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Fundamental Theories about Electrical Properties of the Polar Liquid Crystals: A Review

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Thepolar liquid crystals (PLCs) are characterizednot only about bulk properties, but also about molecular parameters (dielectric permittivity, anisotropy etc.), and their mutual association and rotation under an applied electric field. Dielectric properties of LCs are related to the response of LC molecules to the application of an electric field. Permittivity is a physical quantity that describes how an electric field affects and is affected by a dielectric medium and is determined by the ability of a material to polarize in response to an applied electric field, and thereby to cancel, partially, the field inside the material. In the LC materials consisting of non-polar molecules, there is only an induced polarization, which consists of two parts: the electronic polarization (which is also present at optical frequencies) and the ionic polarization. In the LCs with polar molecules, there is in addition to the total induced polarization, the orientation polarization, due to the tendency of the permanent dipole moments to orient themselves parallel to the field. In the present research article, an introduction to the fundamental theories concerning electrical properties of the polar liquid crystal has been discussed.

LIQUID CRYSTAL AS A DIELECTRIC MATERIAL: A dielectric is the electrically insulating material between the metallic plates of a capacitor. A good dielectric typically contains polar molecules that reorient in external electric field. This dielectric polarization increases the capacitor's capacitance. Generalizing this, any insulating substance can be called a dielectric. While the term "insulator" refers to a low degree of electrical conduction, the "dielectric" is typically used to describe materials with a high polarization density.The orientational order of the liquid crystal molecules, their number density and any interaction between molecules influence their molecular properties. The dielectric behavior of the liquid crystals reflects the collective response of the mesogens as well as their molecular properties, and there is a coupling between the macroscopic polarization and the molecular response through the internal electric field. Consequently, the molecular description of the dielectric properties of the liquid crystal phases requires the specification of the internal electric field in anisotropic media, which is a difficult task.

THE STATIC DIELECTRIC PERMITTIVITY: Liquid crystals are dielectrics and for low electric fields the induced dipole moment per unit volume i.e. polarization (**P**)is proportional to the electric field **E** [**1**].

$$P = \varepsilon_0 \chi E \qquad \textbf{(1)}$$

where χ is the dielectric susceptibility and ε_0 is the dielectric permittivity in free space. There are two types of polarization induced by the applied electric field, both of which contribute to the dielectric permittivity. The field induces a polarization through the relative displacement of the electronic atomic distances, which is represented by the molecular polarizability α. The contribution from these displacements is small and usually ignored. Polar materials, i.e. materials which have local dipole moments bound to the molecules, also induce an orientational polarization in the tendency of the molecular dipole moments to align with the field freedom. For the isotropic dielectric, the electric displacement vector:

$$D = \varepsilon_0 E + P = \varepsilon_0 (\chi + 1) E = \varepsilon_0 \varepsilon E \qquad \textbf{(2)}$$

Where ε is the relative dielectric permittivity or dielectric constant.Now **Equation2** can be written as:

$$\varepsilon - 1 = \frac{P}{\varepsilon_0 E} \qquad \textbf{(3)}$$

$$\text{or,} \qquad \varepsilon_S - 1 = \frac{P_\infty + P_D}{\varepsilon_0 E}$$

Here the subscripts ∞ and Drepresents respectively, the electronic and dipolar polarization, and the subscript s indicates that the frequencies considered are effectively zero (static field). A plot of dielectric permittivity versus frequency is shown in Figure **1**.

