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B.Sc (PS) Computer Science VI Sem
Dielectrics

When $p_x = p \cos \theta$, $d\Omega = 2\pi \sin \theta d\theta$ and $f(\theta)$ is given by eq. (1). Substituting these values, eq. (2) becomes

$$P_d = \frac{\int_{-1}^{+1} p \cos \theta 2\pi \sin \theta \exp(-pE \cos \theta / k_B T) d\theta}{\int_{-1}^{+1} 2\pi \sin \theta \exp(-pE \cos \theta / k_B T) d\theta} \quad (3)$$

Now substituting $a = pE/k_B T$, $t = \cos \theta$ and $dt = -\sin \theta d\theta$

eq. (3) can be written in the form

$$P_d = \frac{p \int_{-1}^{+1} \exp(-at) t dt}{\int_{-1}^{+1} \exp(-at) dt} = p \frac{d}{da} \log \int_{-1}^{+1} \exp(-at) dt$$

$$= p \left[\frac{d}{da} \log(e^a - e^{-a}) \right] \frac{d}{da} \log a$$

$$= p \left[\coth(a) - \frac{1}{a} \right]$$

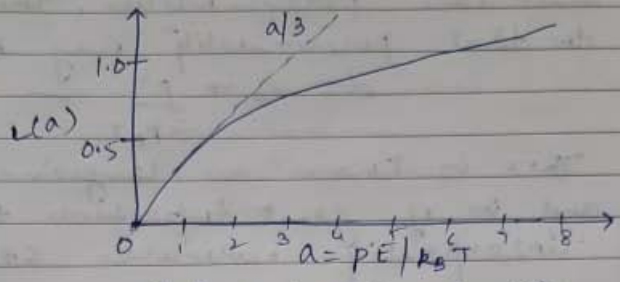
$$\approx p L(a) \quad (4)$$

$$\text{Where } L(a) = \coth(a) - \frac{1}{a}$$

The function $L(a)$ is known as Langevin function. Debye applied this relation to an electric dipole gas. Fig shows a plot of the Langevin function $L(a)$ as a function of a . When a is very large, that is at very high field strength or at low temp, the function $L(a)$ approaches saturation value at unity. This corresponds to the maximum alignment of the dipoles along the direction of the field. For small values of a (i.e. $a \ll 1$ or $pE \ll k_B T$) we have

$$\cosh(a) = \frac{1}{a} + \frac{a}{3} + \frac{a^3}{45} + \dots$$

So that $L(a) = \frac{a}{3} \dots (5)$



Plot of Langevin function.

Actually, in order to approach the value of a to be unity at room temp., the field strength of about 10^9 V/m is required. Thus, for a moderate field ($\sim 10^5 - 10^6$ V/m) and moderate temp. (~ 300 K), the value of a is of the order of $10^{-3} - 10^{-4}$, which is much less than unity and hence the above approx. (eq. 5) could be used safely without losing much of accuracy. This assumption may be justified by showing that the magnitude of $k_B T$ at room temp. is many times larger than the potential energy gain resulting from the alignment of the dipoles at the same temp. Moreover, the value of a found in most experimental situations is of the same order. Now, substituting the value of $L(a)$ in eq. (4) and replacing back the value of a , we obtain

$$P_d = \frac{p^2 E}{3 k_B T} \quad (6)$$

Therefore, the dipole polarizability per dipole becomes

$$\alpha_d = \frac{P_d}{E} = \frac{p^2}{3 k_B T} \quad (7)$$

It is clear from eq. (7) that the dipole or orientation polarization is temperature dependent. If α_0 denotes the sum of the electronic and ionic polarizabilities, then from eq. (7) the total polarizability may be written as

$$\alpha = \alpha_0 + \frac{p^2}{3k_B T} \quad (8)$$

This is known as Langevin-Debye equation and is of great importance to chemists in interpreting molecular structure.

