1013 hPa)
rubber	2.5 - 3.5
glass	5-10
NaCl	5.9
ethanol	25.8
water	81.1
strontium titanate	350

Clausius-Mossotti relation

$$\alpha = \frac{\epsilon - 1}{\epsilon + 2} \frac{3\epsilon_0 V}{N}$$

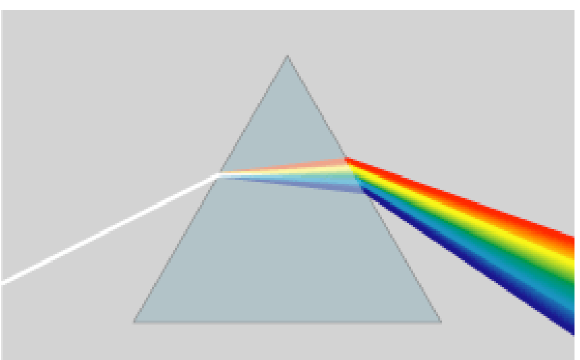
or

$$\epsilon = \frac{3\epsilon_0 V/N + 2\alpha}{3\epsilon_0 V/N - \alpha}$$

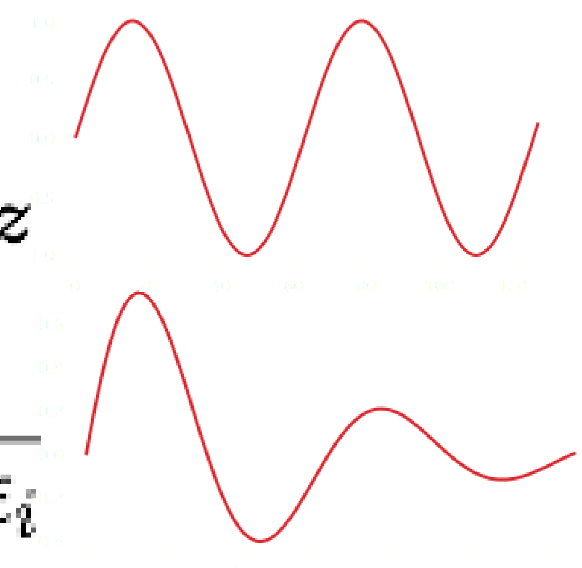
Frequency dependence of the dielectric constant

plane wave $$\mathcal{E}(z,t) = \mathcal{E}_0 e^{i(kz-\omega t)}$$

$$k = \frac{2\pi N}{\lambda_0}$$ complex index of refraction $$N = n + i\kappa$$



$$\mathcal{E}(z,t) = \mathcal{E}_0 e^{i\left(\frac{2\pi n}{\lambda_0}z-\omega t\right)} e^{-\frac{2\pi\kappa}{\lambda_0}z}$$



Maxwell relation $$N = \sqrt{\epsilon} = \sqrt{\epsilon_r + i\epsilon_i}$$

$$\mathcal{E}(z,t) = \mathcal{E}_0 e^{i((2\pi N/\lambda_0)z-\omega t)} = \mathcal{E}_0 e^{i((\omega\sqrt{\epsilon}/c)z-\omega t)}$$

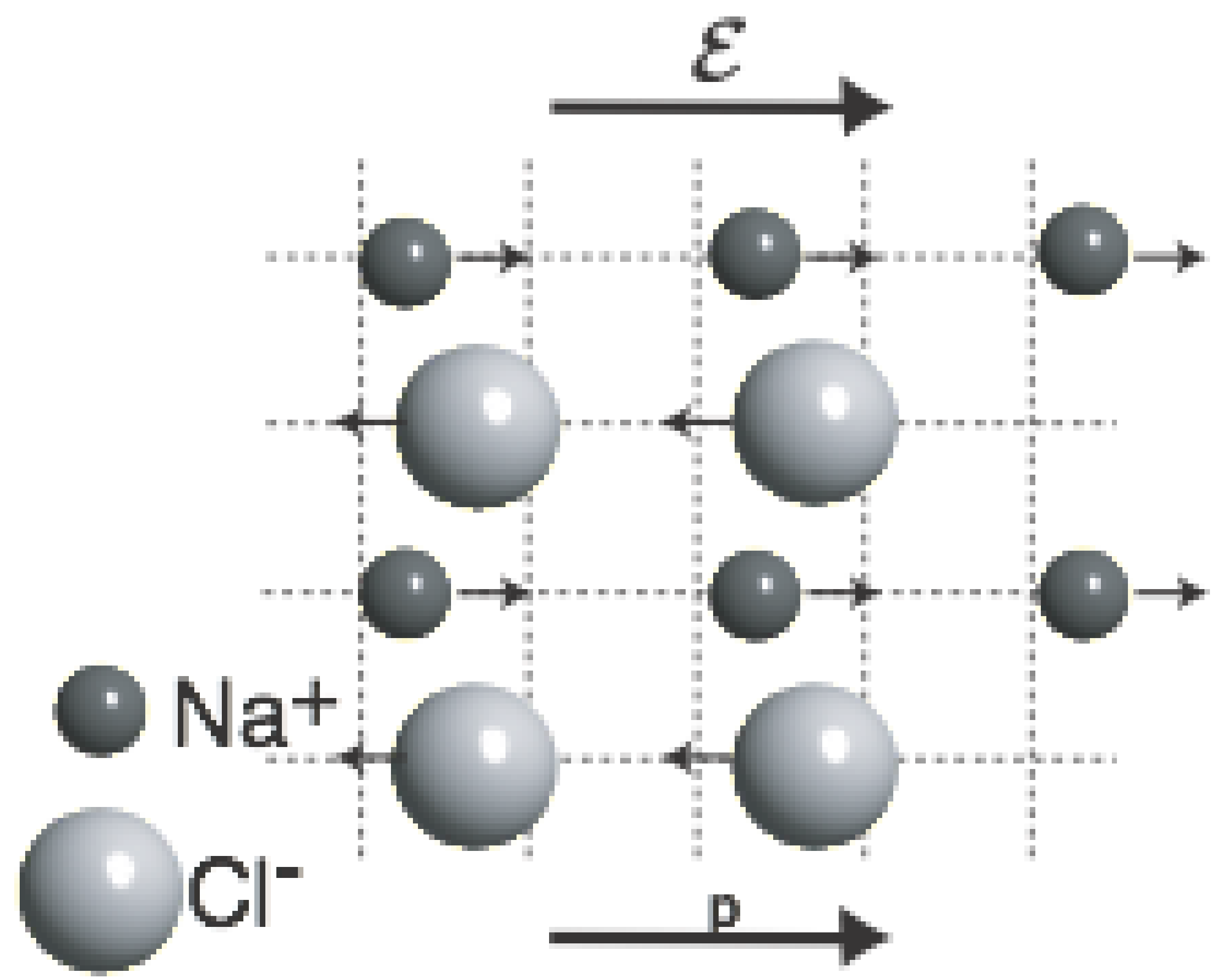
all the interesting physics is in the dielectric function!

Wavelength ratio is given by refraction index: $$\frac{\lambda_{\text{вакуум}}}{\lambda_{\text{образец}}} = \sqrt{\varepsilon\mu}$$

This provides a way to measure high-frequency ε

Frequency dependence of the dielectric constant

- Slowly varying fields: quasi-static behaviour.
- Fast varying fields: polarisation cannot follow anymore (only electronic polarization can).
- Of particular interest is the optical regime.



