Dielectric Solids / Insulators

Macroscopic description

dielectric polarisation $\mathbf{P} = \chi_e \epsilon_0 \boldsymbol{\mathcal{E}}$

$8.854187817 \times 10^{-12}\ \mathrm{C^2 J^{-1} m^{-1}}$

dielectric susceptibility χ_e (> 0)

dielectric constant $\epsilon = \chi_e + 1$

microscopic dipole $\mathbf{p} = q\boldsymbol{\delta}$

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

Plane-plate capacitor

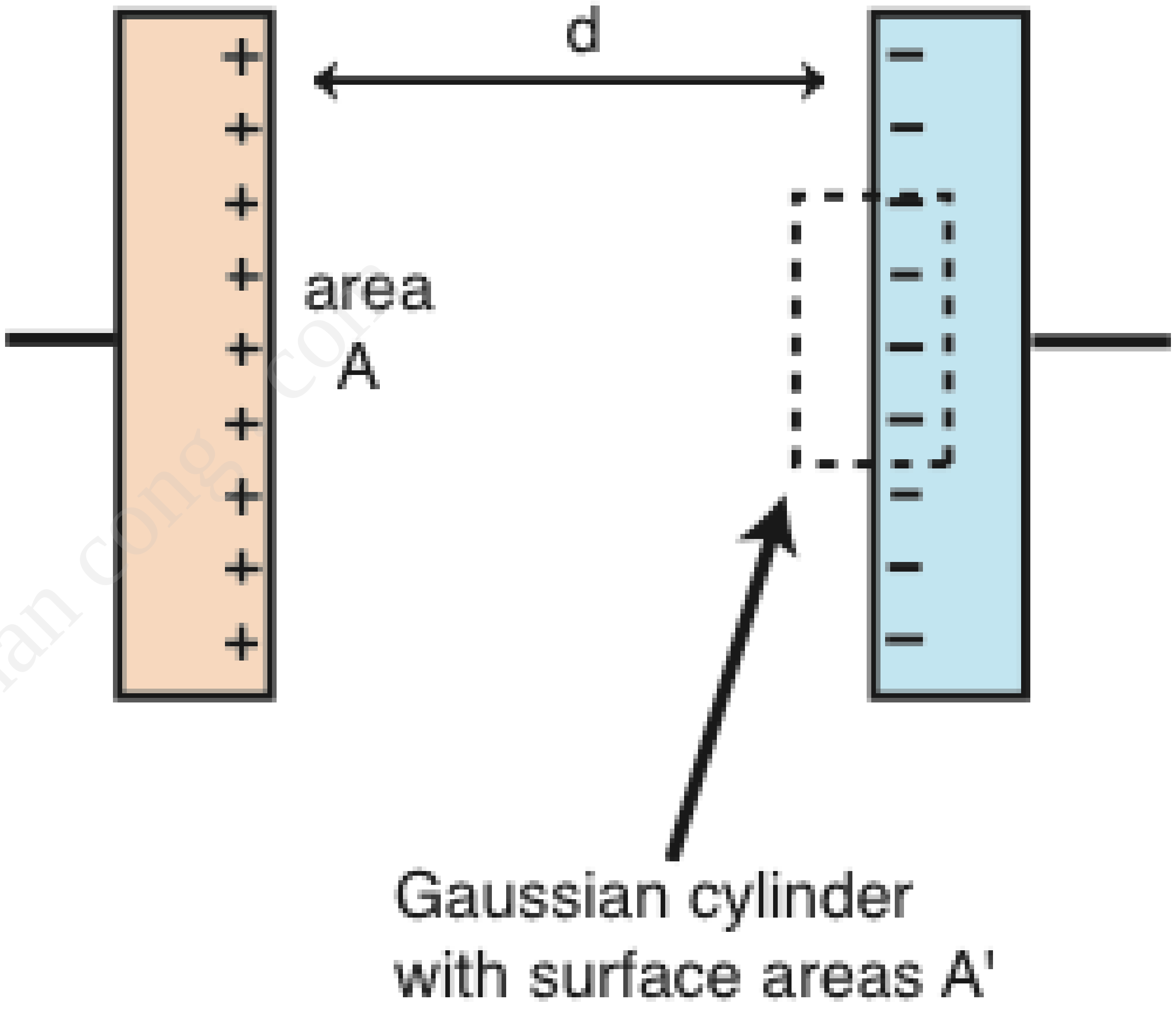
$$\oint \boldsymbol{\mathcal{E}}\, d\mathbf{A} = \oint \mathcal{E}_\perp\, dA = \frac{Q_{encl}}{\epsilon_0}$$

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

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

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

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



Gaussian cylinder
with surface areas A'

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

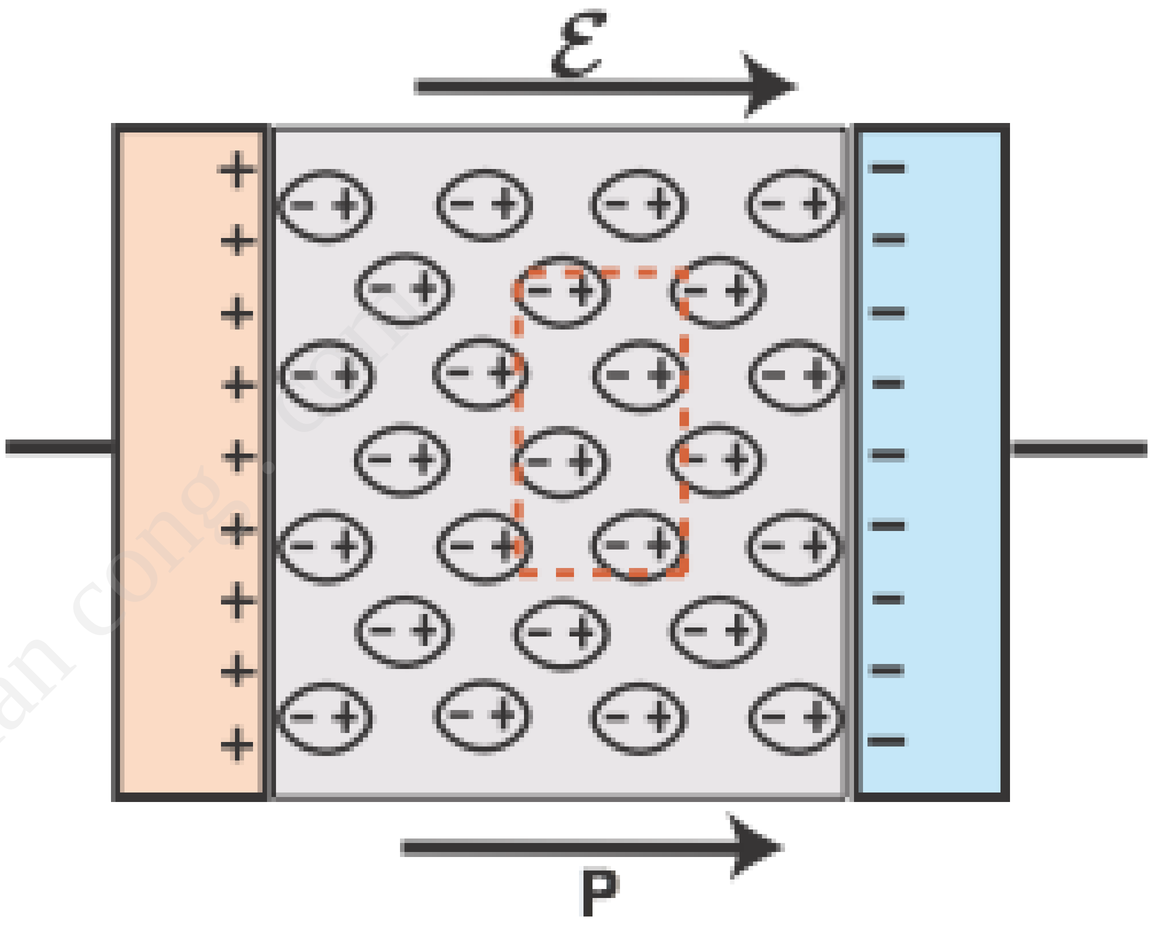
Plane-plate capacitor with dielectric

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

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

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

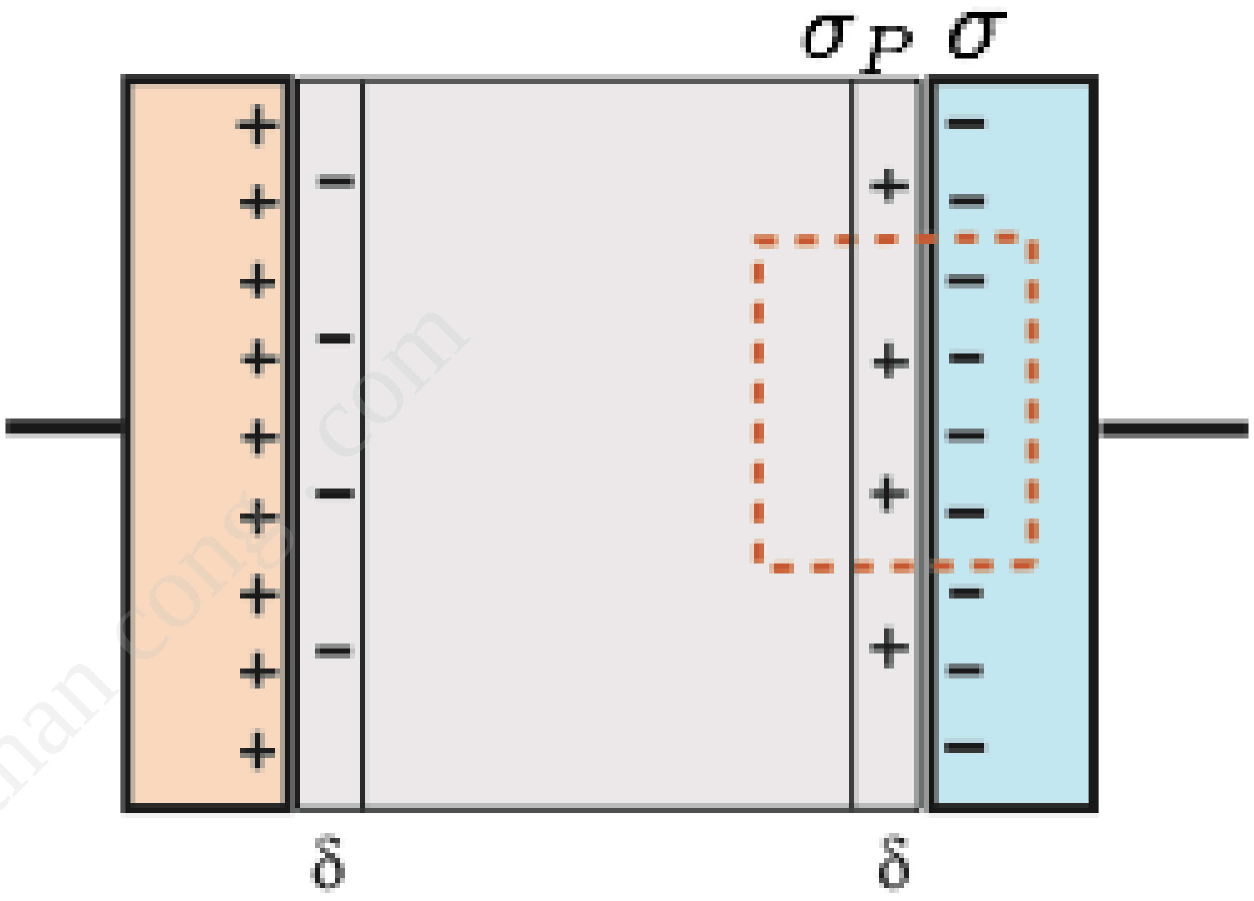
$$\mathcal{E} = \frac{\sigma - \sigma_P}{\epsilon_0} = \frac{1}{\epsilon_0}(\sigma - P)$$