Total polarization:-

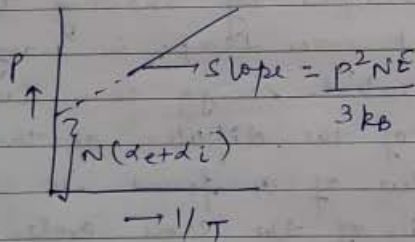
The total polarization is the sum of the electronic, ionic and orientation polarization. Therefore, total polarization is given by

$$P = N \cdot p_e + P_i + P_d$$

Substituting the value of P_d in above eq. we get

$$P = N \alpha_e E + N \alpha_i E + N \alpha_d E$$

$$\text{hence } P = N E \left(4\pi \epsilon_0 R^3 + \alpha_i + \frac{p^2}{3k_B T} \right)$$



Clausius-Mossotti Relation:-

Relation between dielectric constant and polarizability of atoms/molecules comprising the dielectric. The dipole moment of an atom per unit polarizing field is called atomic polarizability (if molecule, then molecular polarizability).

thus dipole moment $= \vec{p} = \alpha \vec{E}_{loc}$

Where α is atomic polarizability. If there are N atoms per unit volume, then polarization vector

$$\vec{P} = N\vec{p} = N\alpha \vec{E}_{loc}$$

Where \vec{E}_{loc} is called the local Electric field.

From we know that

$$\vec{P} = \epsilon_0 \vec{E} (\epsilon_r - 1) = N\alpha \vec{E}_{loc}$$

$$\vec{E} \epsilon_r \epsilon_0 - \vec{E} \epsilon_0 = N\alpha \vec{E}_{loc}$$

$$\vec{E} \epsilon_r \epsilon_0 = N\alpha \vec{E}_{loc} + \vec{E} \epsilon_0$$

$$\epsilon_r = 1 + \frac{N\alpha \vec{E}_{loc}}{\epsilon_0 \vec{E}} \quad (1)$$

The local field \vec{E}_{loc} is given by

$$\vec{E}_{loc} = \vec{E} + \frac{\vec{P}}{3\epsilon_0} = \vec{E} + \frac{N\alpha \vec{E}_{loc}}{3\epsilon_0}$$

$$\text{OR } \vec{E} = \vec{E}_{loc} - \frac{N\alpha \vec{E}_{loc}}{3\epsilon_0} = \vec{E}_{loc} \left[1 - \frac{N\alpha}{3\epsilon_0} \right]$$

$$\frac{\vec{E}_{loc}}{\vec{E}} = \frac{1}{1 - \left(\frac{N\alpha}{3\epsilon_0} \right)} \quad (2)$$

substituting \vec{E}_{loc} / \vec{E} in equation (1)

$$\epsilon_r = 1 + \frac{N\alpha}{\epsilon_0} \left[\frac{1}{\left(1 - \frac{N\alpha}{3\epsilon_0} \right)} \right]$$

$$\epsilon_r = \frac{\epsilon_0 \left[1 - \frac{N\alpha}{3\epsilon_0} \right] + N\alpha}{\epsilon_0 \left[1 - \frac{N\alpha}{3\epsilon_0} \right]}$$

$$\epsilon_r = \frac{\epsilon_0 \left[1 - \frac{N\alpha}{3\epsilon_0} \right] + \frac{N\alpha \epsilon_0}{\epsilon_0}}{\epsilon_0 \left[1 - \frac{N\alpha}{3\epsilon_0} \right]} = \frac{1 - \frac{N\alpha}{3\epsilon_0} + \frac{N\alpha}{\epsilon_0}}{1 - \frac{N\alpha}{3\epsilon_0}}$$

$$= \frac{1 + \frac{2}{3} \left(\frac{N\alpha}{\epsilon_0} \right)}{1 - \frac{1}{3} \left(\frac{N\alpha}{\epsilon_0} \right)}$$