Frequency dependence of the dielectric constant

- Slowly varying fields: quasi-static behaviour.
- Fast varying fields: polarisation cannot follow anymore (only electronic).
- Of particular interest is the optical regime.

material	static ε	ε_{opt}
diamond	5.68	5.66
NaCl	5.9	2.34
LiCl	11.95	2.78
TiO_2	94	6.8
quartz	3.85	2.13

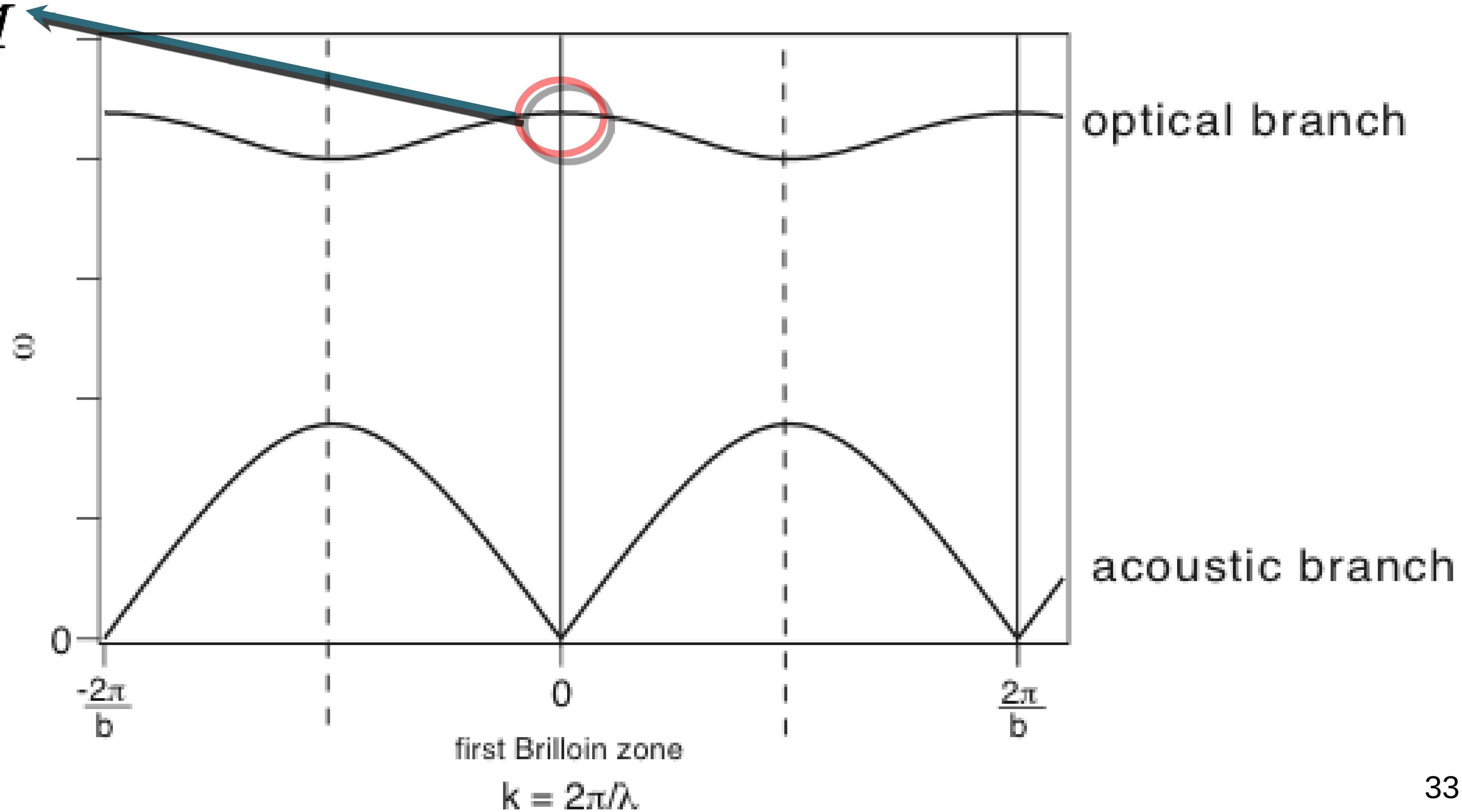
Frequency dependence of the dielectric constant: driven and damped harmonic motion

- We obtain an expression for the frequency-dependent dielectric function as given by the polarization of the lattice.
- The lattice motion is just described as one harmonic oscillator.

light E-field

(almost constant over very long distance)

$$\omega_o = \sqrt{\frac{2\gamma}{M}}$$



Frequency dependence of the dielectric constant: driven and damped harmonic motion (1)

We start with the usual differential equation

$$\frac{d^2x}{dt^2} + \eta\frac{dx}{dt} + \omega_0^2 x = \frac{e\mathcal{E}_0}{M}e^{-i\omega t}$$

friction term

harmonic restoring term

driving field (should be local field)

This equation describes the motion of ions, atoms, or electrons in quadratic potential.

$$\omega_o = \sqrt{\frac{2\gamma}{M}}$$

Frequency dependence of the dielectric constant: driven and damped harmonic motion (2)

Equation $$\frac{d^2x}{dt^2} + \eta\frac{dx}{dt} + \omega_0^2 x = \frac{e\mathcal{E}_0}{M}e^{-i\omega t}$$

has solution $$x = Ae^{-i\omega t}$$

with complex amplitude $$A = \frac{e\mathcal{E}_0}{M}\frac{1}{\omega_0^2 - \omega^2 - i\eta\omega}$$ or

$$A = \frac{e\mathcal{E}_0}{M}\left(\frac{\omega_0^2 - \omega^2}{(\omega_0^2 - \omega^2)^2 + \eta^2\omega^2} + \frac{i\eta\omega}{(\omega_0^2 - \omega^2)^2 + \eta^2\omega^2}\right)$$

real part imaginary part

Frequency dependence of the dielectric constant: driven and damped harmonic motion (3)

Polarization $P(t) = P_i(t) + P_e(t) = \frac{N}{V} e A e^{-i\omega t} + \frac{N}{V} \alpha \mathcal{E}_0 e^{-i\omega t}$

ionic / lattice part **electronic / atomic part**

$$\epsilon = \frac{P(t)}{\epsilon_0 \mathcal{E}_0 e^{-i\omega t}} + 1 = \frac{NeA}{V\epsilon_0 \mathcal{E}_0} + \frac{N\alpha}{V\epsilon_0} + 1$$

for sufficiently high frequencies we know that $P_i = 0$

$$\epsilon_{\mathrm{opt}} = \frac{N\alpha}{V\epsilon_0} + 1 \quad , \qquad \epsilon(\omega) = \frac{NeA}{V\epsilon_0 \mathcal{E}_0} + \epsilon_{\mathrm{opt}}$$

Frequency dependence of the dielectric constant: driven and damped harmonic motion (4)

combine

$$\epsilon(\omega) = \frac{NeA}{V\epsilon_0\mathcal{E}_0} + \epsilon_{\text{opt}}$$

with $$A = \frac{e\mathcal{E}_0}{M}\left(\frac{\omega_0^2 - \omega^2}{(\omega_0^2 - \omega^2)^2 + \eta^2\omega^2} + \frac{i\eta\omega}{(\omega_0^2 - \omega^2)^2 + \eta^2\omega^2}\right)$$