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

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

$\varepsilon = 1 + \chi_e$

so the E-field decreases by a factor of ε



capacitance increase by a factor of ε

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

The quest for materials with high Σ

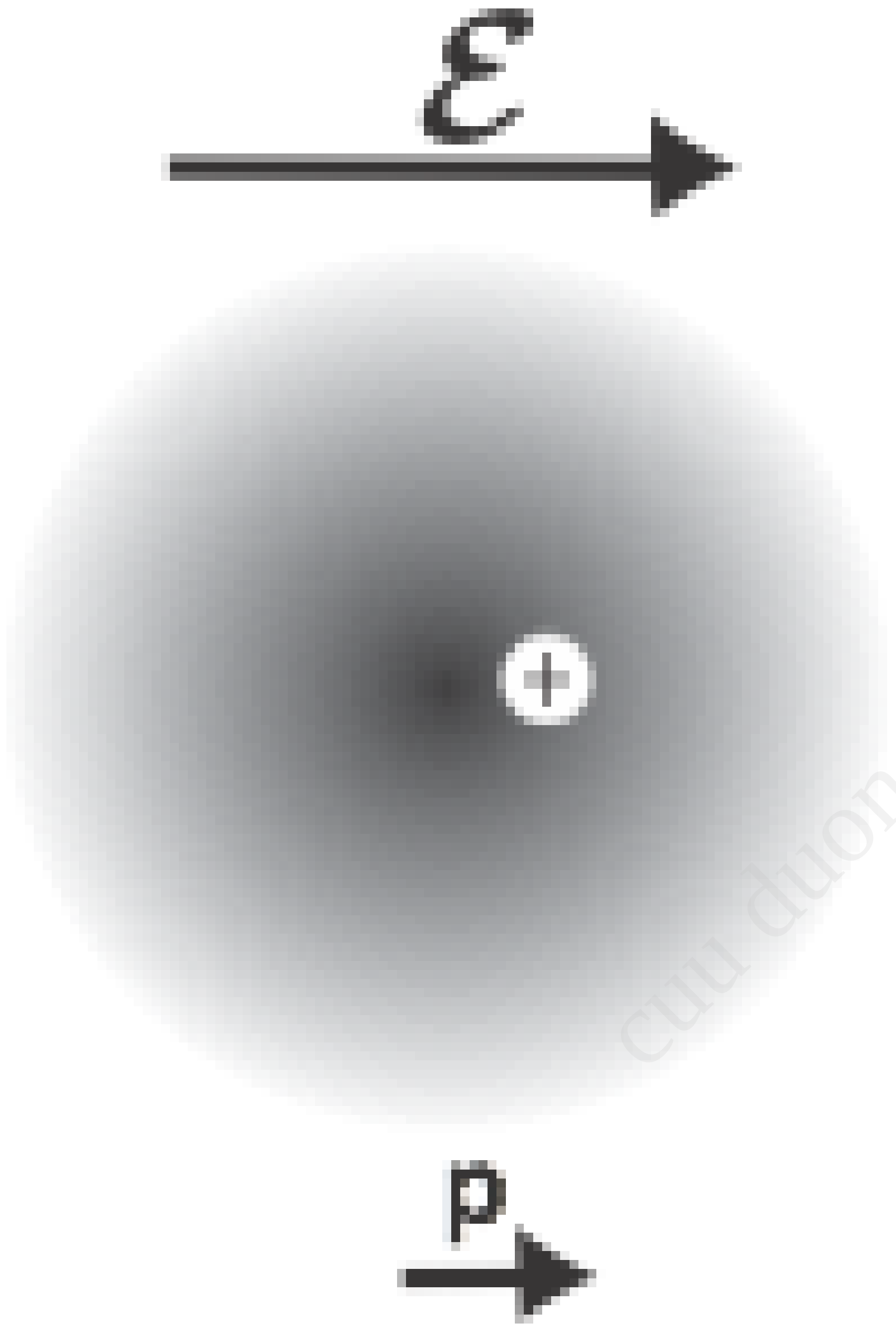
gate area $A = l^2$

required charge to make it work $Q = CU = \frac{UA\epsilon\epsilon_0}{d}$

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

Microscopic origin: electronic polarization



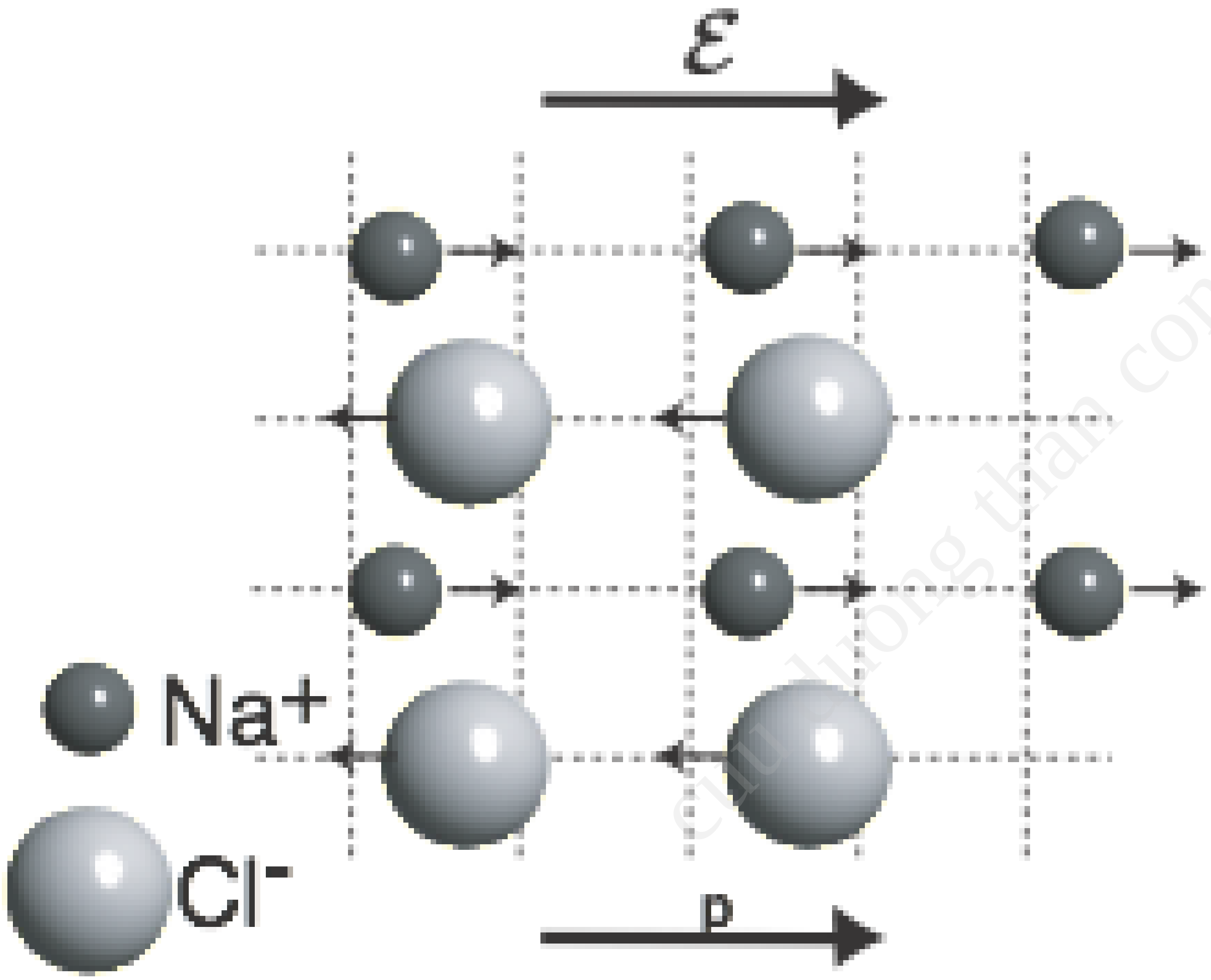
for one atom

$$\mathbf{p} = \alpha \boldsymbol{\mathcal{E}}$$

for the solid

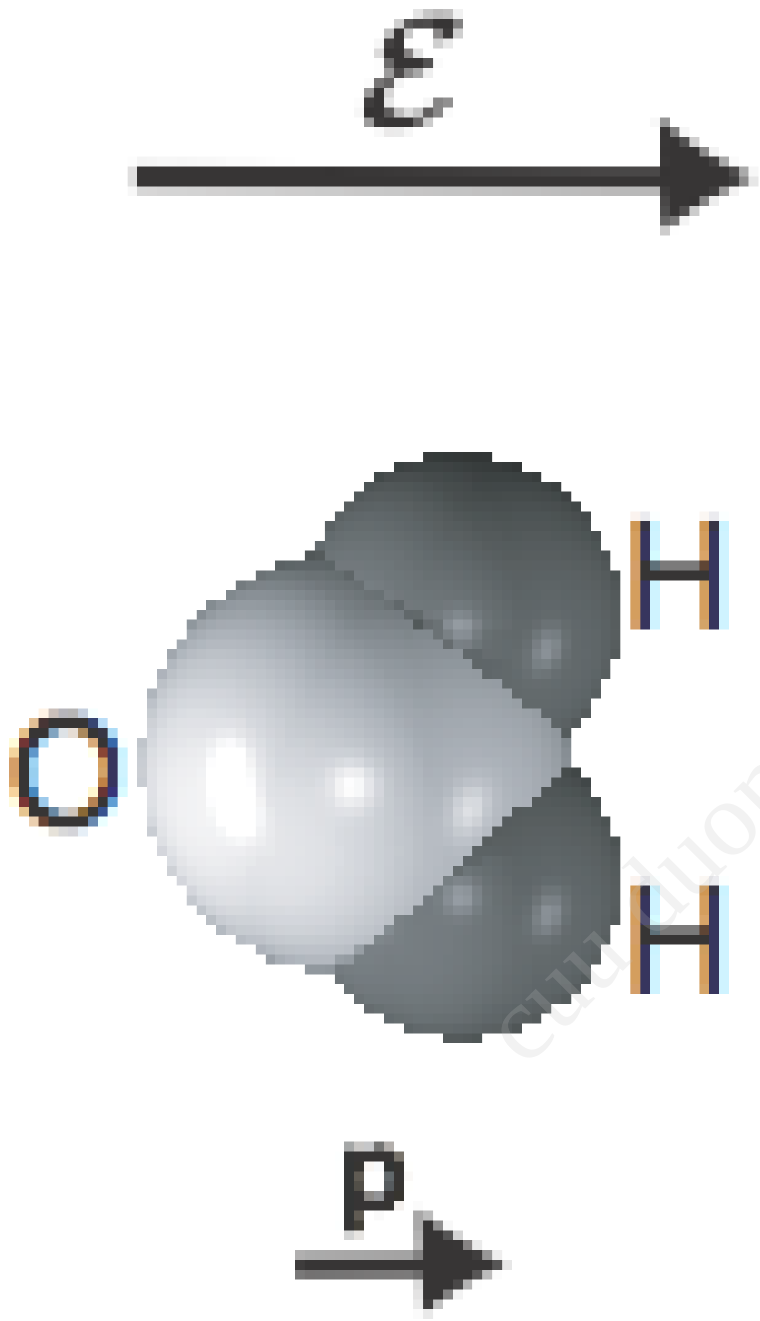
$$\mathbf{P} = \frac{N}{V} q\boldsymbol{\delta} = \frac{N}{V}\mathbf{p}$$

