FoP 3B Part II

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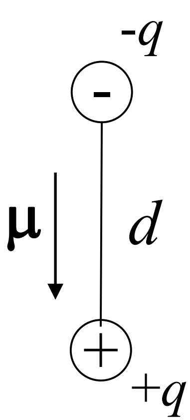
Room 151

Lecture 11: Ferroelectric crystals

Summary of lecture 10

Electric dipole moment:

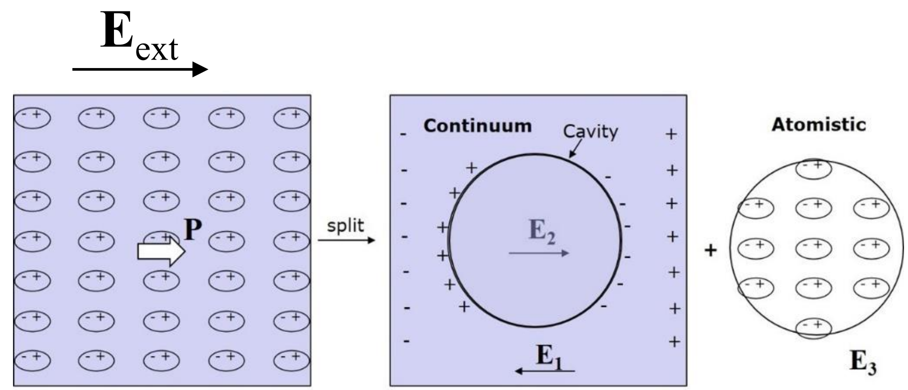


$$|\boldsymbol{\mu}| = qd$$

Local vs macroscopic fields:

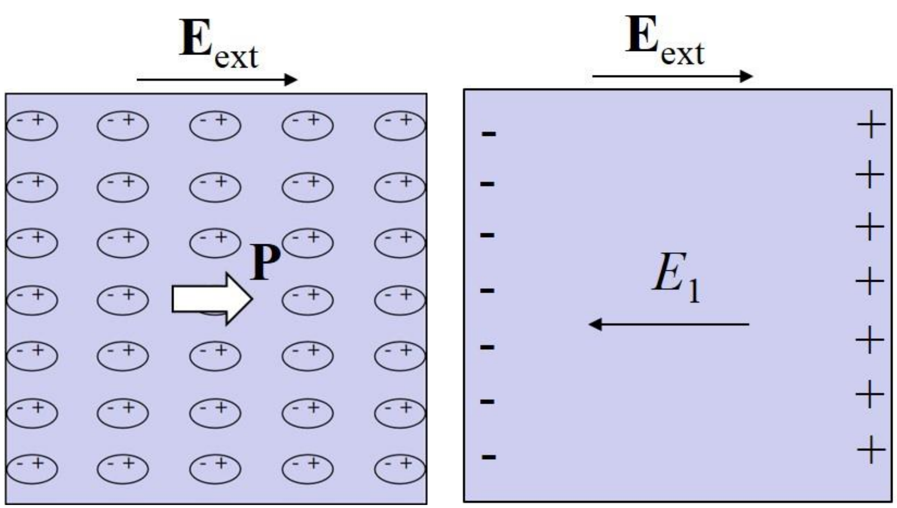
$$\boldsymbol{\mu} = \alpha \mathbf{E}_{\text{local}}$$

polarisability



$$E_{\text{local}} = \underbrace{\left(E_{\text{ext}} - \frac{\sigma}{\epsilon_0}\right)}_{E_{\text{macro}}} + \frac{P}{3\epsilon_0}$$

Polarisation and depolarising fields:



Aim of today's lecture

► Discuss polarisability, polarisation mechanisms and ferroelectric crystals

Key concepts:

-Clausius-Mossoti relationship and polarisability

-Electronic polarisation: frequency dependence of dielectric function

-Ferroelectric crystals

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Clausius-Mossotti relation

The polarisation magnitude P is given by:

Local electric field

$$P = N\mu = N\alpha E_{\text{local}}$$

Dipole density

Dipole moment

Polarisability

Using $E_{\text{local}} = E_{\text{macro}} + (P/3\epsilon_o)$ gives*:

$$N\alpha = \frac{(P/E_{\text{macro}})}{1 + \frac{1}{3\epsilon_o}(P/E_{\text{macro}})}$$