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

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

$$= \frac{1 + \frac{2}{3} \left(\frac{N\alpha}{\epsilon_0} \right) + 2 - \frac{2}{3} \left(\frac{N\alpha}{\epsilon_0} \right)}{1 - \frac{1}{3} \left(\frac{N\alpha}{\epsilon_0} \right)}$$

$$= \frac{3 + \frac{2}{3} \left(\frac{N\alpha}{\epsilon_0} \right) - \frac{2}{3} \left(\frac{N\alpha}{\epsilon_0} \right)}{1 - \frac{1}{3} \left(\frac{N\alpha}{\epsilon_0} \right)}$$

$$= \frac{N\alpha / \epsilon_0}{3} = \frac{N\alpha}{3\epsilon_0}$$

$$\boxed{\frac{\epsilon_r - 1}{\epsilon_r + 2} = \frac{N\alpha}{3\epsilon_0}} \quad \text{--- (3)}$$

$$\alpha = \frac{3\epsilon_0 (\epsilon_r - 1)}{N(\epsilon_r + 2)} \quad \text{--- (4)}$$

Eq (3) is Clausius - Mossotti relation which relates the macroscopic dielectric constant with the microscopic polarizabilities.

Multiplying both sides of eq. (3) by the molar volume, we get

$$\left[\frac{\epsilon_r - 1}{\epsilon_r + 2} \right] \frac{M_A}{\rho} = \left[\frac{N_A}{3\epsilon_0} \right] \frac{M_A}{\rho} \quad \text{where } M_A \text{ is the molecular weight}$$

$$\frac{M_A N}{\rho} = N_A$$

$$\left[\frac{\epsilon_r - 1}{\epsilon_r + 2} \right] \frac{M_A}{\rho} = \frac{N_A \alpha}{3\epsilon_0} = P_m$$

Called molar polarization. In the presence of orientational polarization, the Clausius-Mossotti equation can be written as

$$P_m = \left[\frac{\epsilon_r - 1}{\epsilon_r + 2} \right] \frac{M_A}{\rho} = \frac{N}{3\epsilon_0} (\alpha_e + \alpha_i + \alpha_o)$$

$$\left[\frac{\epsilon_r - 1}{\epsilon_r + 2} \right] \frac{M_A}{\rho} = \frac{N \alpha}{3\epsilon_0} = \frac{N}{3\epsilon_0} (\alpha' + \alpha_o) \quad \text{--- (5)}$$

This equation is called Debye's equation and it forms the basis for the method of determining permanent dipole moment.

Relation between dielectric constant and refractive index

$$\text{We know } v = \frac{1}{\sqrt{\mu\epsilon}}$$

μ = magnetic permeability of the medium

ϵ = absolute permittivity

μ_0 = permeability of non-magnetic media

$$\text{hence } v = \frac{1}{\sqrt{\mu_0 \epsilon}}$$

$$\text{ref. index of } n = \frac{\text{velocity of waves in vacuum}}{\text{velocity of waves in medium}}$$

$$n = \frac{1/\sqrt{\mu_0 \epsilon_0}}{1/\sqrt{\mu_0 \epsilon}} = \sqrt{\epsilon/\epsilon_0} = \sqrt{\epsilon_r}$$

Thus $n = \sqrt{\epsilon_r}$, where ϵ_r is the relative permittivity. Using this value of ϵ_r in equation (3).

$$\frac{n^2 - 1}{n^2 + 2} = \frac{N\alpha}{3\epsilon_0} \quad (6)$$

This is called ~~lorentz~~ Lorentz-Lorentz formula.

Behaviour of Dielectrics in Alternating field -

When a dielectric material is placed in an alternating field the orientation of the dipoles and hence the polarization will tend to reverse when the polarity of the field changes. As long as the frequency remains low ($< 10^6$ Hz) there is no significant lag in polarization with alterations of the field. The permittivity is independent of freq. and has same magnitude as in the static field. When the freq. is increased, the dipoles will not be able to rotate rapidly and their oscillators will lag behind those of the field. With further inc. in freq., the permanent dipoles in the medium will be unable to follow the field and contribution to static permittivity from this molecular process i.e. the orientation polarization stops. This usually happens in the radio frequency range ($10^6 - 10^{10}$ Hz).

→ At still higher freq. i.e. in the infra-red range