Microscopic origin: ionic polarization



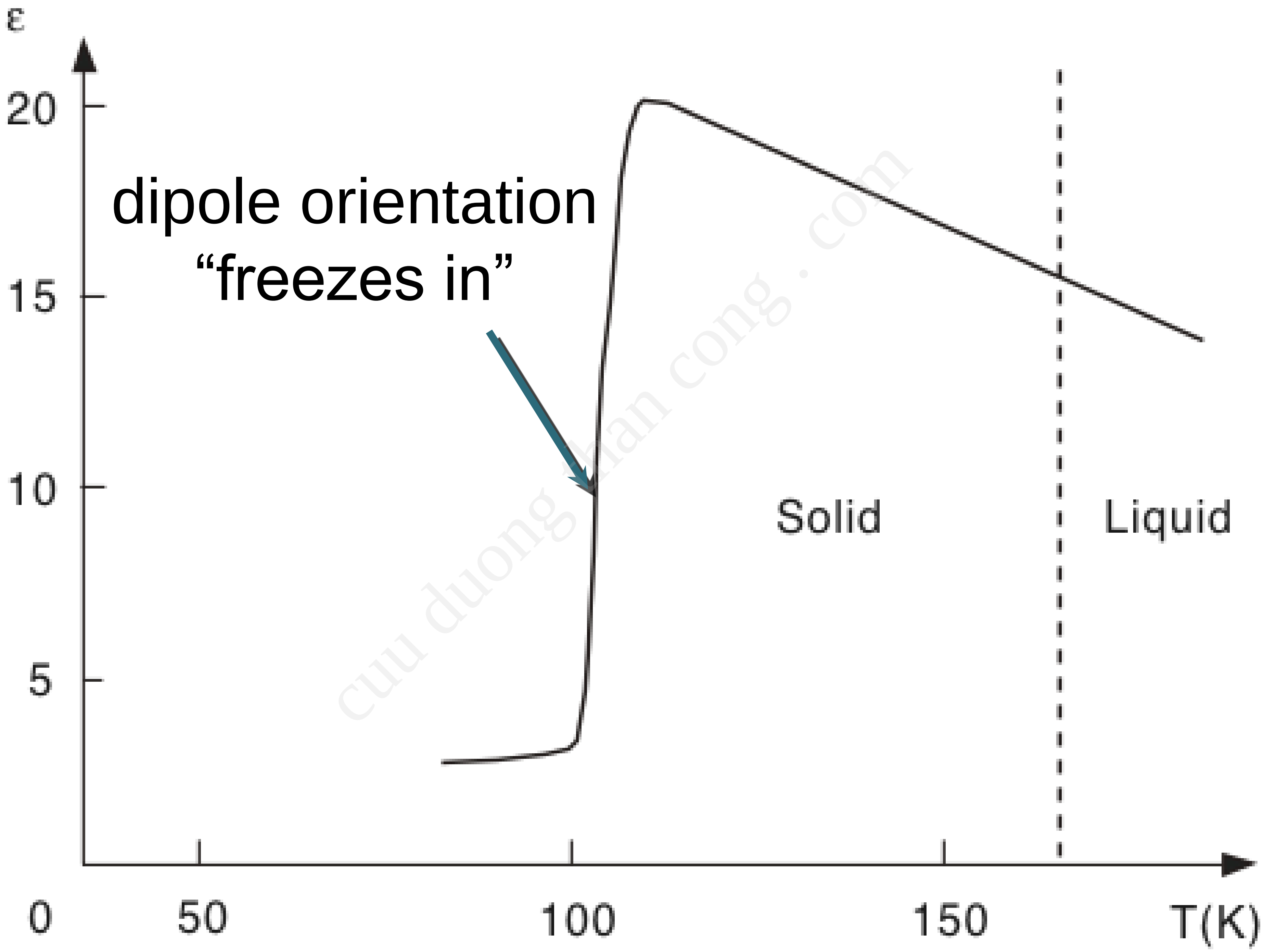
$$\mathbf{P} = \frac{N}{V} q\delta = \frac{N}{V}\mathbf{p}$$

Microscopic origin: orientational polarization



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

Example: Hydrogen chloride

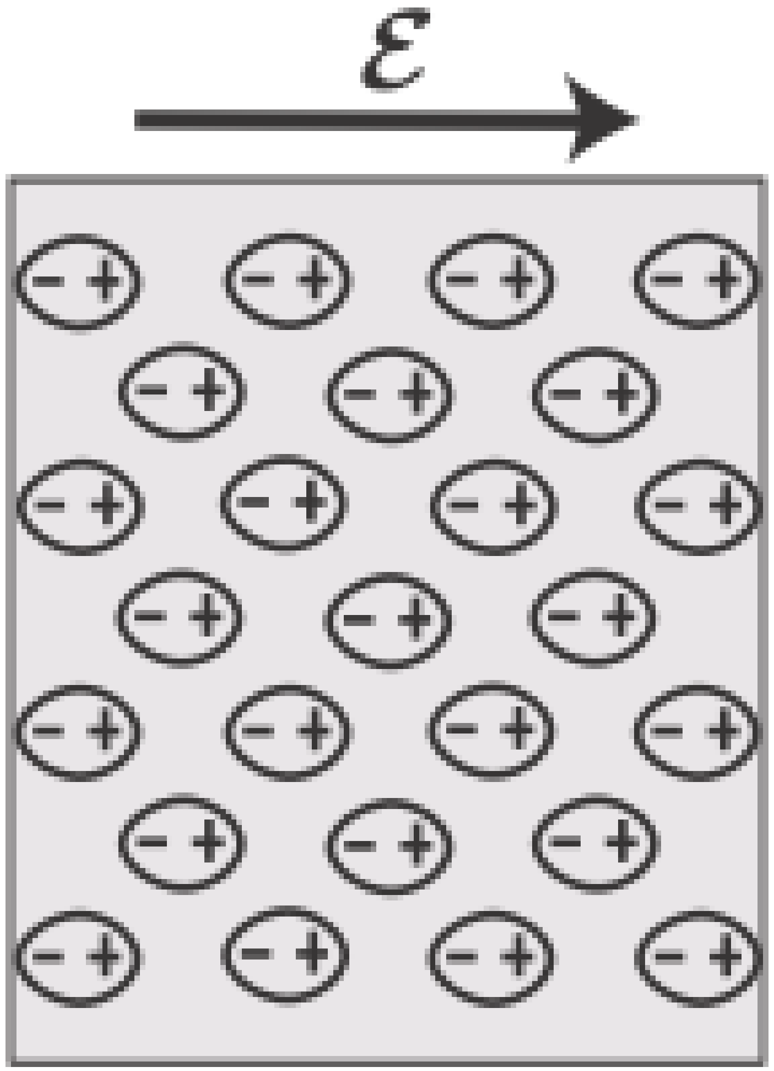


dipole orientation
"freezes in"

The local field

From the measured ε can we figure out α?

average field:
external plus internal



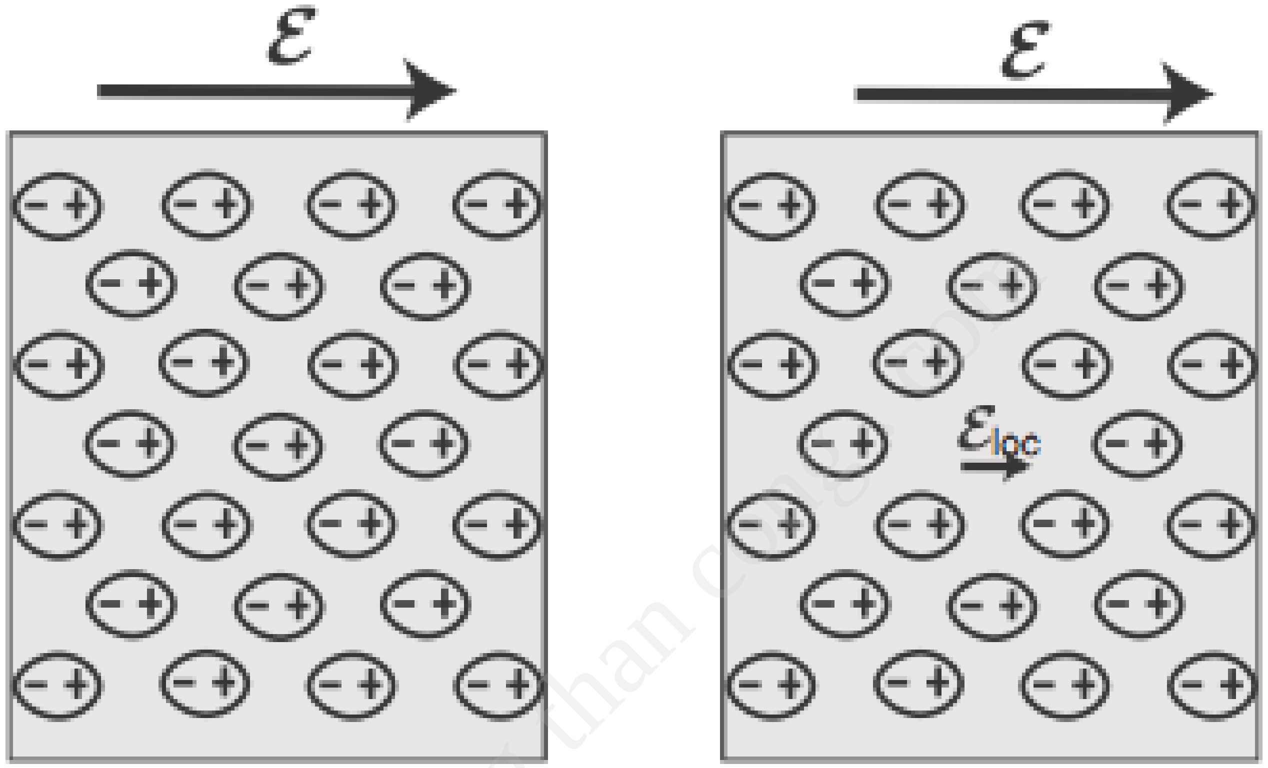
$$\mathbf{P} = (\epsilon - 1)\epsilon_0 \boldsymbol{\mathcal{E}} = \frac{N}{V}\mathbf{p} = \frac{N}{V}\alpha\boldsymbol{\mathcal{E}}$$

$$\alpha = \frac{(\epsilon - 1)\epsilon_0 V}{N}$$

simple but unfortunately also incorrect!

The local field

What is the electric field each dipole ‘feels’ in a dielectric?



the actual local field is higher

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

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

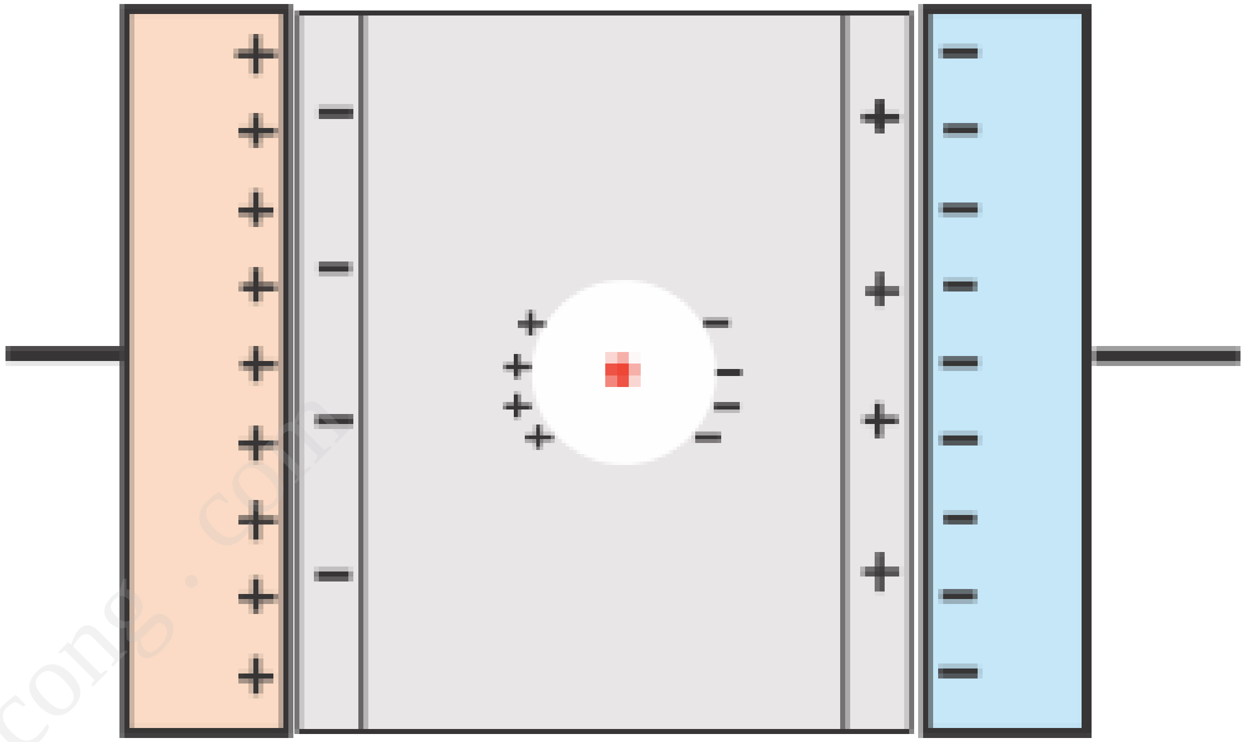
$$\mathbf{P} = (\epsilon - 1)\epsilon_0\boldsymbol{\mathcal{E}}$$