to get the complex dielectric function to be

$$\epsilon = \epsilon_r + i\epsilon_i$$

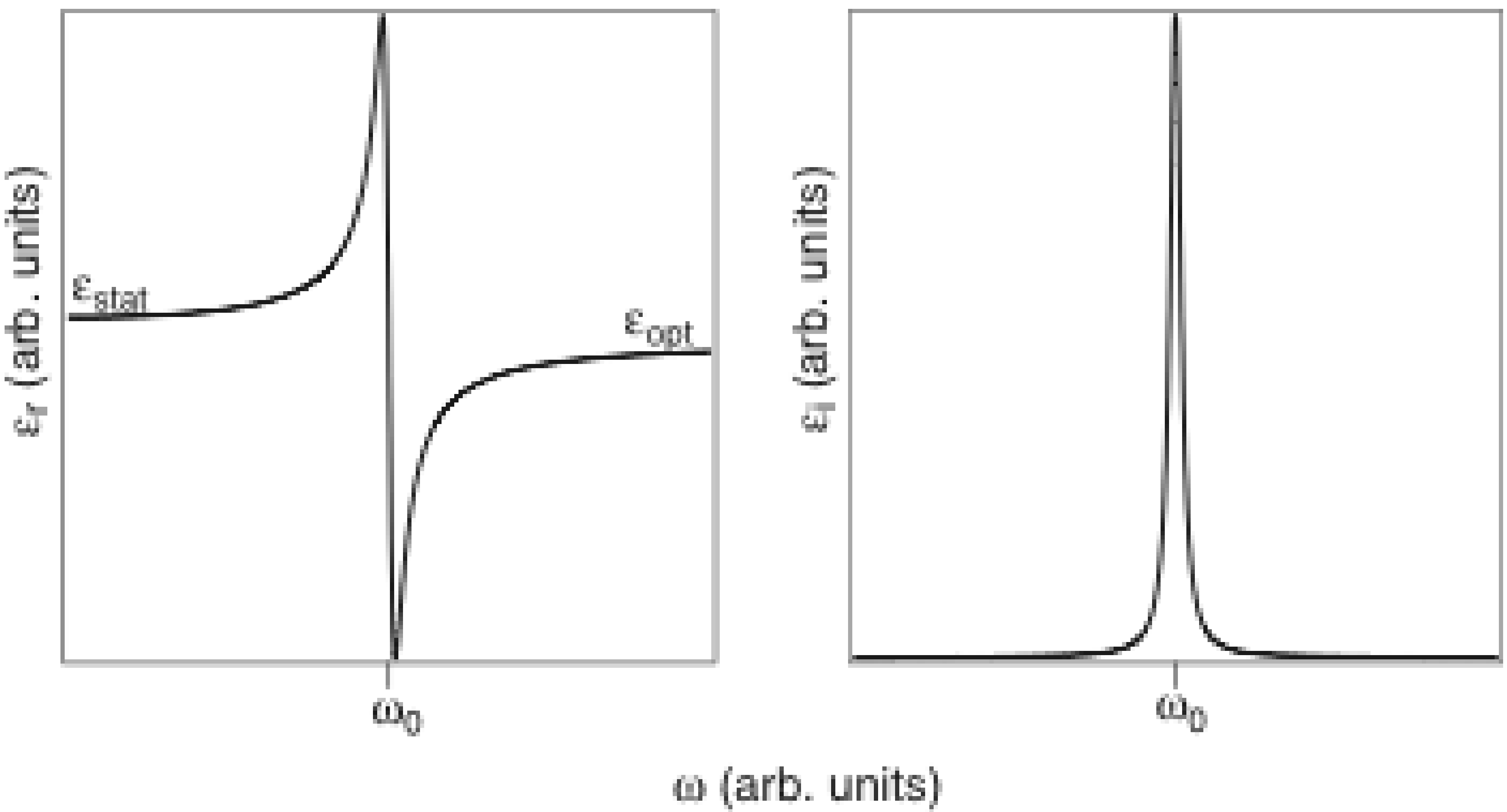
$$\epsilon_r(\omega) = \frac{Ne^2}{V\epsilon_0 M}\frac{\omega_0^2 - \omega^2}{(\omega_0^2 - \omega^2)^2 + \eta^2\omega^2} + \epsilon_{opt}$$

$$\epsilon_i(\omega) = \frac{Ne^2}{V\epsilon_0 M}\frac{\eta\omega}{(\omega_0^2 - \omega^2)^2 + \eta^2\omega^2}$$

Frequency dependence of the dielectric constant: driven and damped harmonic motion (5)

Dielectric constant (function) $\epsilon = \epsilon_r + i\epsilon_i$

$$\epsilon_r = \frac{Ne^2}{V\epsilon_0 m}\frac{\omega_0^2 - \omega^2}{(\omega_0^2 - \omega^2)^2 + \eta^2\omega^2} + \epsilon_{opt} \qquad \epsilon_i = \frac{Ne^2}{V\epsilon_0 m}\frac{\eta\omega}{(\omega_0^2 - \omega^2)^2 + \eta^2\omega^2}$$



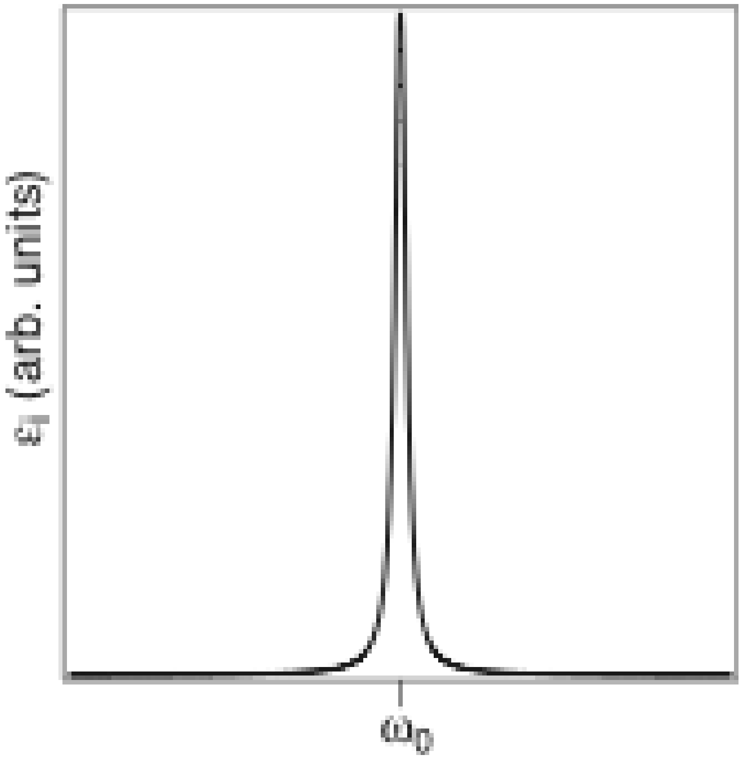
Remember the plasma oscillation in a metal: even higher frequencies

values of the plasma energy $\hbar\omega_P$

	measured	calculated
K	3.72 eV	4.29 eV
Mg	10.6 eV	10.9 eV
Al	15.3 eV	15.8 eV
Si	16.6 eV	16.0 eV
Ge	16.2 eV	16.0 eV

- We have seen that metals are transparent above the plasma frequency (in the UV).
- This lends itself to a simple interpretation: above the plasma frequency the electrons cannot keep up with the rapidly changing field and therefore they cannot keep the metal field-free, like they do in electrostatics.

The physical meaning of ε_i



instantaneous power dissipation (per unit volume)

$$p(t) = j(t)\mathcal{E}(t)$$

We use $\mathcal{E}(t) = \mathcal{E}_0 \exp(-i\omega t)$ and

the Maxwell equation (in SI) $\mathbf{j} = \mathrm{curl}\mathbf{H} - \frac{\partial \mathbf{D}}{\partial t}$

$$j(t) = -\frac{\partial D}{\partial t} = -\frac{\partial}{\partial t}\epsilon\epsilon_0\mathcal{E}(t) = \epsilon_0\mathcal{E}(t)\left(i\omega\epsilon_r - \omega\epsilon_i\right)$$

On average the dissipated power is $\bar{p} = \frac{1}{T}\int_0^T \mathcal{E}(t)j(t)dt$

$$\bar{p} = \frac{\omega}{T}\int_0^T E_0^2 \cos(\omega t)\left[\varepsilon_r \sin(\omega t) - \varepsilon_i \cos(\omega t)\right]dt = \varepsilon_i \omega \frac{E_0^2}{2} = \sigma \frac{E_0^2}{2}$$

=> electric conductivity $\sigma = \varepsilon_i \varepsilon_0 \omega$ (in SI), or $\sigma = \varepsilon_i \omega / 4\pi$ (in CGS)