From the definition of electric displacement $D = \epsilon_o E_{\text{macro}} + P = \epsilon_o \epsilon_r E_{\text{macro}}$:

$$\boxed{\frac{\epsilon_r - 1}{\epsilon_r + 2} = \frac{N\alpha}{3\epsilon_o}}$$

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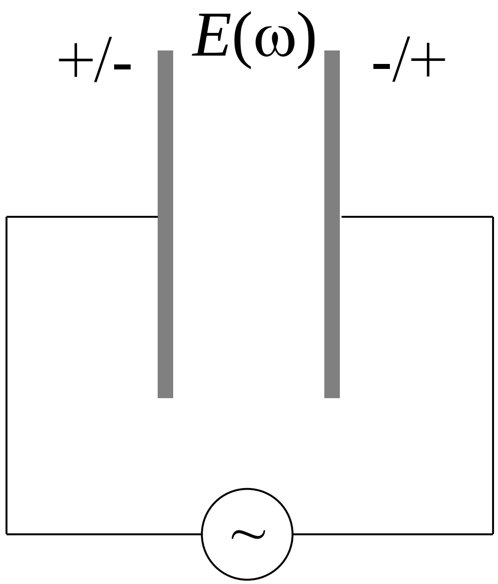
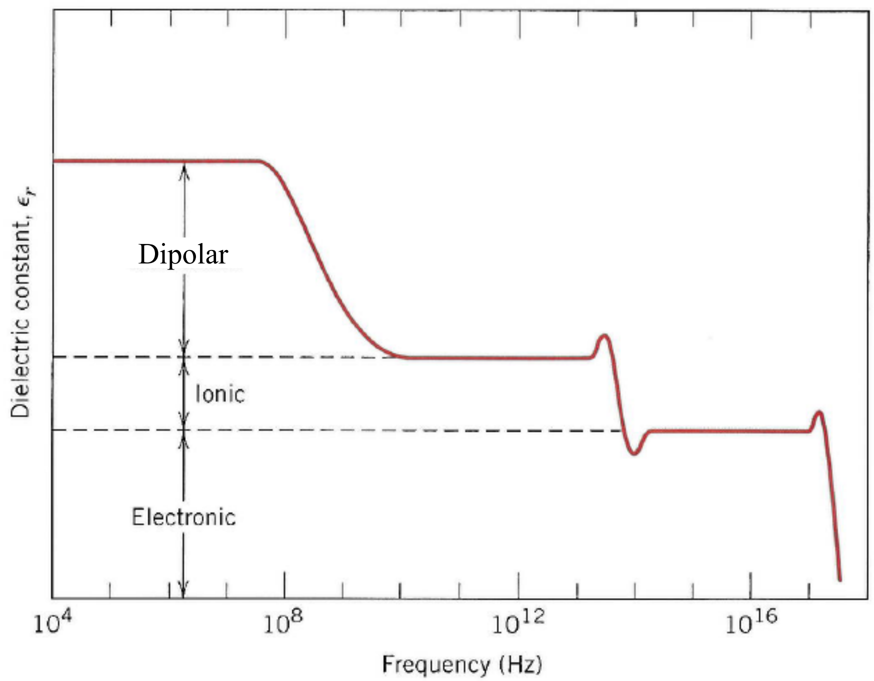
* E_{macro} here is the *internal macroscopic* field, i.e. sum of external and depolarising (E_1) fields

Polarisation mechanisms





-If the capacitor is connected to an AC circuit polarisation of medium will oscillate with electric field *E* (frequency ω).

-Hence:

$$C = \epsilon_o \epsilon_r(\omega)\ \frac{A}{d}$$

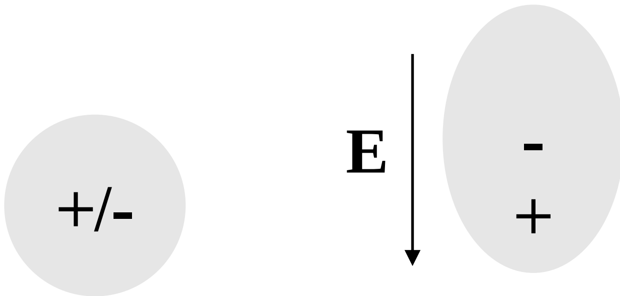
dielectric constant for frequency ω

Electronic: polarisation of electron cloud w.r.t nucleus

Ionic: polarisation of oppositely charged ions

Dipolar: polarisation and re-orienting of molecules (e.g. H_2O) with permanent electric dipoles

Electronic polarisation



Unpolarised atom
Electric field OFF

Polarised atom
Electric field ON

-Electron-nuclear bond treated as an oscillating spring (spring constant $K = m\omega_o^2$).