Clausius-Mossotti relation

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

(next few slides optional)

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 $\mathbf{E} = \mathbf{E}_0 + \mathbf{E}_1$

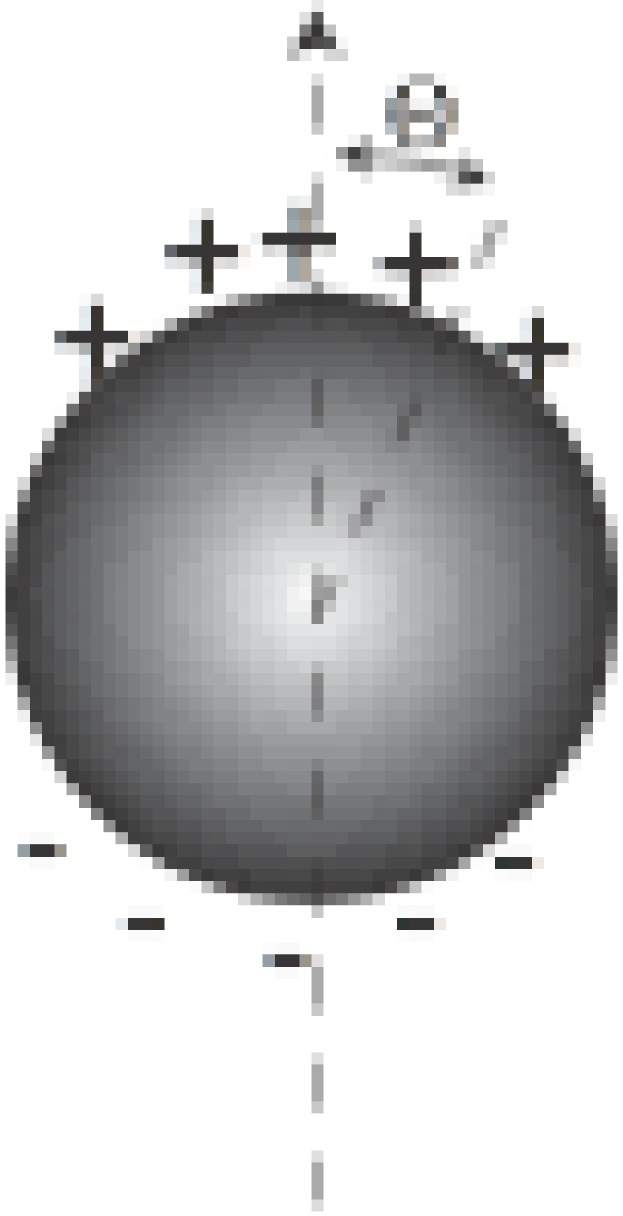
field from the surface dipoles of a spherical cavity large against microscopic dimensions $\mathbf{E}_2$

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

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

The local field at a point in the dielectric

calculation of the cavity field
(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

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

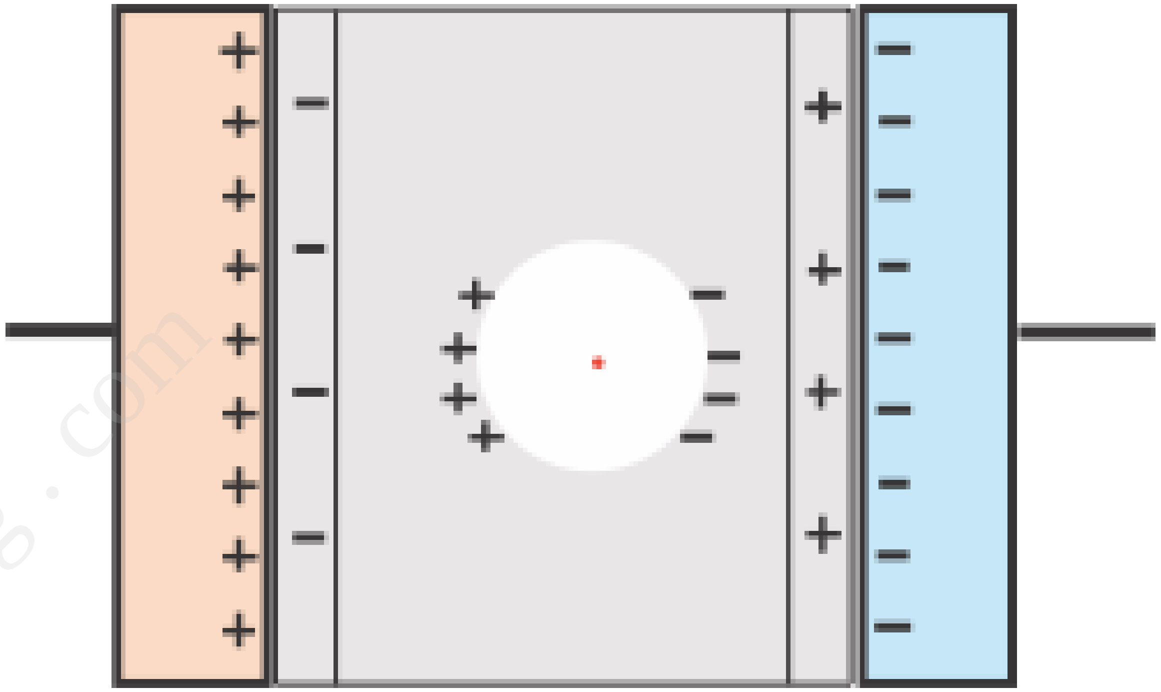
surface charge density on sphere

$$\sigma = P\cos\Theta$$

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

The local field at a point in the dielectric

calculation of the field
inside the cavity for a cubic lattice



field of a dipole (along z)

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

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

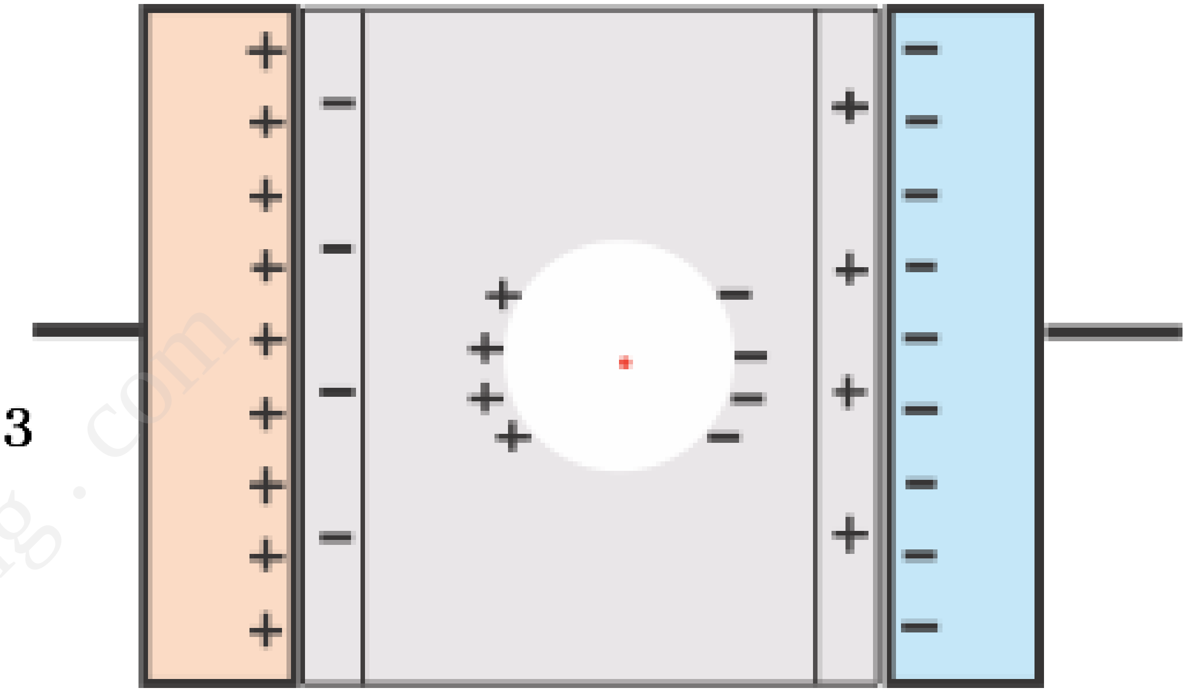
field at centre for all dipoles in cavity

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

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

The local field at a point in the dielectric

calculation of the total local field



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

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

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

it follows that

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

(end of optional slides)

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 or

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

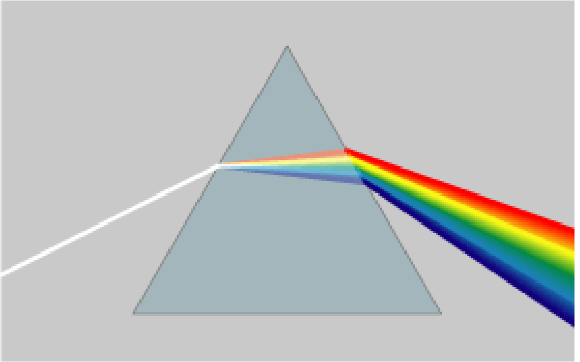
$$\epsilon = \frac{3\epsilon_0 V/N + 2\alpha}{3\epsilon_0 V/N - \alpha}$$

Frequency dependence of the dielectric constant

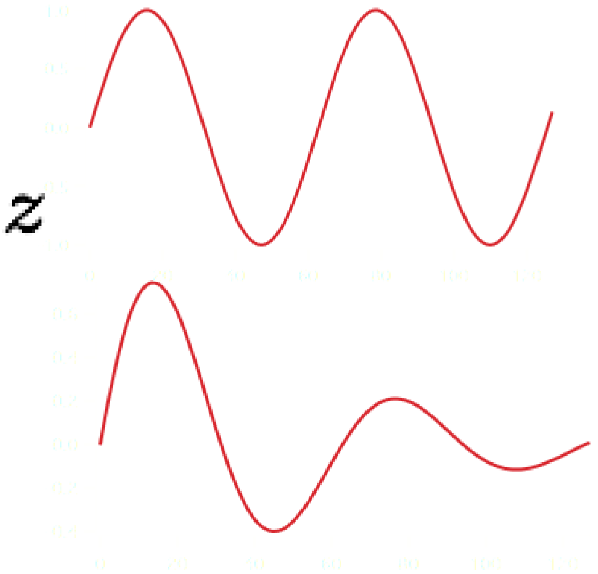
plane wave $$\mathcal{E}(z,t) = \mathcal{E}_0 e^{i(kz-\omega t)}$$