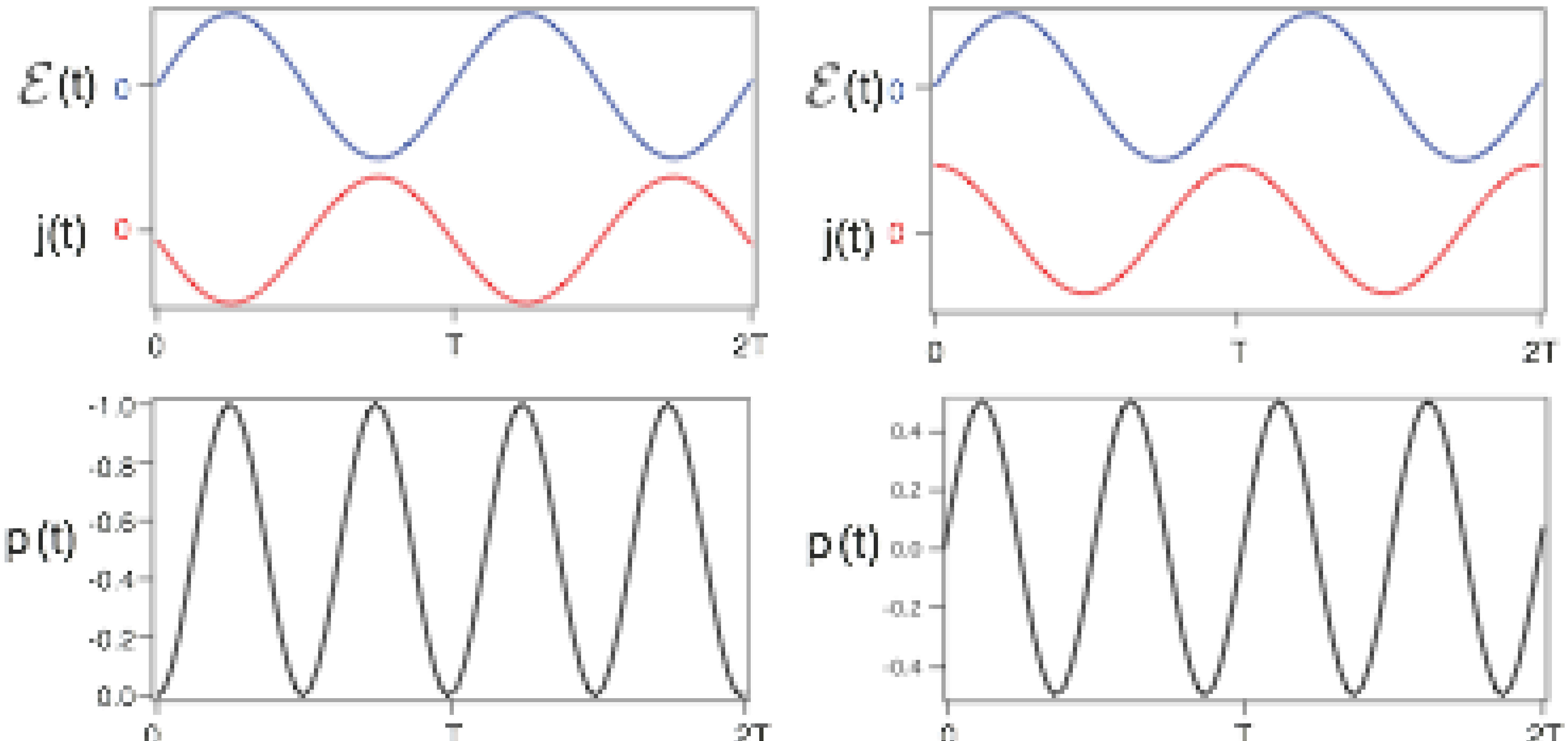
$$j(t) = \epsilon_0 \mathcal{E}(t) \left(i\omega\epsilon_r - \omega\epsilon_i \right)$$

energy dissipation

$$\overline{p} = \frac{1}{T} \int_0^T \mathcal{E}(t) j(t) dt$$

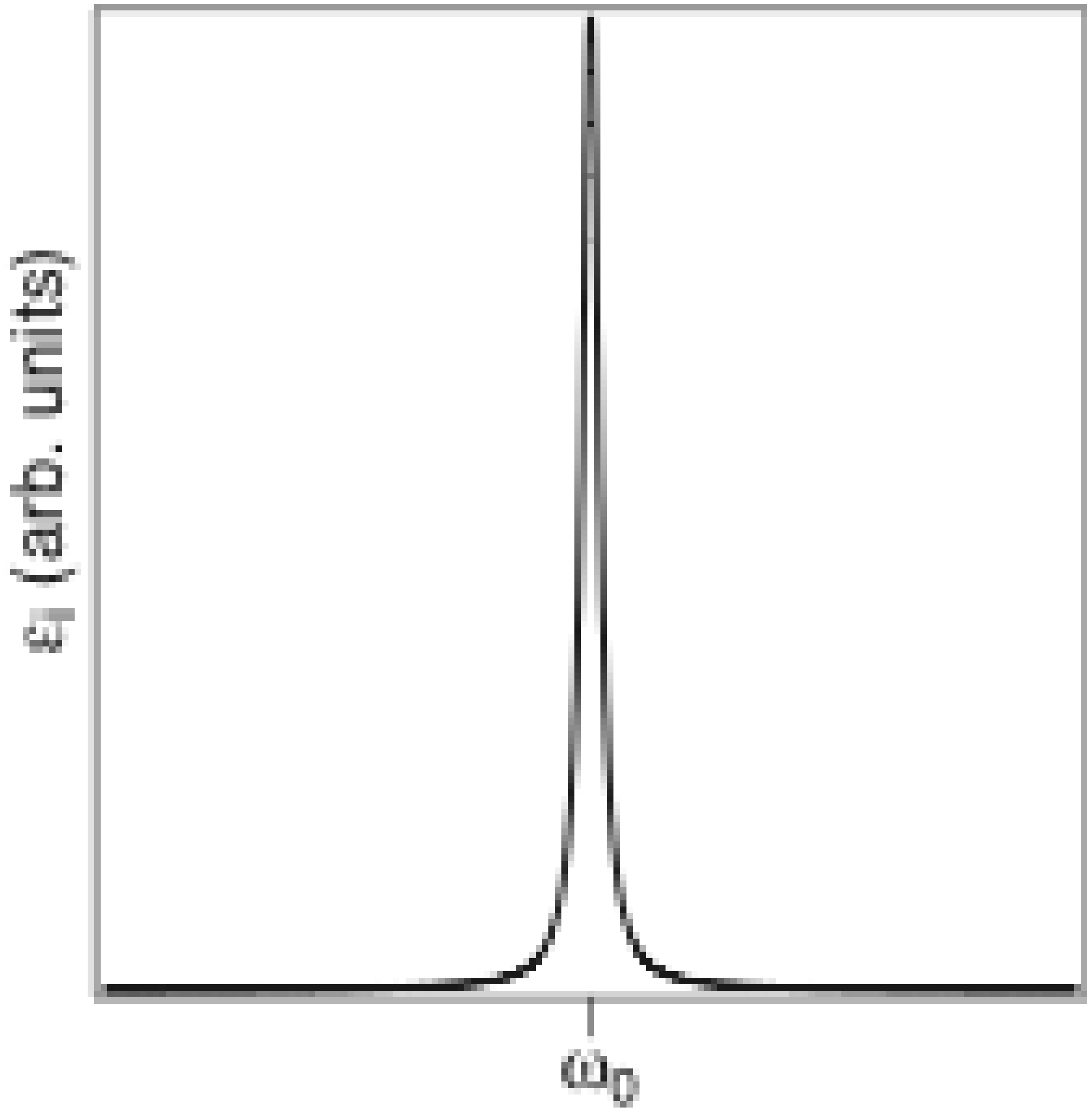
ε imaginary

ε real



The meaning of ε_i

energy dissipation, especially at resonance frequency



Frequency dependence of the dielectric constant: even higher frequencies (optical)