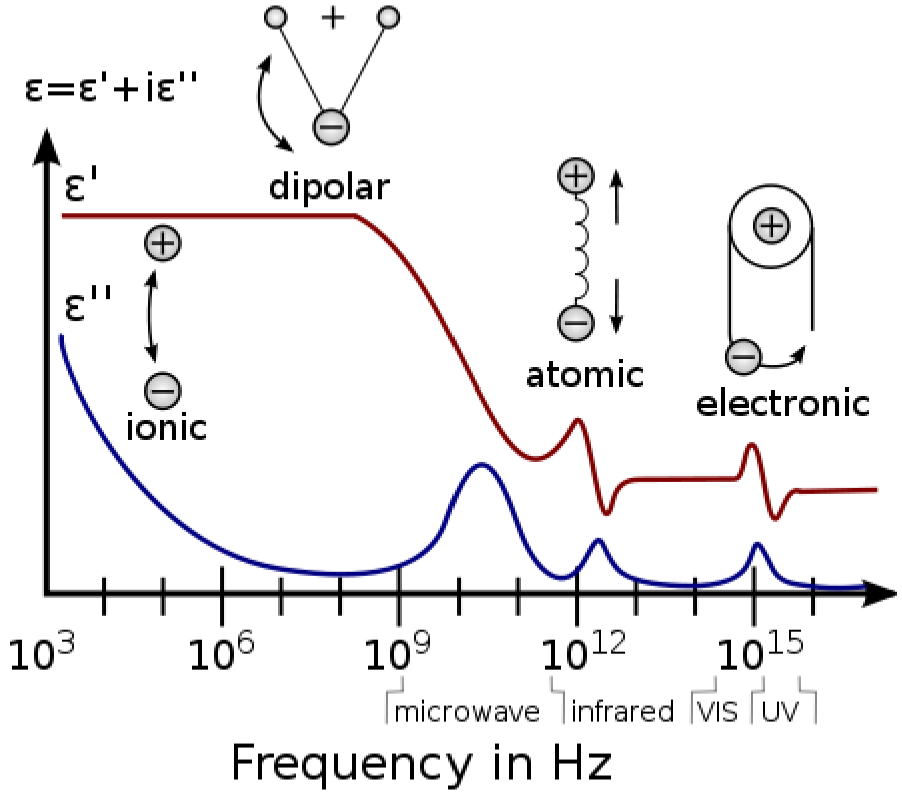

Figure 1: Simplified plot of the complex dielectric permittivity parts and versus frequency.

The infinity sign results the fact that the electronic reorientation usually occurs at high frequencies or optical frequencies, whereas the dipolar contribution is restricted to relatively low frequencies. If we consider the medium to be anisotropic and without polar order in the field free case, both the constituent parts of the total dielectric polarization P_∞ and P_D can be written in terms of the molecular parameters:

$$P_\infty = N\varepsilon E_i$$

$$P_D = N < \mu >= N\mu < \cos\theta > \quad \textbf{(4)}$$

where N is the number of particles per unit volume, ε is the electric polarizability, <μ> is the thermal average of the dipole moment and θ is the angle between the individual dipoles and E_i is the internal field is not identical to the external field E. The dependence of <μ> on E_i can be calculated from the Boltzmann probability distribution function $e^{-W/kT}$

where $$W = -\vec{\mu}.\vec{E} = -\mu E \cos\theta$$

is the energy of the dipole in the internal field. Integrated over the distribution of a sphere, this gives

$$\langle \cos\theta \rangle = \frac{\mu E}{3kT}$$

Therefore $$P_D = \frac{N\mu^2}{3kT} E_i \tag{5}$$

Inserting **Equations4** and **5** in **Equation3** we get,

$$(\varepsilon_S - 1)E = \frac{N}{\varepsilon_0}\left(\alpha + \frac{\mu^2}{3kT}\right)E_i \tag{6}$$

If E$_i$ is identical to E, then **Equation 6** can be written as (the incorrect)

$$(\varepsilon_S - 1) = \frac{N}{\varepsilon_0}\left(\alpha + \frac{\mu^2}{3kT}\right) \tag{7}$$

The correct relation requires knowledge of the relation of E$_i$ and E. This relation is

$$E_i = \left(\frac{\varepsilon_S + 2}{3}\right)E \tag{8}$$

Putting Equation **8** in Equation **6** we get,

$$\frac{\varepsilon_S - 1}{\varepsilon_S + 2} = \frac{N}{3\varepsilon_0}\left(\alpha + \frac{\mu^2}{3kT}\right) \tag{9}$$

This is the well-known Debye equation. In the case of non-polar dielectrics $\mu = 0$ and Equation **9** reduces to

$$\frac{\varepsilon_S - 1}{\varepsilon_S + 2} = \frac{N}{3\varepsilon_0}\alpha \tag{10}$$

Equation 10 has been derived earlier first by Mossotti [**2**] in 1847 and independently by Clausius [**3**] in 1879, but in a different way and without any explicit notation of internal field. For high frequency, $\varepsilon_S \rightarrow \varepsilon_\infty$ refractive index n is related to

$$\varepsilon_\infty = n^2$$

So **Equation 10**can be written as:

$$\frac{\varepsilon_S - 1}{\varepsilon_S + 2} = \frac{n^2 - 1}{n^2 + 2} = \frac{N}{3\varepsilon_0}\alpha \qquad \textbf{(11)}$$

This is Lorenz-Lorentz equation.The theory relating molecular properties and macroscopic permittivity for an isotropic liquid was revised in 1936 by Onsager [**4**]. He was first to make a further distribution between the internal field E_i as an average field acting locally to result in a displacement, and the field E_d called directing field, exerting torque on the dipoles, showing that these fields are not necessarily identical. **Equation 6** then has to be related by:

$$(\varepsilon_S - 1)E = \frac{N}{\varepsilon_0}\left(\alpha E_i + \frac{\mu^2}{3kT}E_d\right) \qquad \textbf{(12)}$$

with the parameters

$$h = \frac{3\varepsilon_s}{2\varepsilon_s + 1} \qquad \textbf{(13)}$$

$$g = \frac{2N}{3\varepsilon_0}\left(\frac{\varepsilon_s - 1}{2\varepsilon_s + 1}\right) \qquad \textbf{(14)}$$

and

$$F = \frac{1}{1 - \alpha g} \qquad \textbf{(15)}$$

Onsager was able to express the relation between the fields as:

$$E_i = hFE \qquad \textbf{(16)}$$

and

$$E_d = hF^2E \qquad \textbf{(17)}$$

Inserted in **Equation 12** this gives the basic expression:

$$\varepsilon_s - 1 = \frac{NhF}{\varepsilon_0}\left(\alpha + \frac{F\mu^2}{3kT}\right) \quad \textbf{(18)}$$

Above equation is widely used for isotropic media and which has to be further generalized for liquid crystals being an anisotropic media.