$$k = \frac{2\pi N}{\lambda_0}$$

complex index of refraction $$N = n + i\kappa$$



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



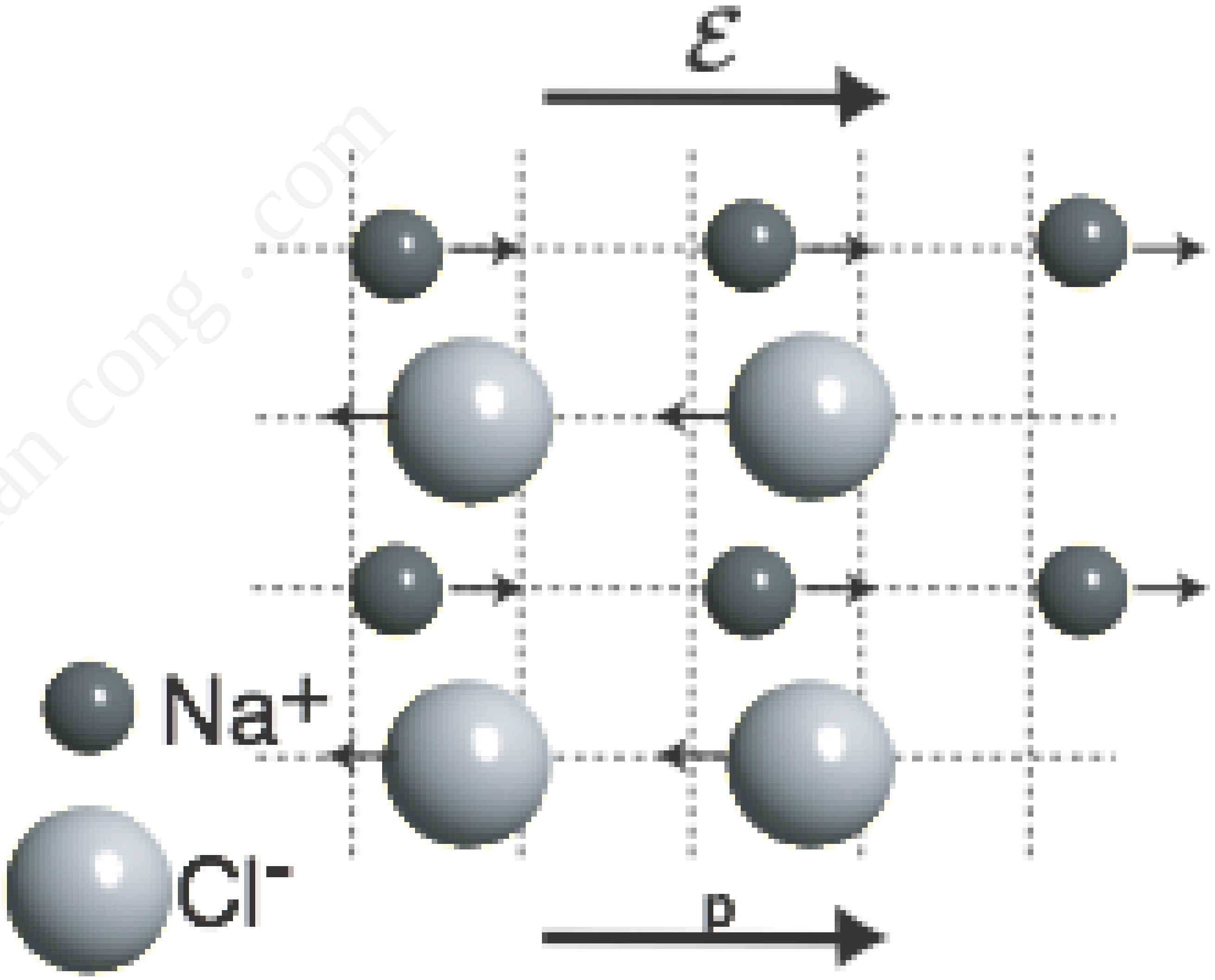
Maxwell relation $$N = \sqrt{\epsilon} = \sqrt{\epsilon_r + i\epsilon_i}$$

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

all the interesting physics in in the dielectric function!

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

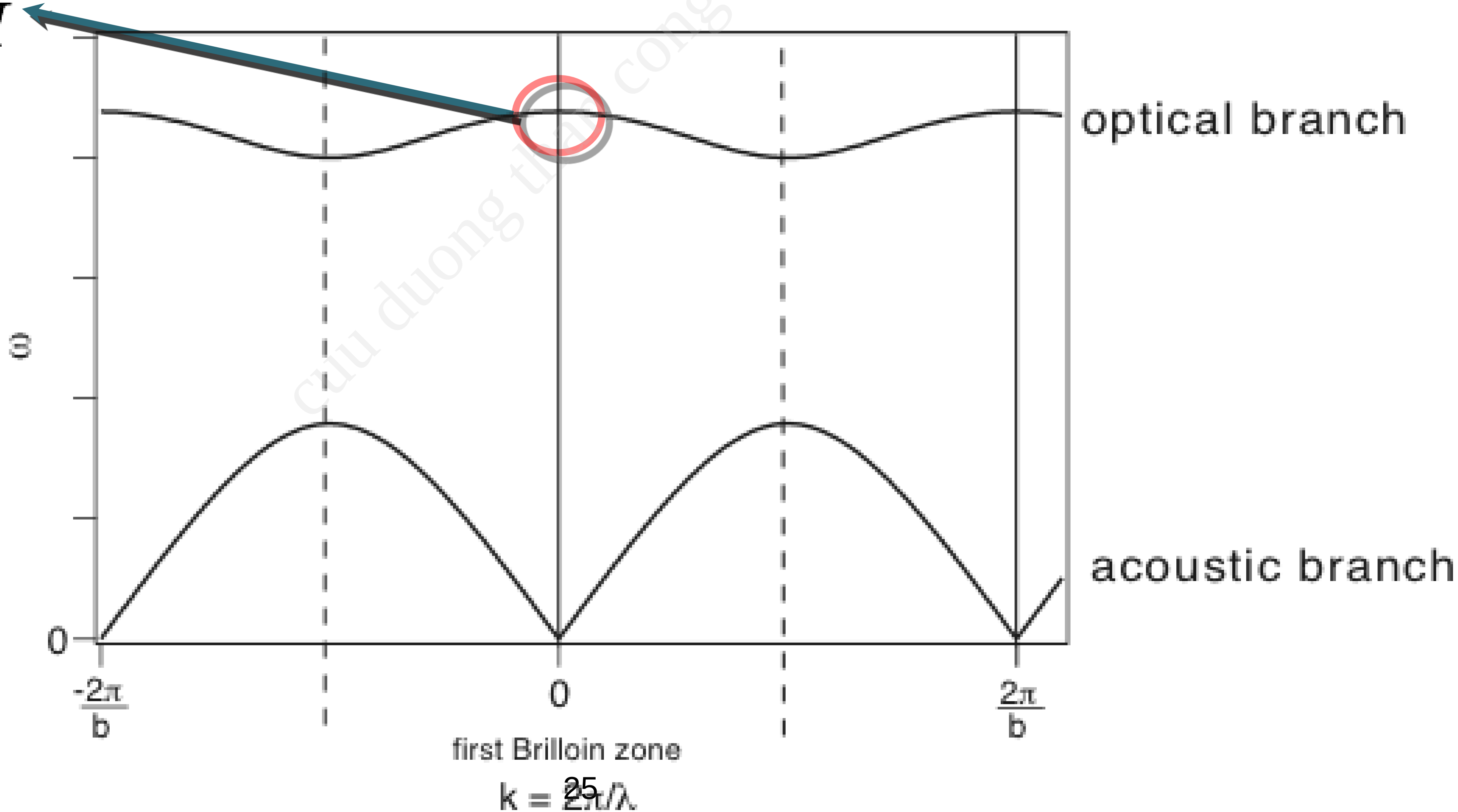
Frequency dependence of the dielectric constant: driven and damped harmonic motion

- 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

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)

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

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

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

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

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

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

real part imaginary part

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

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

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

$$P_i = 0$$

$$\epsilon_{\text{opt}} = \frac{N\alpha}{V\epsilon_0} + 1$$

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

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

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

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

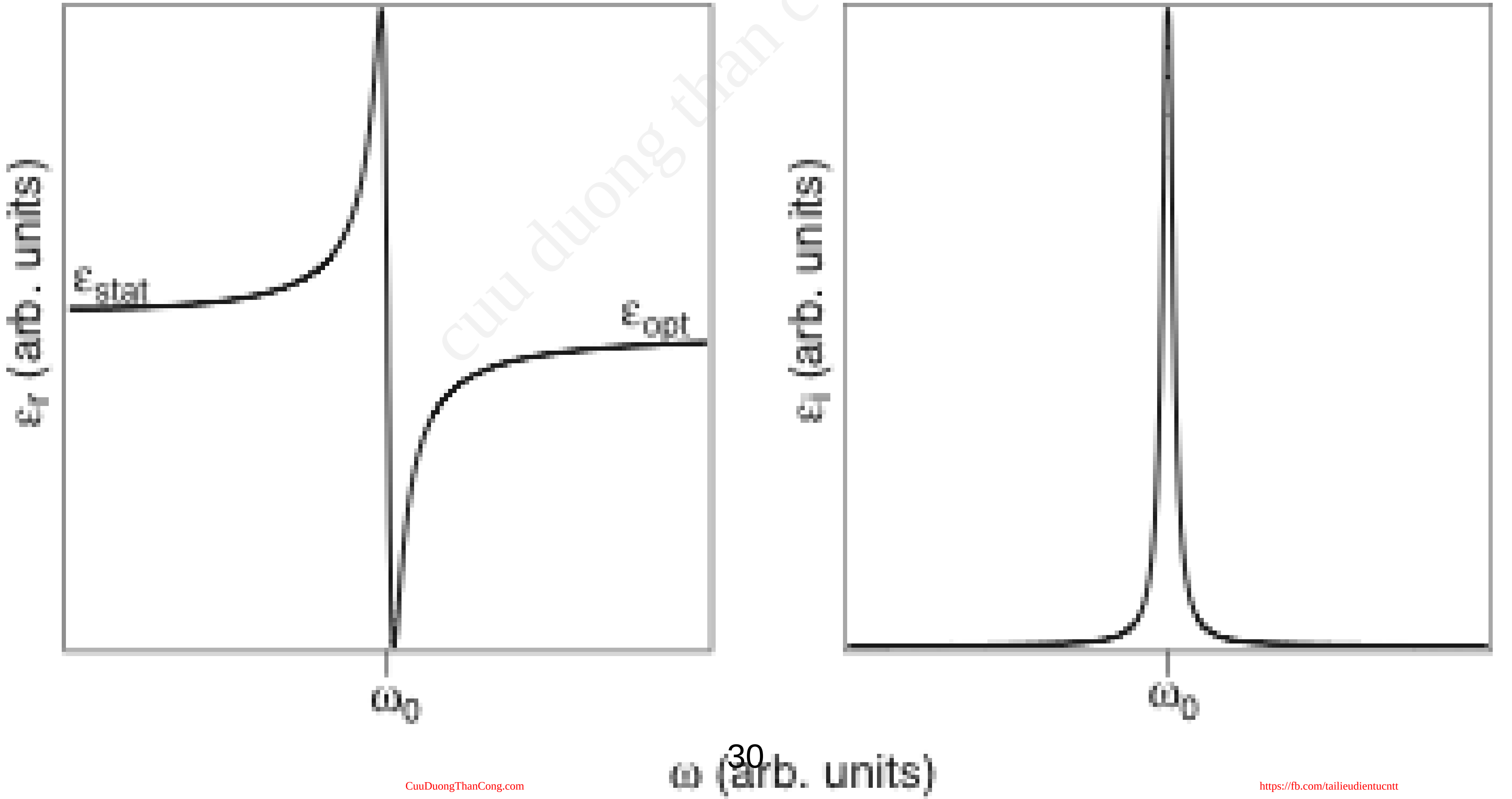
$$\epsilon_r(\omega) = \frac{Ne^2}{V\epsilon_0 M}\frac{\omega_0^2-\omega^2}{(\omega_0^2-\omega^2)^2+\eta^2\omega^2} + \epsilon_{opt}$$