-Assume an oscillating *local* electric field $\mathbf{E}_{\text{local}}(\omega) = \mathbf{E}_o \exp(i\omega t)$.

-Electron position is $\mathbf{r}(\omega) = \mathbf{r}_o \exp(i\omega t)$.
$\therefore\ \boldsymbol{\mu}(\omega) = -e\,\mathbf{r}(\omega)$

-Equation of motion for electron:

$$m\ddot{\mathbf{r}} = -K\mathbf{r} - e\mathbf{E}_{\text{local}}$$

SHM restoring force   Force due to electric field

- Substituting for $\mathbf{r}$ and using $\boldsymbol{\mu}(\omega) = \alpha(\omega)\mathbf{E}_{\text{local}}(\omega)$ gives:

$$\alpha(\omega) = \frac{e^2}{m(\omega_o^2 - \omega^2)} \qquad \left(\omega_o = \sqrt{K/m}\right)$$

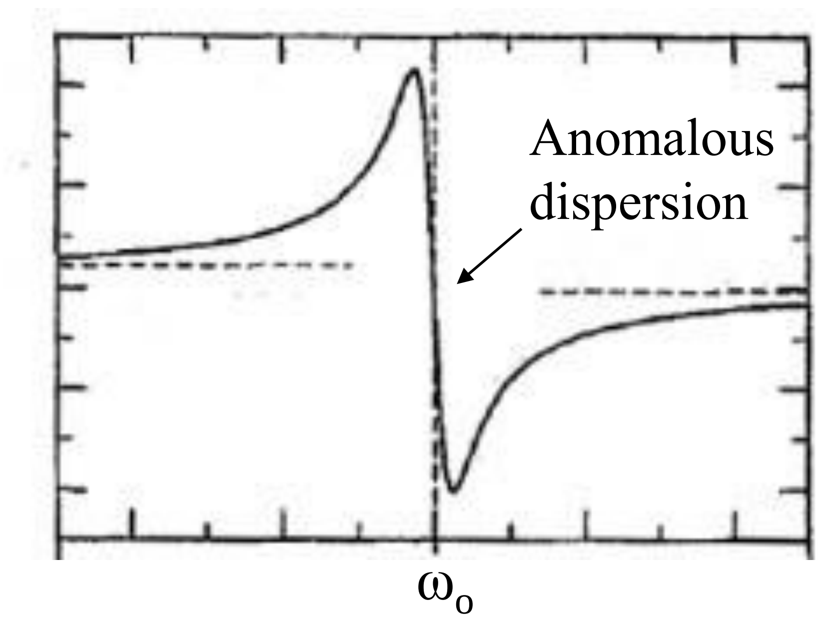
Dielectric function due to electronic polarisation

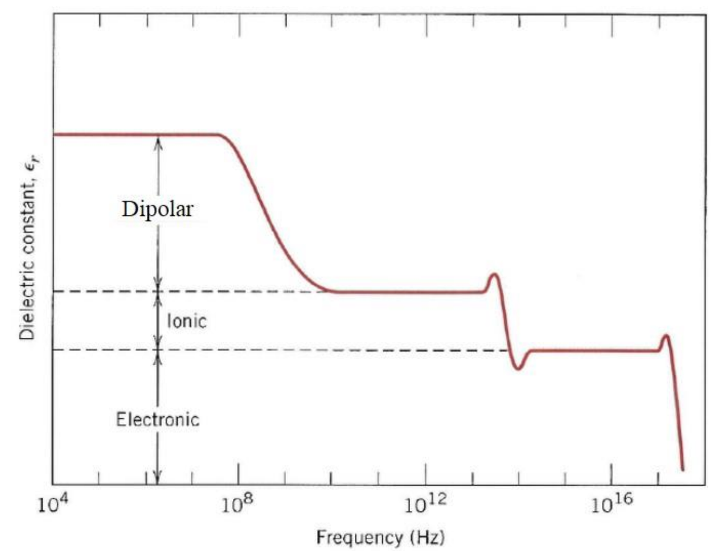
From the Clausius-Mossotti relation:

$$\epsilon_r(\omega) = 1 + \frac{N\alpha(\omega)}{\epsilon_o - [N\alpha(\omega)/3]}$$