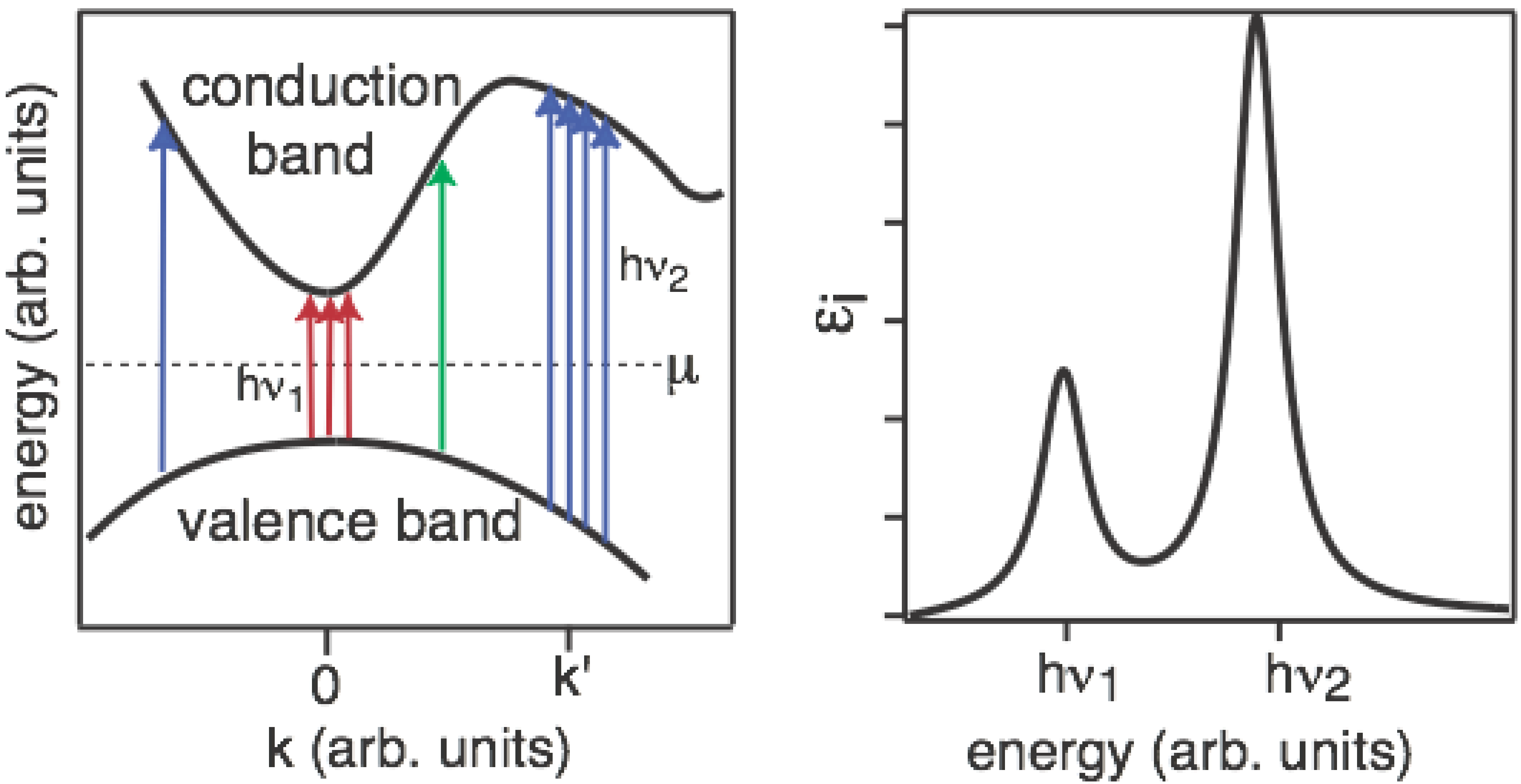
Si

CdSe

CdS

image source: wikipedia (Si) and http://woelen.homescience.net (CdSe, CdS)

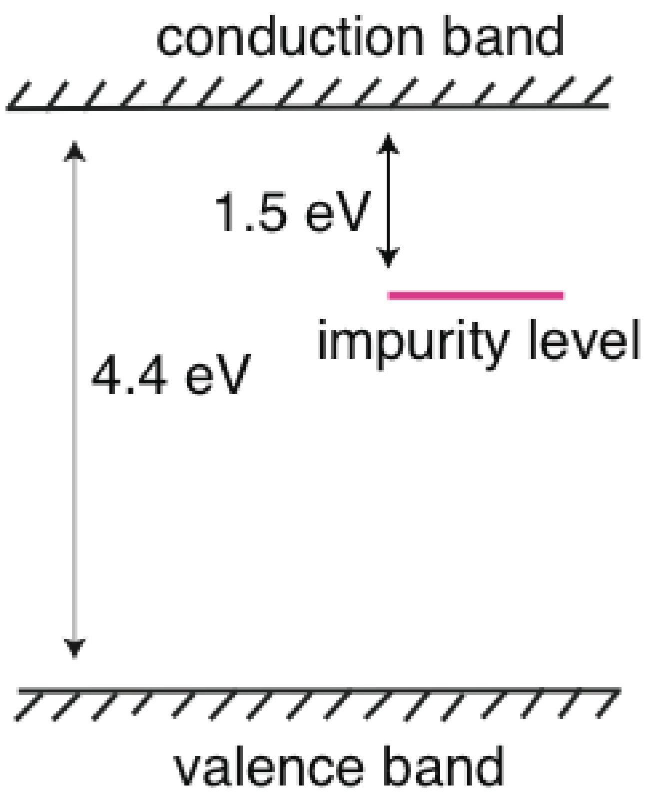
Frequency dependence of the dielectric constant: even higher frequencies (optical)



$$\epsilon_i(h\nu) \propto \sum_{\mathbf{k}} M^2 \delta(E_C(\mathbf{k}) - E_V(\mathbf{k}) - h\nu)$$

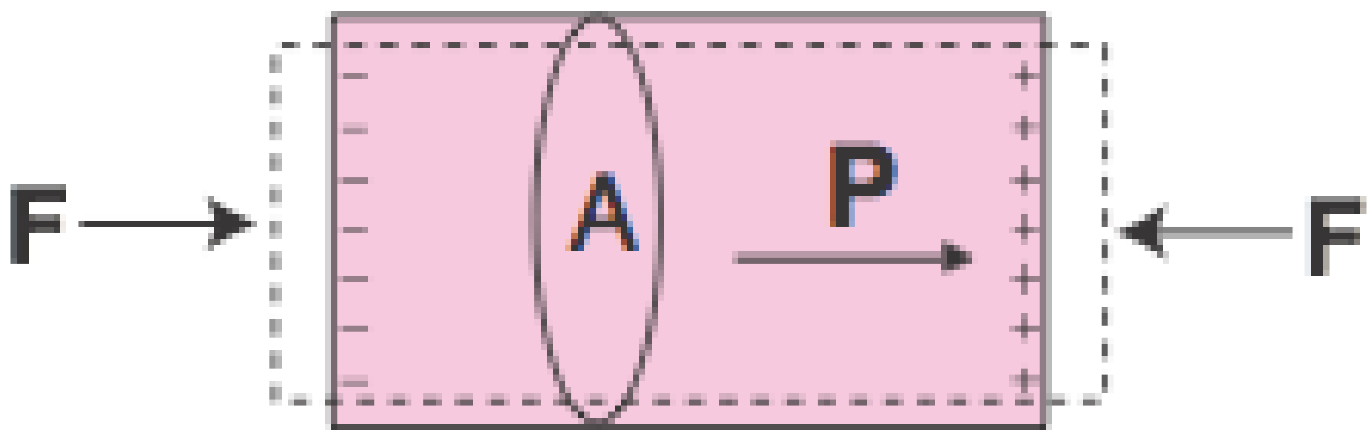
Impurities in dielectrics

- Single-crystals of wide-gap insulators are optically transparent (diamond, alumina)
- Impurities in the band gap can lead to absorption of light with a specific frequency
- Doping with shallow impurities can also lead to semiconducting behaviour of the dielectrics. This is favorable for high-temperature applications because one does not have to worry about intrinsic carriers (e.g. in the case of diamond or more likely SiC)