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

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

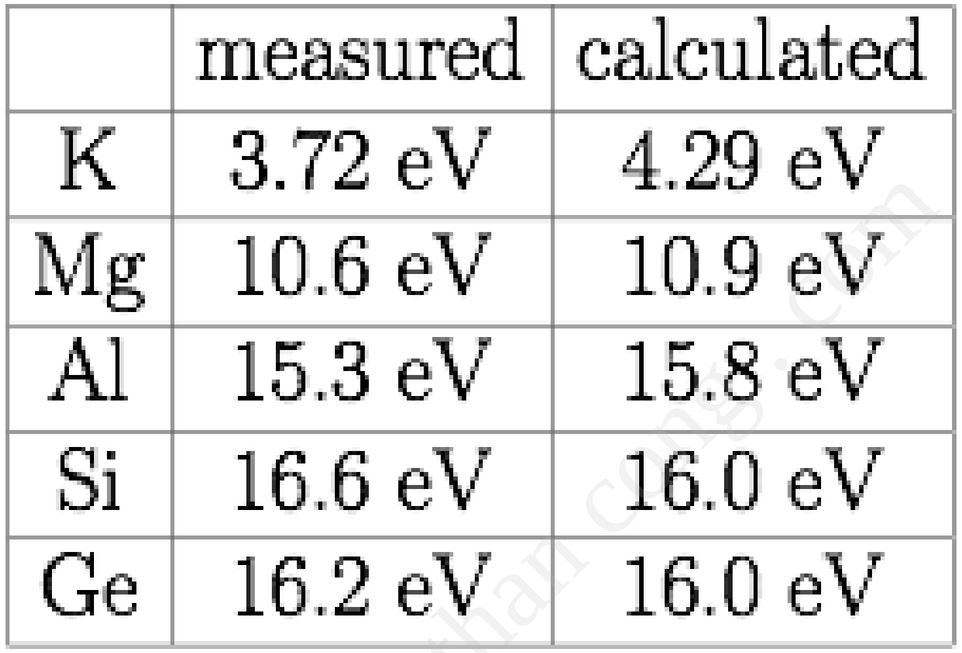
$$\epsilon = \epsilon_r + i\epsilon_i$$

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



remember the plasma oscillation in a metal: even higher frequencies

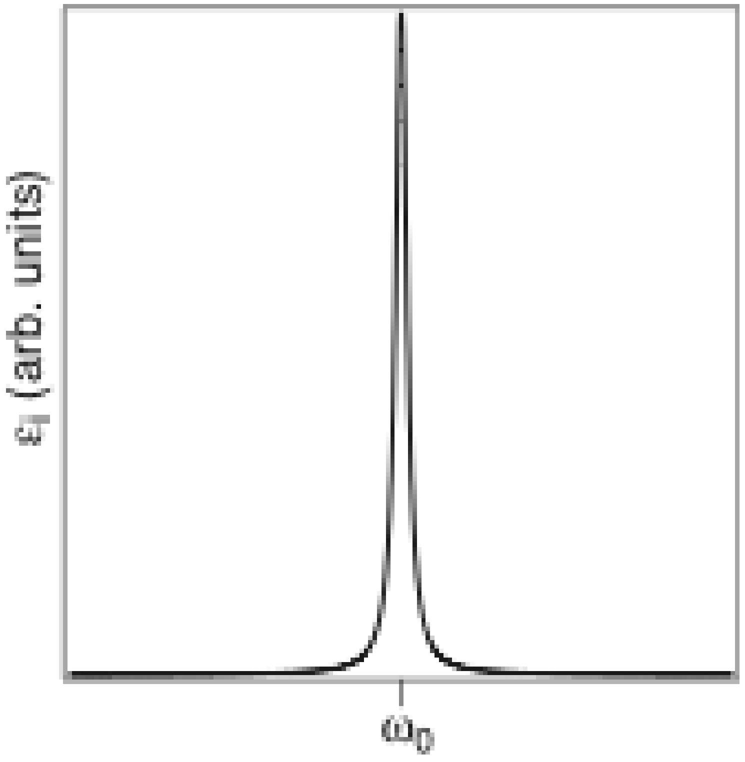
values for the plasma energy $\hbar\omega_P$



	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 meaning of ε_i



instantaneous power dissipation (per unit volume)

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

use

$$\mathcal{E}(t) = \mathcal{E}_0 \exp(-i\omega t) \qquad \mathbf{j} = \mathrm{curl}\mathbf{H} - \frac{\partial \mathbf{D}}{\partial t}$$