Substituting for α(ω):

$$\epsilon_r(\omega) = 1 + \frac{Ne^2}{m\epsilon_o(\omega_o^2 - \omega^2) - (Ne^2/3)}$$

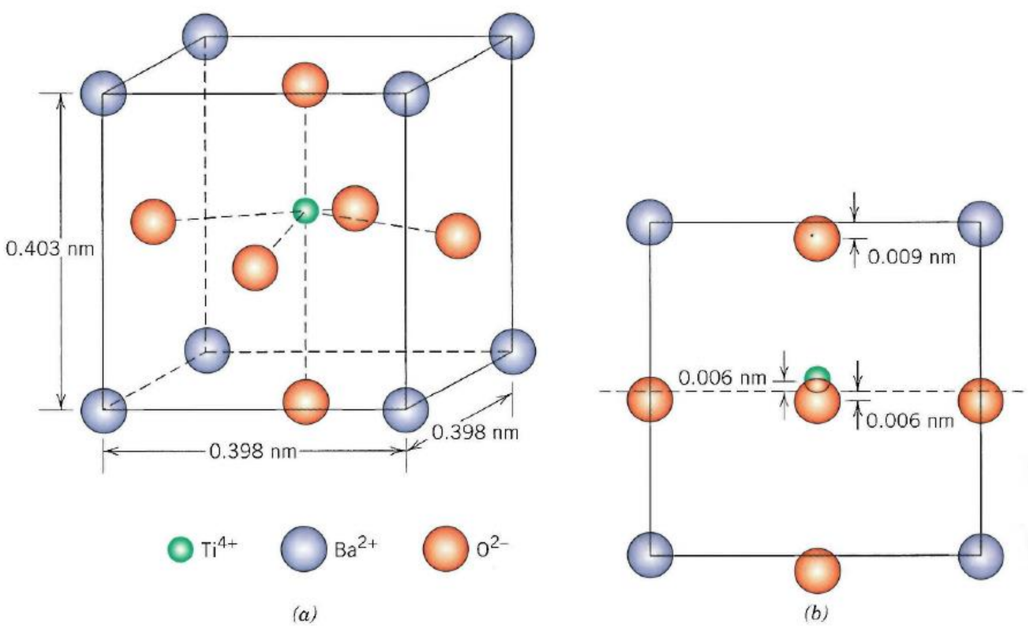




Ferroelectric crystals

Material	Dielectric Constant	Material	Dielectric Constant
Vacuum	1	Benzene	2.28
Helium	1.000065	Diamond	5.7
Neon	1.00013	Salt	5.9
Hydrogen	1.00025	Silicon	11.8
Argon	1.00052	Methanol	33.0
Air (dry)	1.00054	Water	80.1
Nitrogen	1.00055	Ice (-30° C)	99
Water vapor (100° C)	1.00587	$KTaNbO_3$ (0° C)	34,000

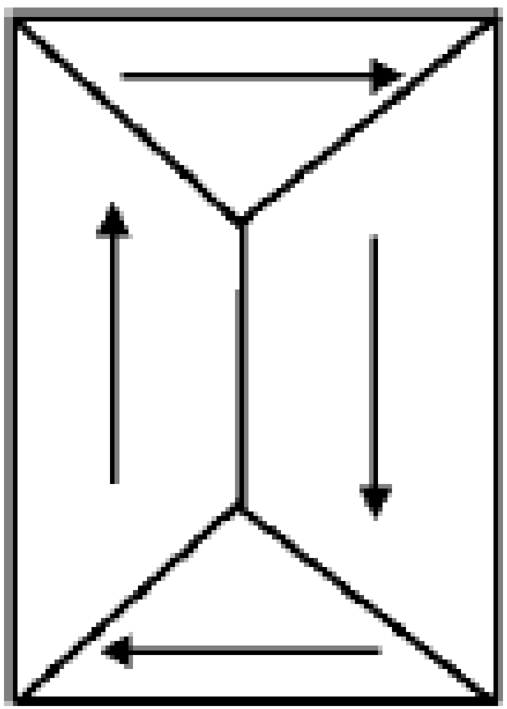
$BaTiO_3$ } Ferroelectric
$PbTiO_3$ } 'perovskites'



$\mathbf{P}_s$ (spontaneous polarisation)