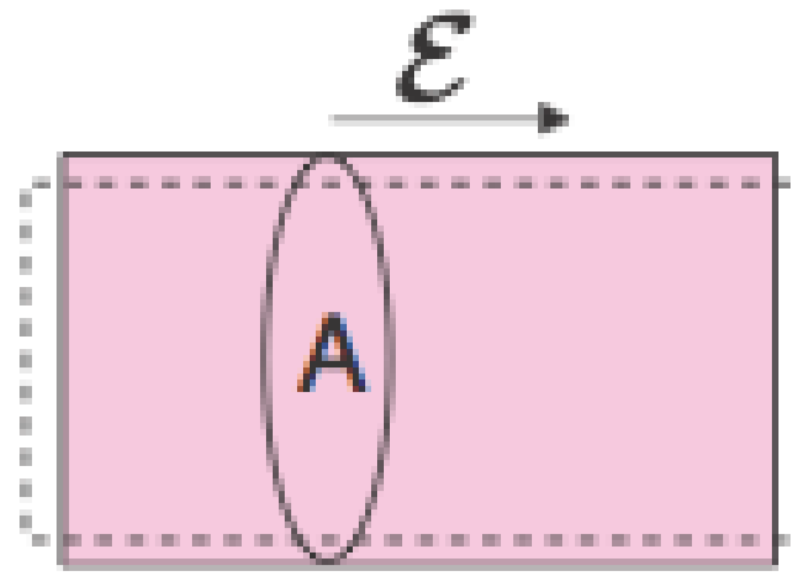


Red light: E = 1.8 eV
Blue light: E = 2.76 eV

Piezoelectricity

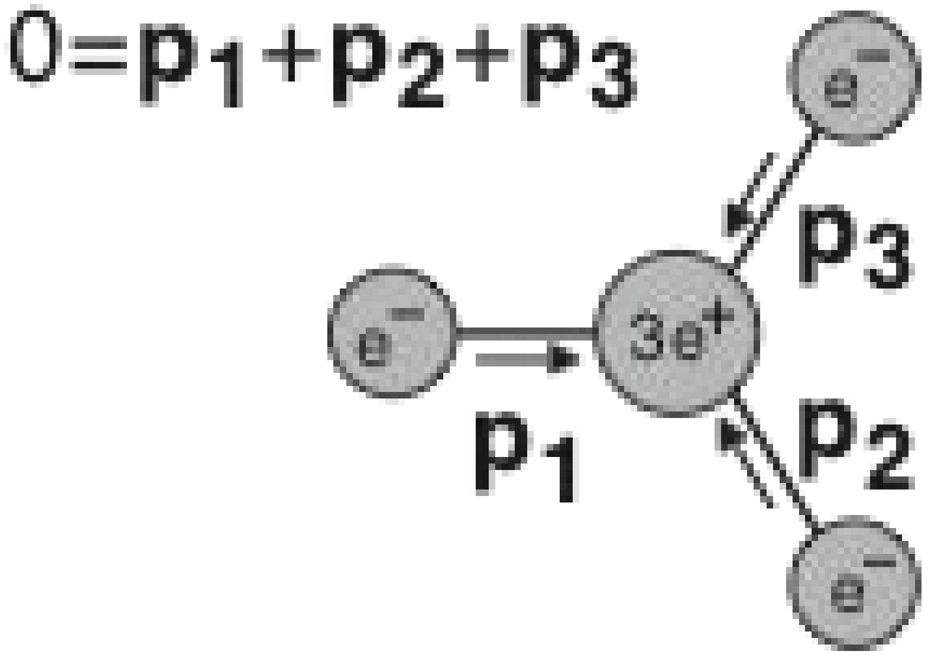


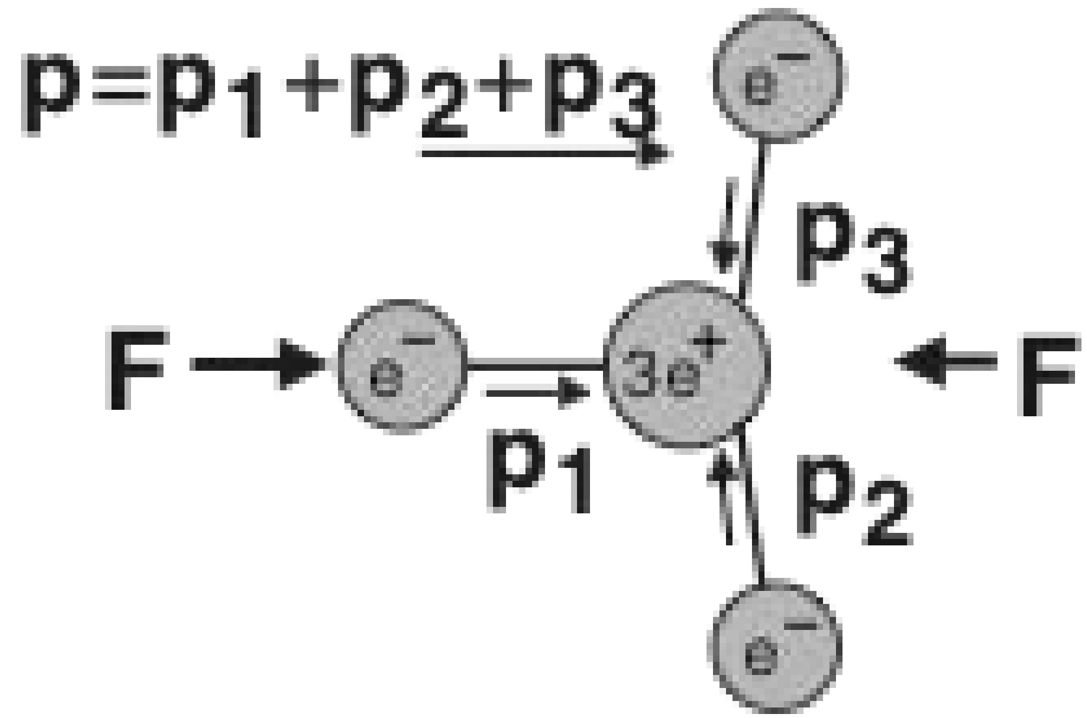
applying stress gives rise to a polarization