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

on average the dissipated power is

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

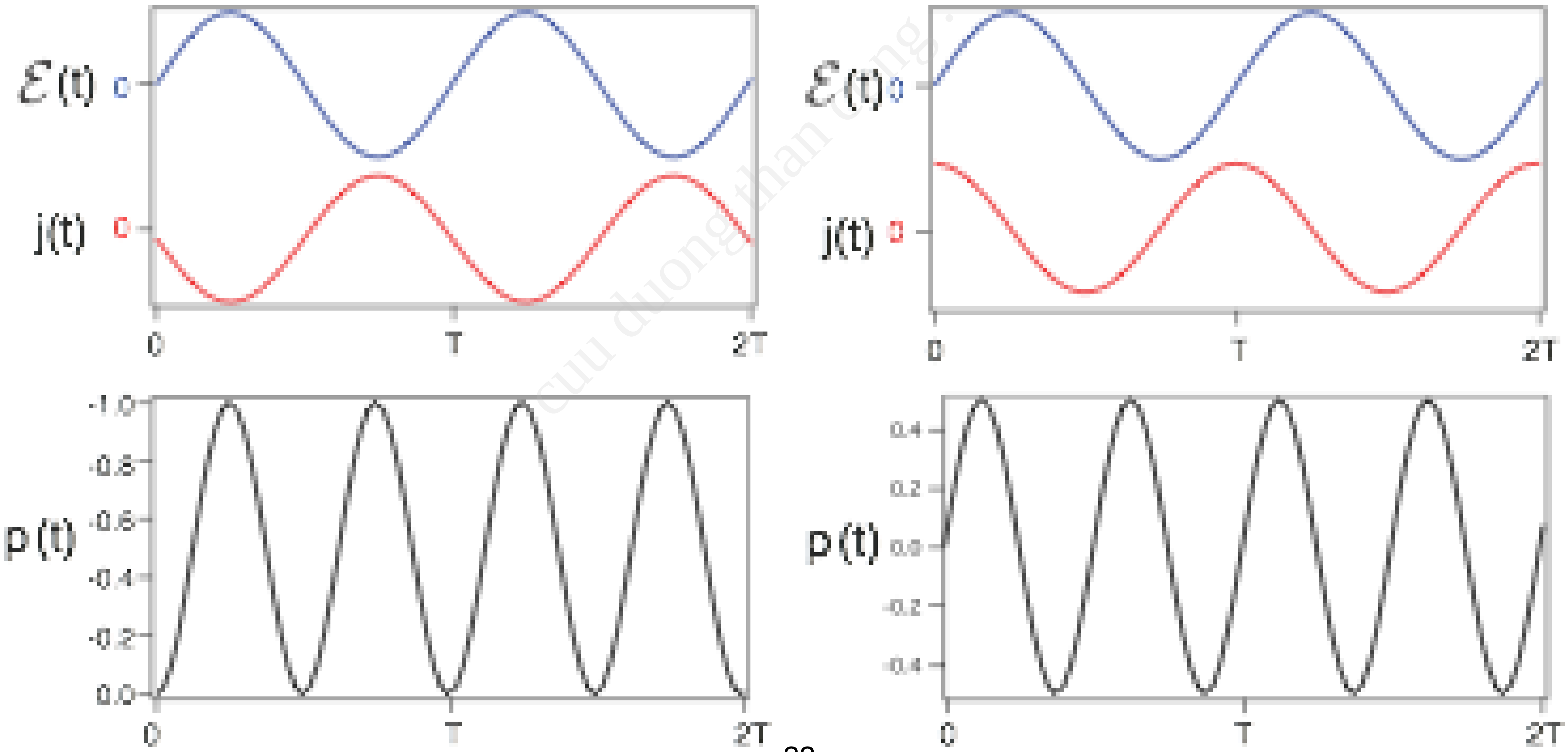
energy
dissipation

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

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

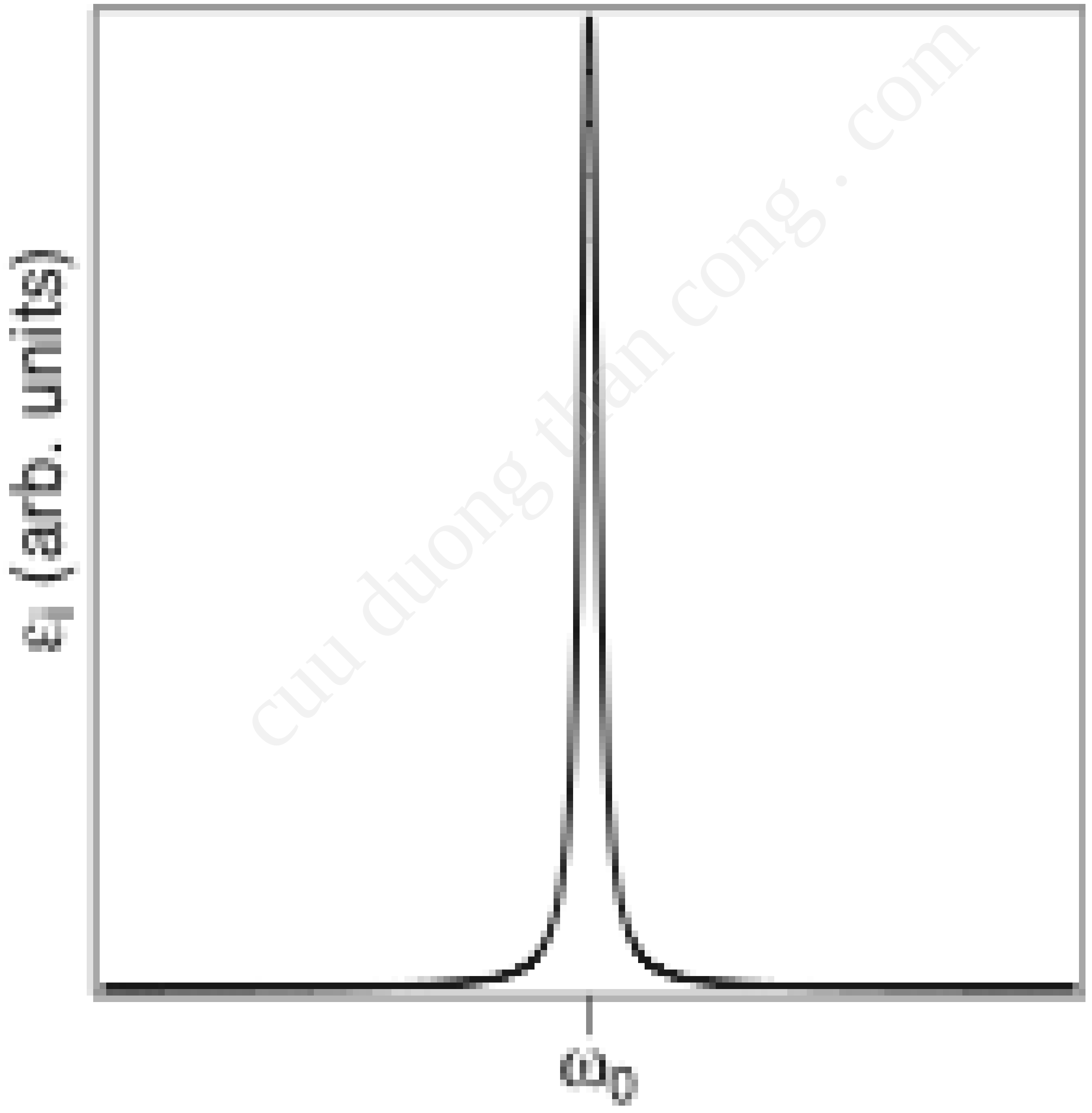
ε imaginary

ε real



The meaning of ε_i

energy dissipation



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

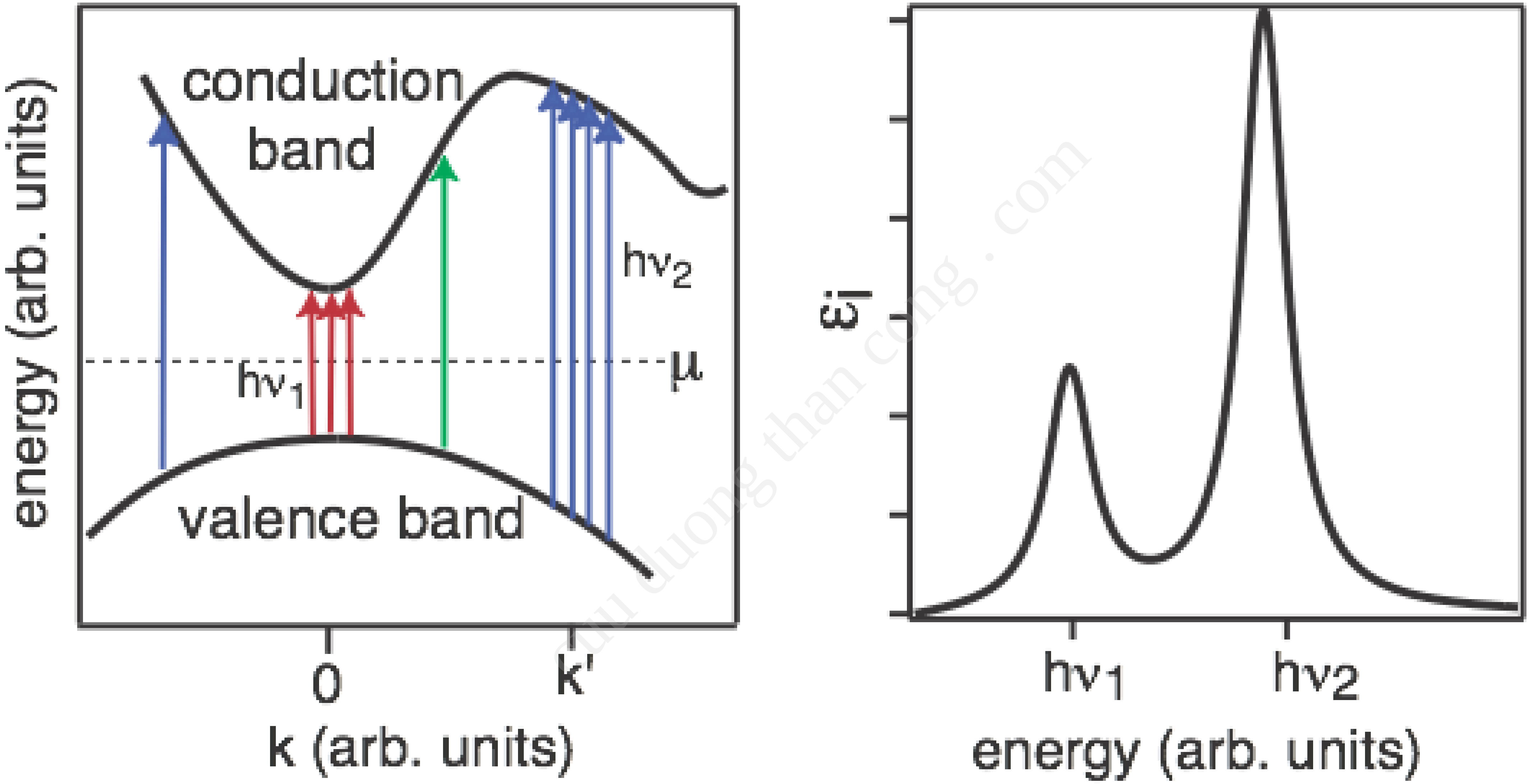
Si

CdSe

CdS

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

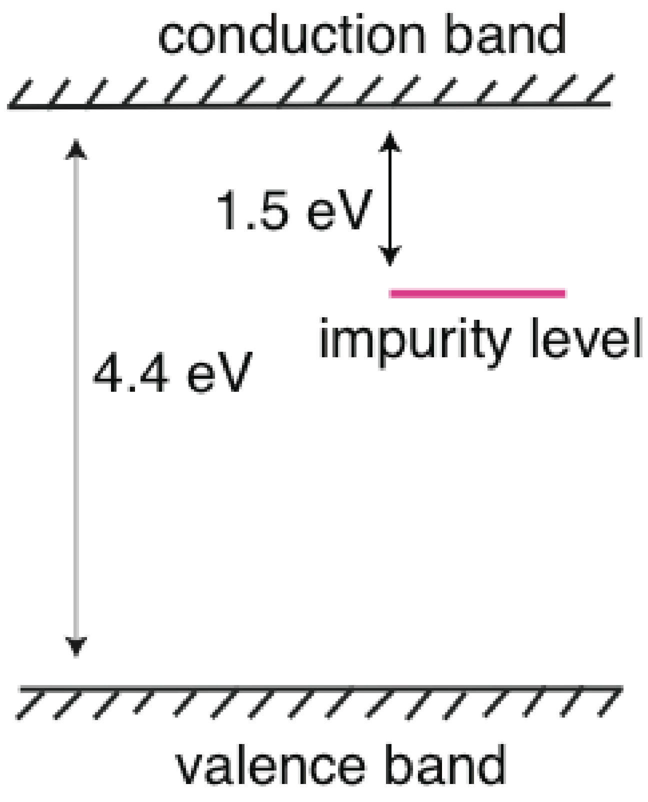
Frequency dependence of the dielectric constant: even higher frequencies (optical)



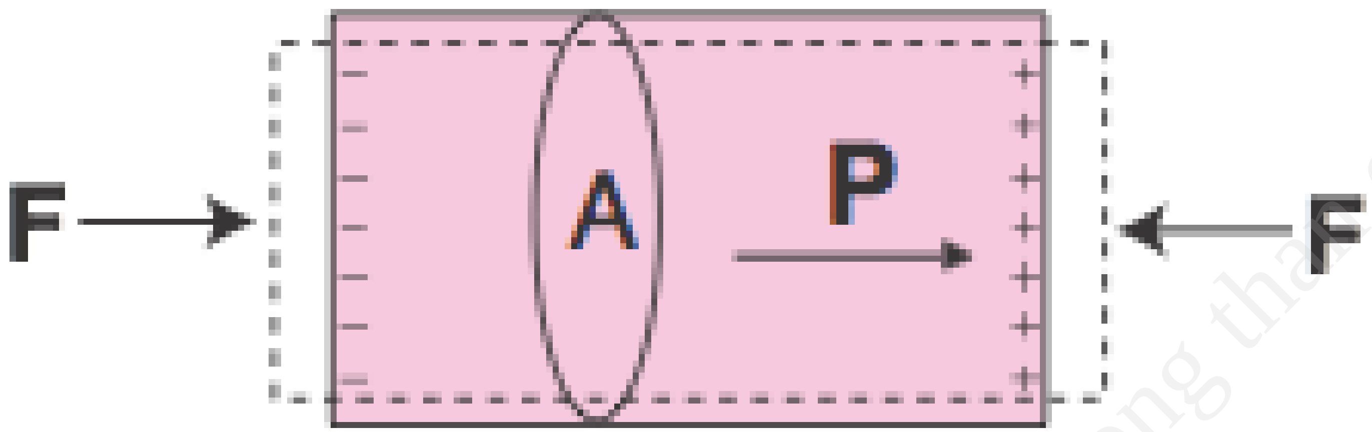
$$\epsilon_i(h\nu) \propto \sum_{\mathbf{k}} M^2 \delta(E_C(\mathbf{k}) - E_V(\mathbf{k}) - h\nu)$$

Impurities in dielectrics

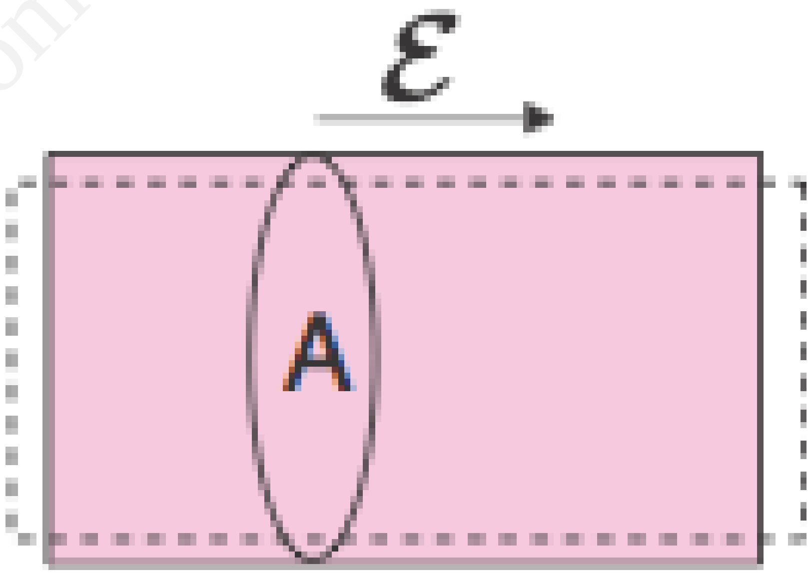
- Single-crystals of wide-gap insulators are optically transparent (diamond, alumina)
- Impurities in the band gap can lead to absorption of light with a specific frequency
- Doping with shallow impurities can also lead to semiconducting behaviour of the dielectrics. This is favourable for high-temperature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