Crystal structure of $BaTiO_3$

Domain formation



For a dielectric with no free carriers:

$$\vec{\nabla} \cdot \mathbf{D} = 0$$

electric displacement field

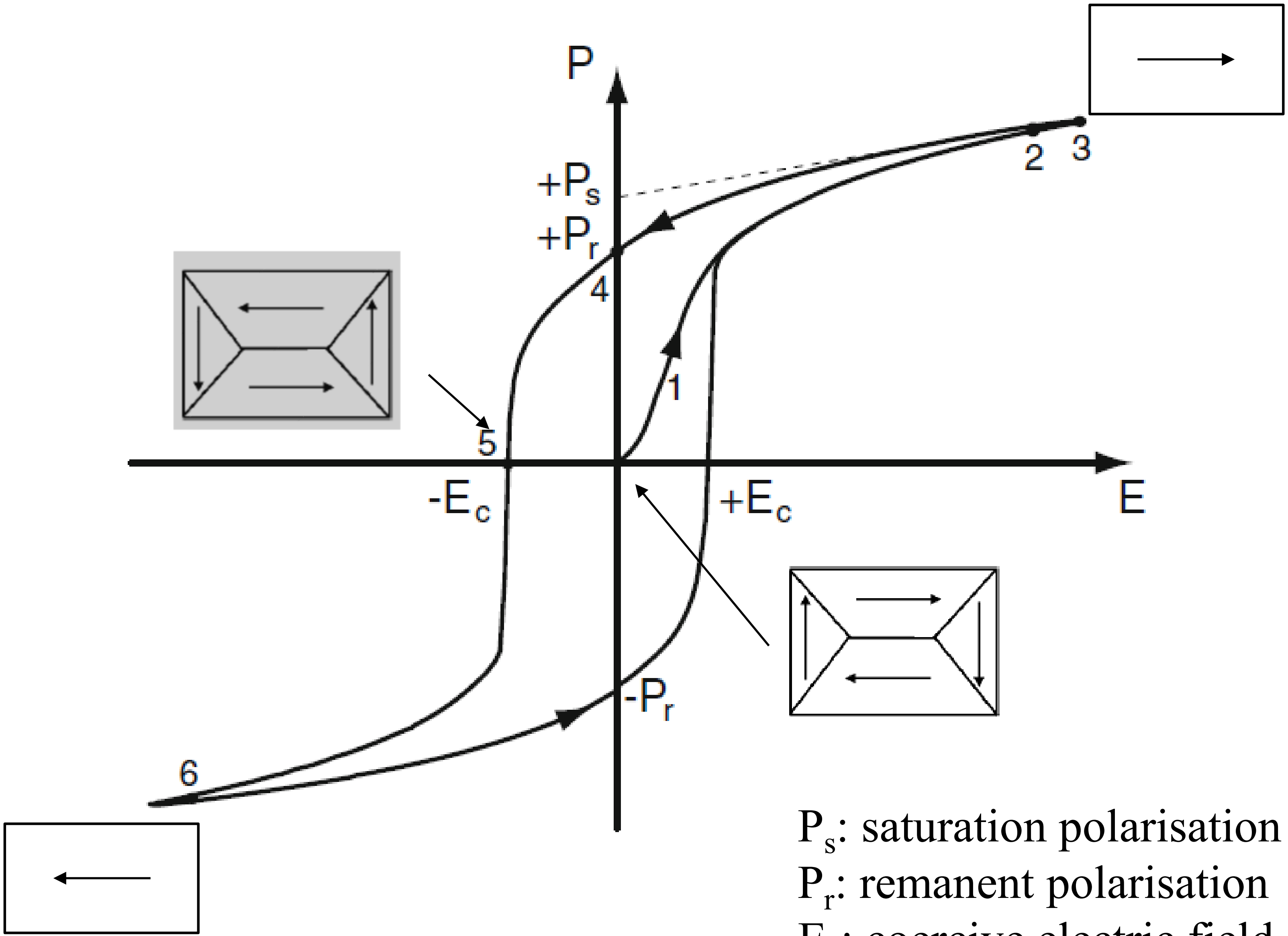
Therefore:

$$\epsilon_o \vec{\nabla} \cdot \mathbf{E} = -\vec{\nabla} \cdot \mathbf{P}$$

At sample surface $\nabla \cdot \mathbf{P} \neq 0$, so that electric field induced within sample.

Domains form to minimise energy due to internal electric field (cf. ferromagnetic domains).

Hysteresis curve



P_s: saturation polarisation
P_r: remanent polarisation
E_c: coercive electric field