applying an electric field gives rise to strain

Piezoelectricity



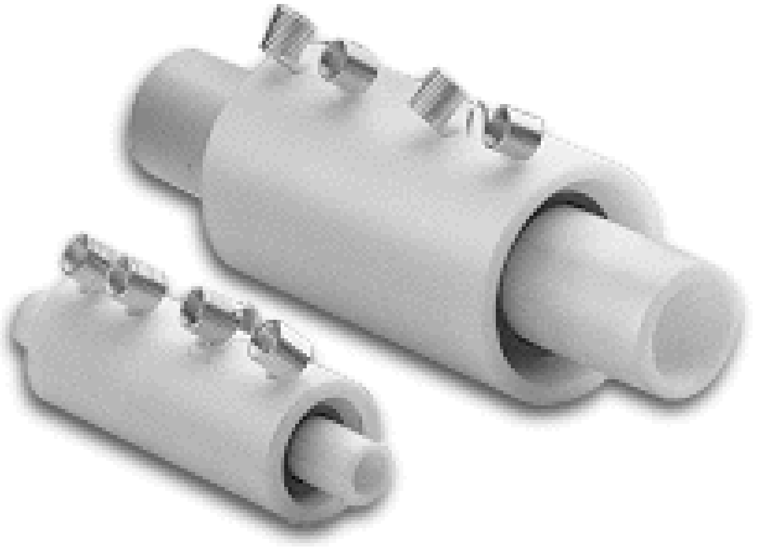


equilibrium structure
no net dipole

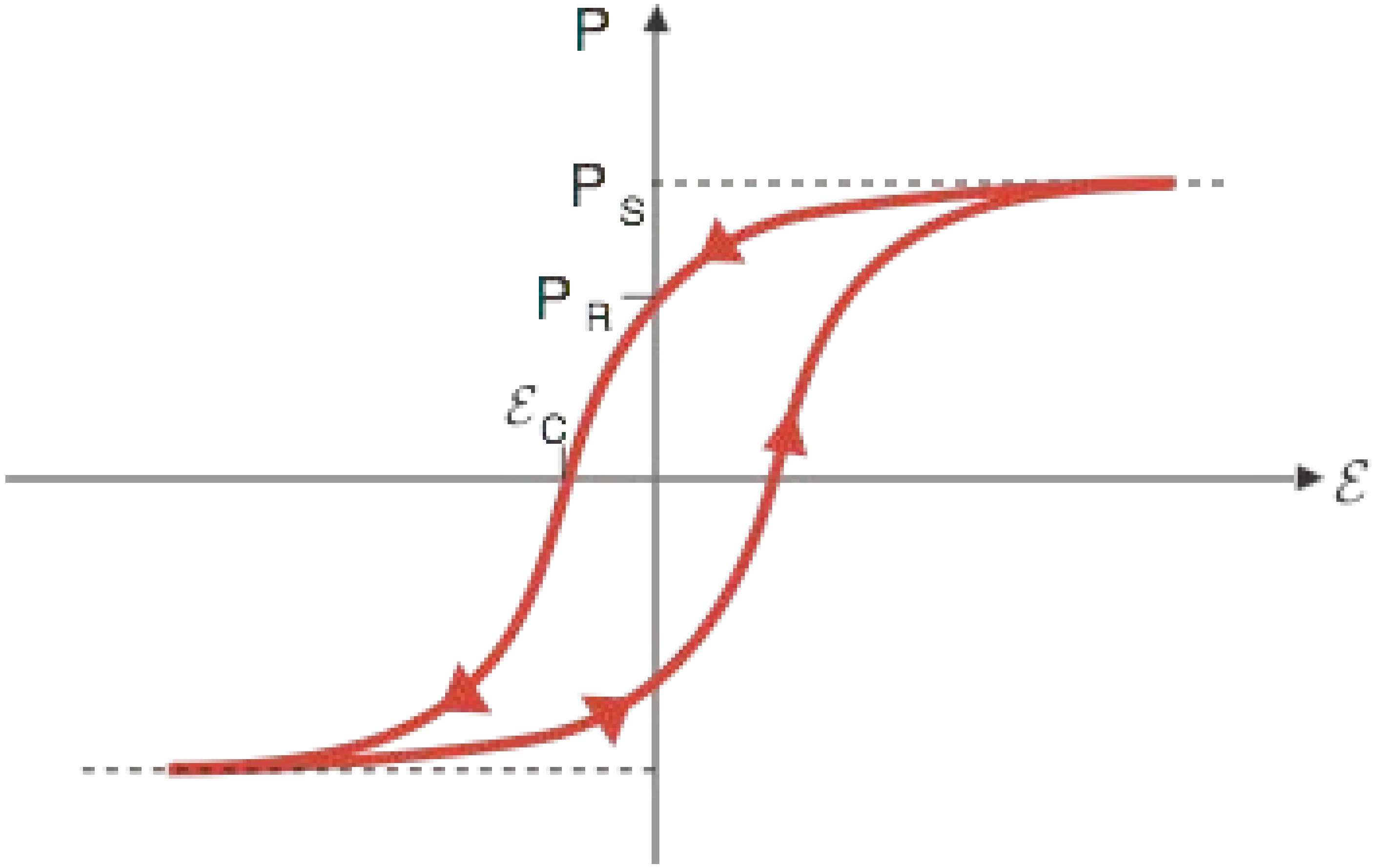
applying stress leads
finite net dipole

Applications (too many to name all....)

- Quartz oscillators in clocks (1 s deviation per year) and micro-balances (detection in ng range)
- microphones, speakers
- positioning: mm range (by inchworms) down to 0.01 nm range

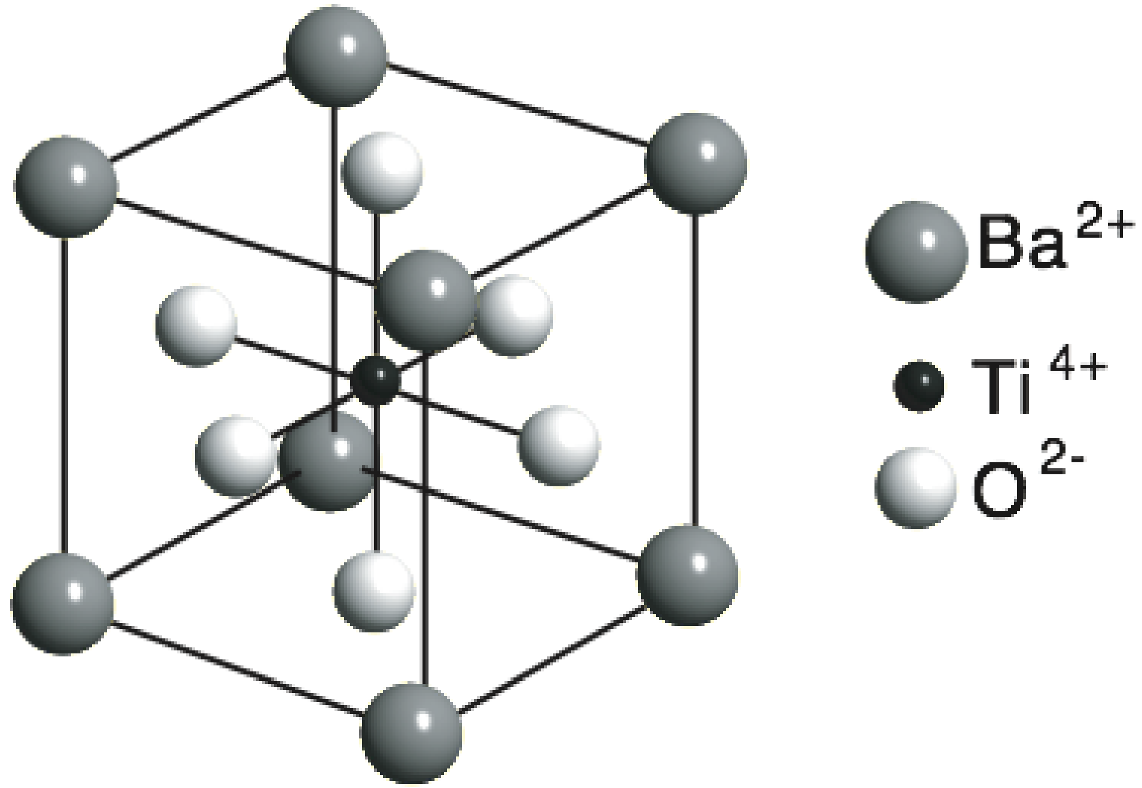


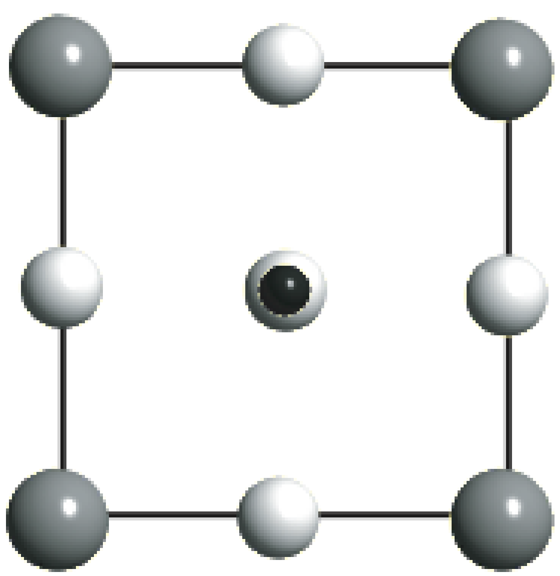
Ferroelectrics

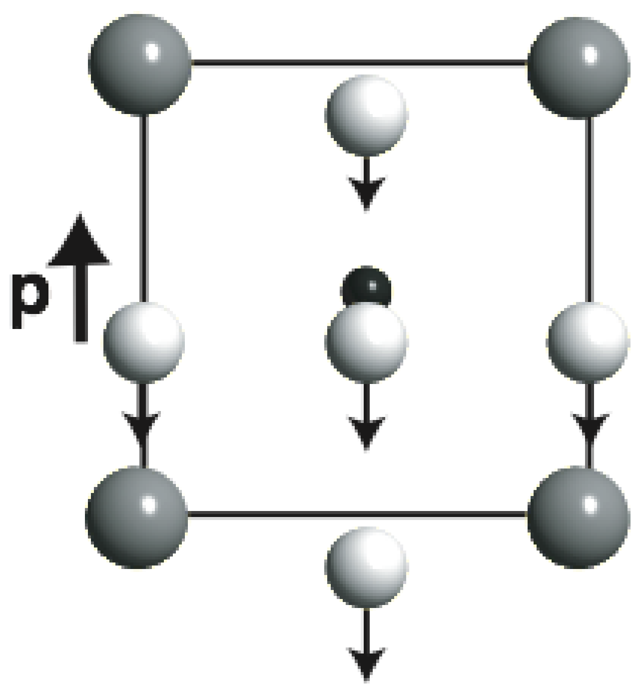


- Spontaneous polarization without external field or stress
- Very similar to ferromagnetism in many aspects: alignment of dipoles, domains, ferroelectric Curie temperature, “paraelectric” above the Curie temperature....
- But: here direct electric field interactions. Direct magnetic field interactions were far too weak to produce ferromagnetism.