Piezoelectricity

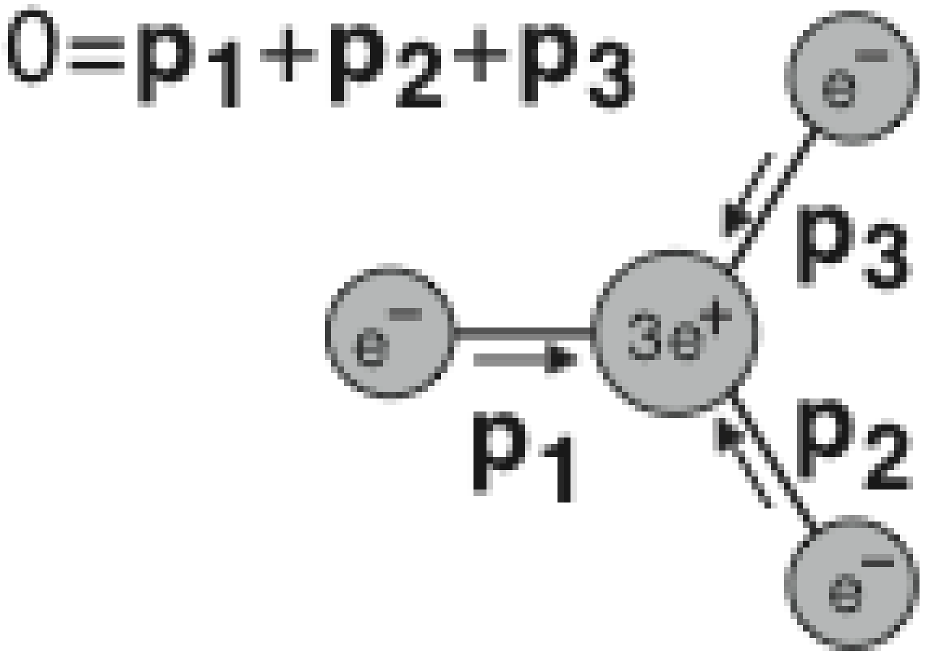


applying stress gives rise to a polarization

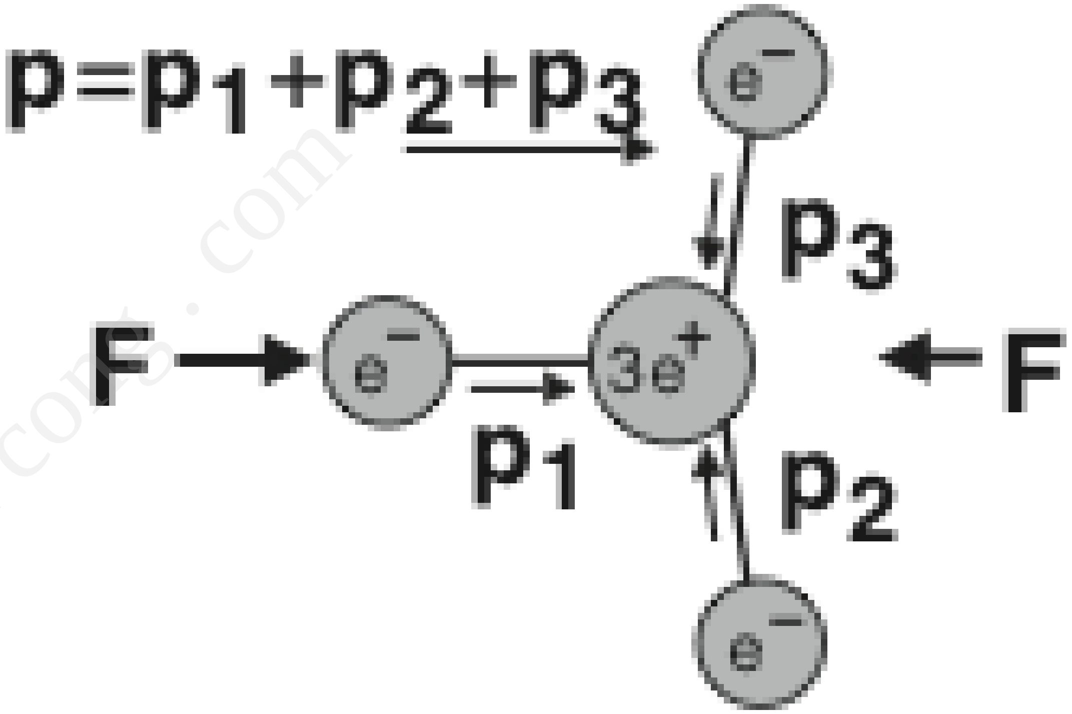


applying an electric field gives rise to strain

Piezoelectricity



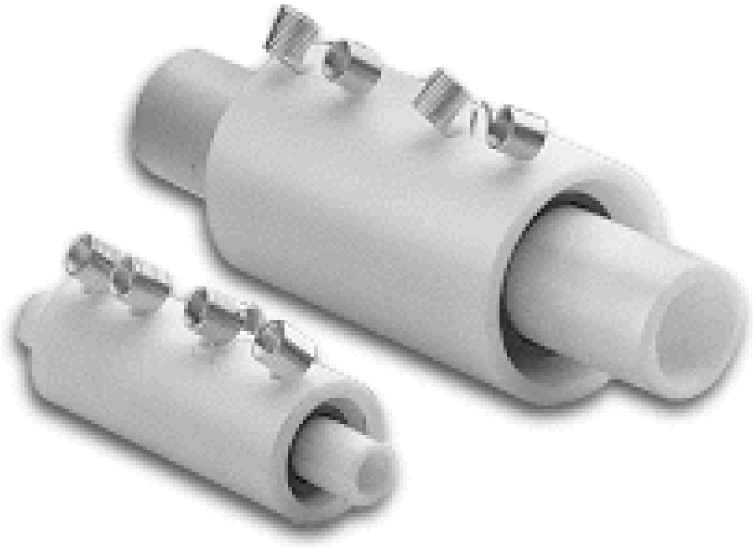
equilibrium structure
no net dipole



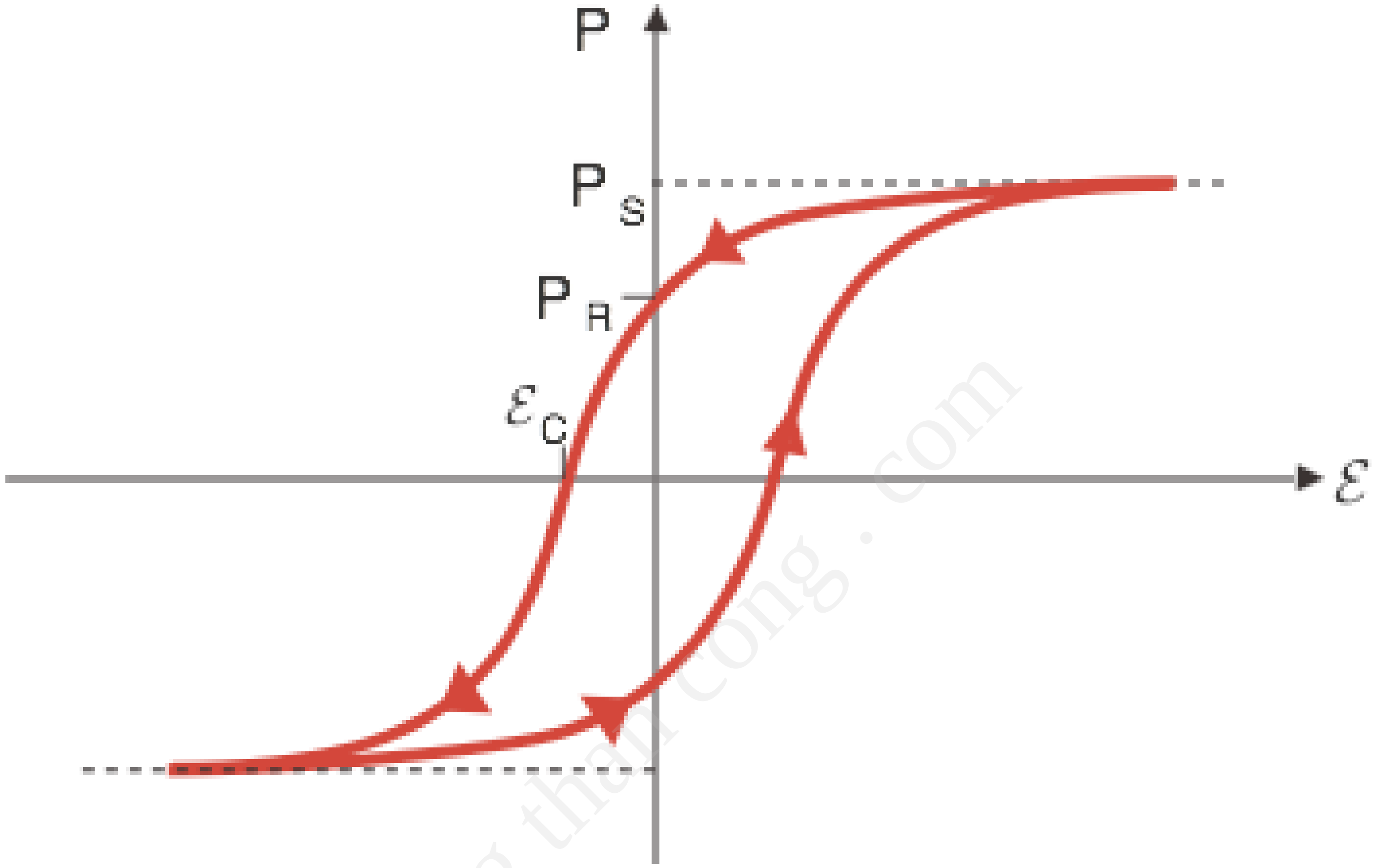
applying stress leads
finite net dipole

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

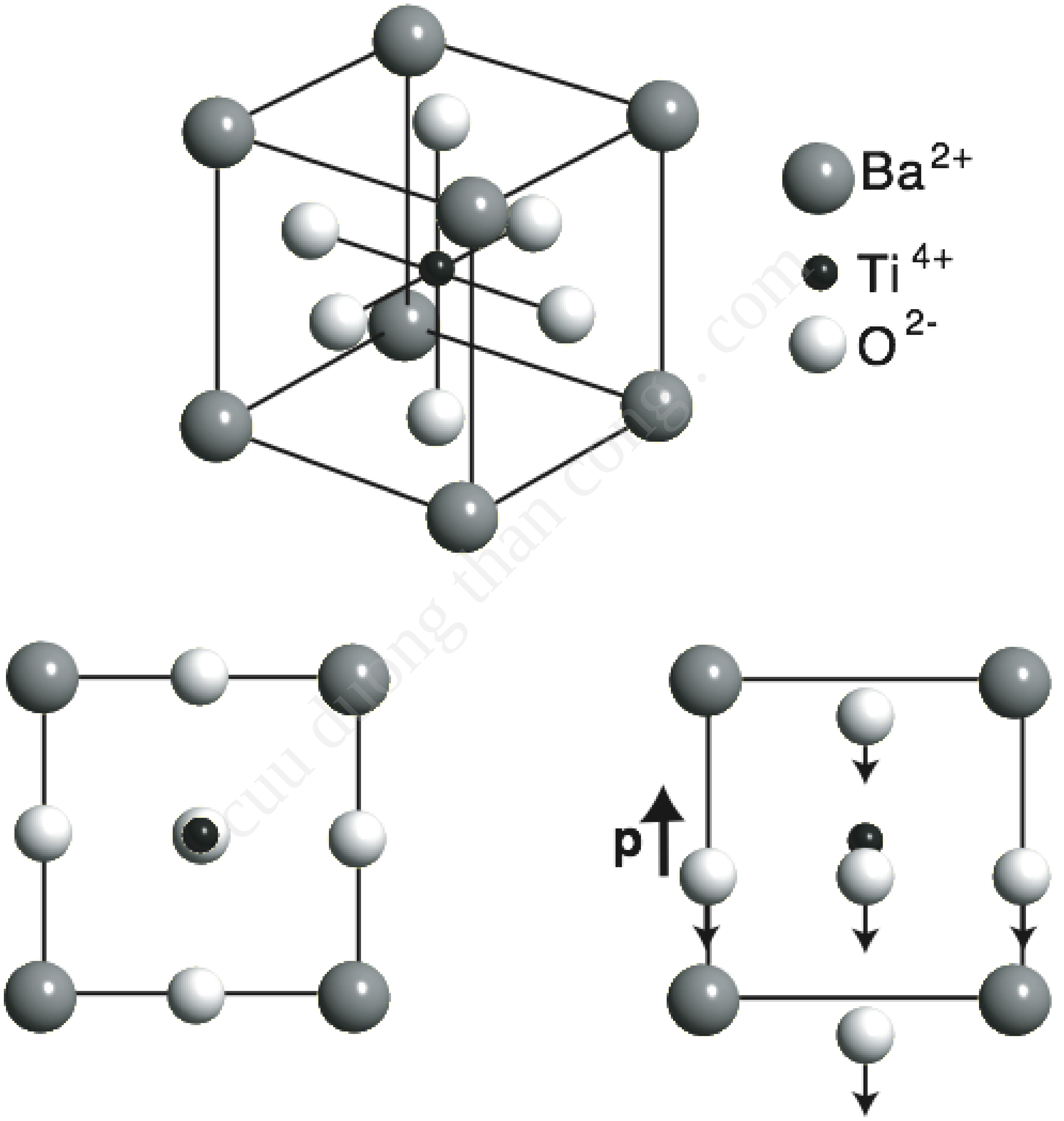


Ferroelectrics



- 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



ferroelectric

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

we start with the usual differential equation

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

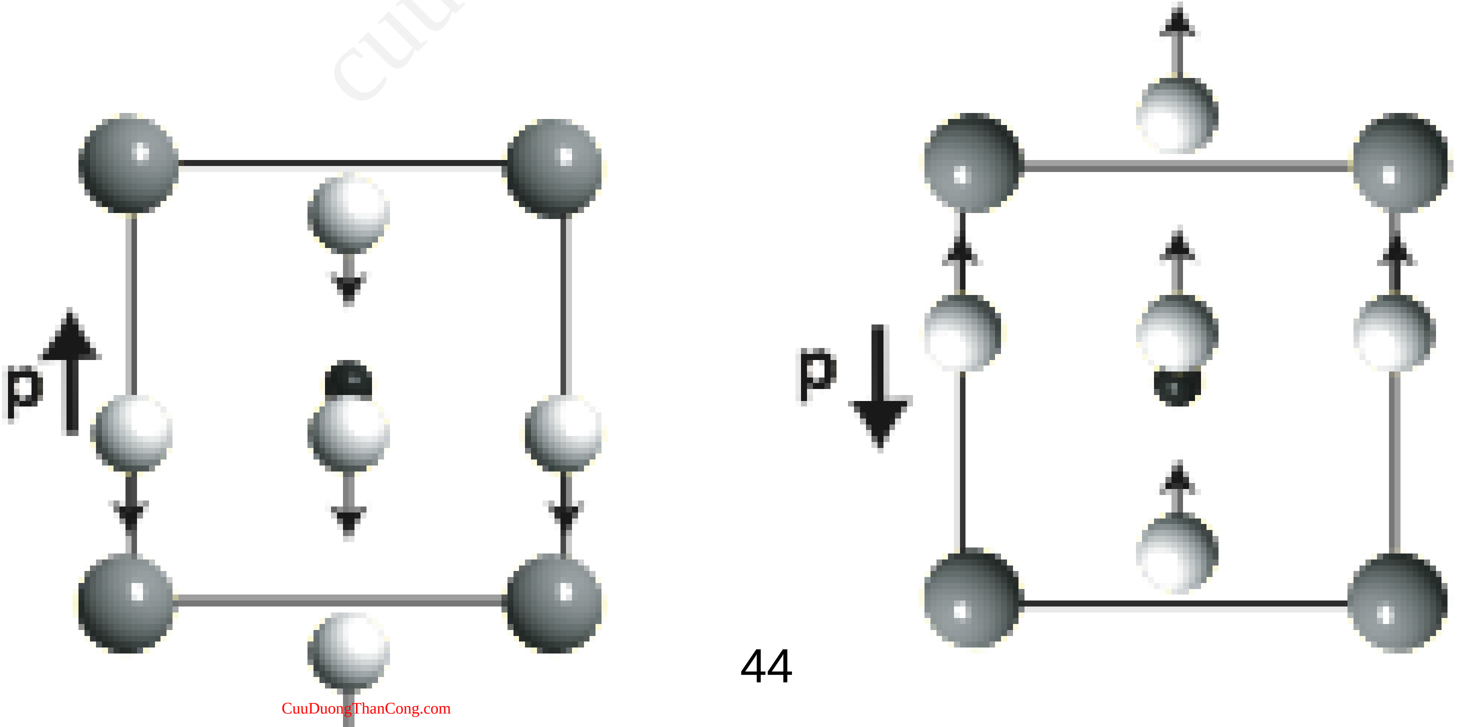
friction term

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)