Example: barium titanate ($BaTiO_3$)







ferroelectric

Frequency dependence of the dielectric constant: driven and damped harmonic motion

we start with the usual differential equation

$$\frac{d^2x}{dt^2} + \eta\frac{dx}{dt} + \omega_0^2 x = \frac{e\mathcal{E}_{loc}(x)}{M}$$

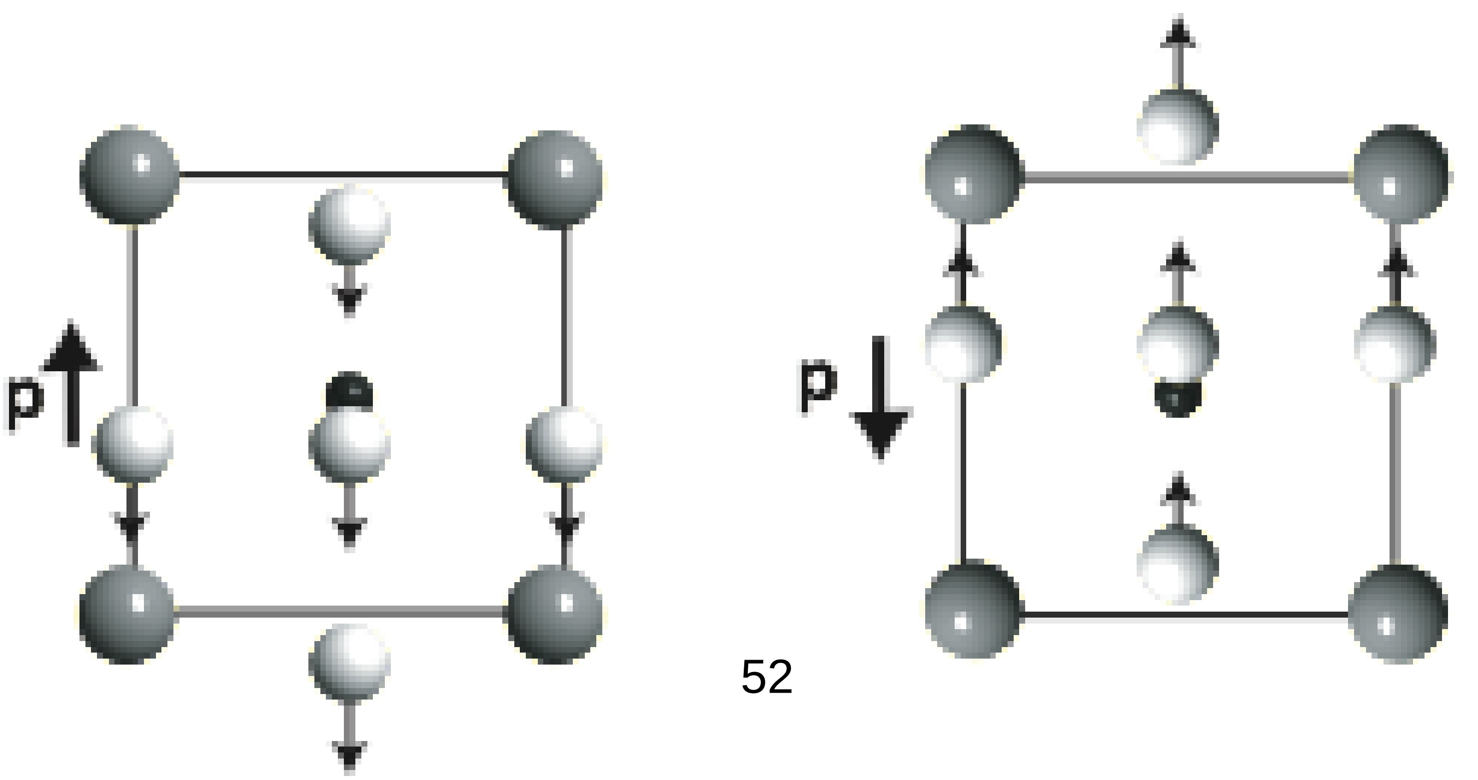
friction term

harmonic restoring term

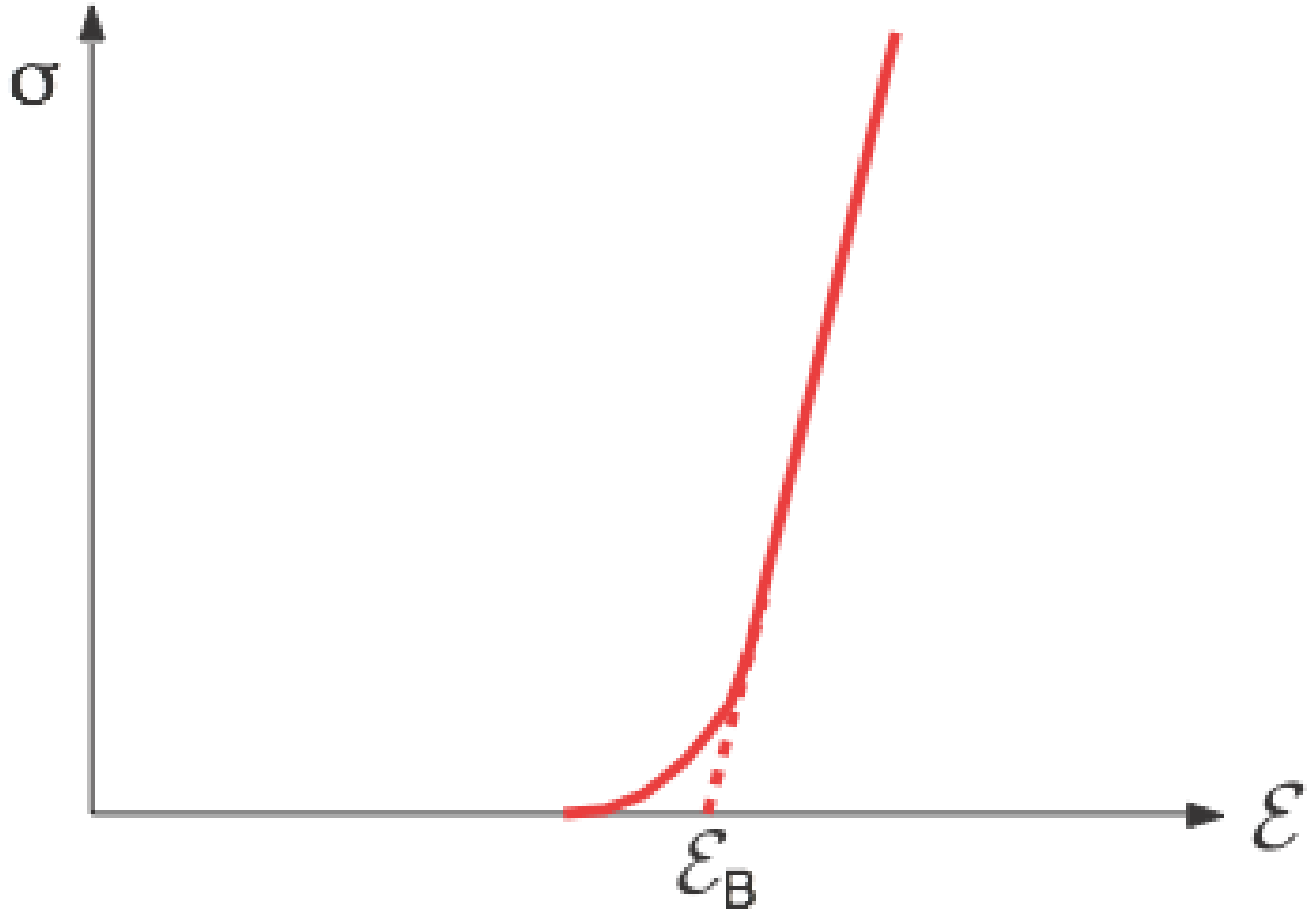
LOCAL field

Applications of ferroelectric materials

- Most ferroelectrics are also piezoelectric (but not the other way round) and can be applied accordingly.
- Ferroelectrics have a high dielectric constant and can be used to build small capacitors.
- Ferroelectrics can be switched and used as non-volatile memory (fast, low-power, many cycles).



Dielectric breakdown



- For a very high electric field, the dielectric becomes conductive.
- Mostly by kinetic energy: if some free electrons gather enough kinetic energy to free other electrons, an avalanche effect sets in (intrinsic breakdown)