ANISOTROPY PROPERTY: It is known that in an isotropic liquid, there is a special direction in space in which the molecules point. But liquid crystals spontaneously exhibit anisotropy property. As there is a special direction in which a molecule points i.e. the properties of longitudinal and transverse components differ.

DIELECTRIC ANISOTROPY OF THE LIQUID CRYSTALS: In an anisotropy medium the scalar permittivity ε must be replaced by a tensor of ranktwo. ε* and D* is usually not parallel to the direction of the electric field E.

$$D^* = \varepsilon_0 \varepsilon^* E^* \quad \textbf{(19)}$$

The dielectric permittivity of the undisturbed nematic liquid crystal as well as for undisturbed non-tilted smectic liquid crystal has two independent principal components.

$$\varepsilon^* = \begin{pmatrix} \varepsilon_\perp & 0 & 0 \\ 0 & \varepsilon_\perp & 0 \\ 0 & 0 & \varepsilon_\parallel \end{pmatrix} \quad \textbf{(20)}$$

A component of the tensor parallel to the director **n** is denoted by the $\varepsilon_\parallel$ and that in the plane perpendicular to the director is denoted by $\varepsilon_\perp$. Phases having this type of symmetry are called uniaxial. The dielectric anisotropy for the uniaxial phase is defined as:

$$\Delta\varepsilon = \varepsilon_\parallel - \varepsilon_\perp \quad \textbf{(21)}$$

Phases having a biaxial symmetry (biaxial phase) has three independent components of the dielectric permittivity tensor the component parallel to the director n is denoted by ε_3. The two components lying in a plane perpendicular to the director are now different in magnitude and denoted by ε_2 and ε_1.

$$\varepsilon^* = \begin{pmatrix} \varepsilon_1 & 0 & 0 \\ 0 & \varepsilon_2 & 0 \\ 0 & 0 & \varepsilon_3 \end{pmatrix} \tag{22}$$

The difference between the tensor components perpendicular to the director n is called dielectric biaxiality and can be written as δε. By convention it is defined as:

$$\delta\varepsilon = \varepsilon_2 - \varepsilon_1 \tag{23}$$

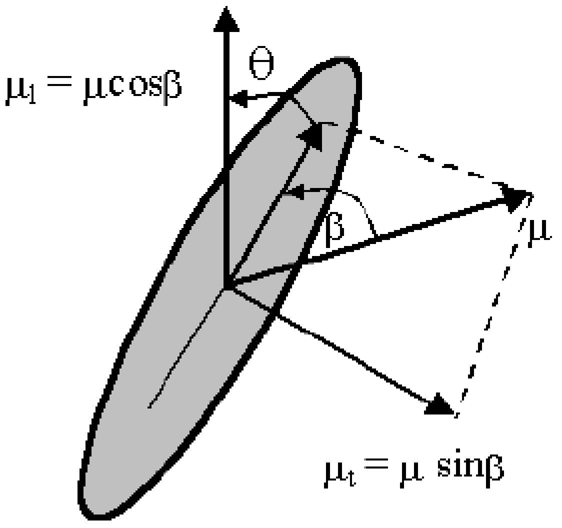

Figure 2: The elongated molecule tilted at an angle θrelative to the director. The molecule is assumed to possess a dipole moment μattached at an angle βto its long axis.

The dielectric anisotropy:

$$\Delta\varepsilon = \varepsilon_3 - \varepsilon_1 \tag{24}$$

Usually, the average dielectric permittivity for a biaxial phase is defined as:

$$\bar{\varepsilon} = \frac{\varepsilon_1 + \varepsilon_2 + \varepsilon_3}{3} \tag{25}$$

with the corresponding expression:

$$\bar{\varepsilon} = \frac{\varepsilon_{\parallel} + 2\varepsilon_{\perp}}{3} \tag{26}$$

for an uniaxial phase.The theoretical treatment describing the dielectric properties of the uniaxial nematicliquid crystal was first given by Maier and Maier [**5**], who reformulated the Onsager treatmentfor the isotropic liquid. They introduce the molecular anisotropy together with the nematicorder parameter S described by the equation:

$$S = 1/2 < 3\cos^2\theta - 1 >$$

The molecular dipole μ has two components parallel to the longitudinal and the transverse molecular axes (denoted by the subscript l and t). Maier and Maier were able to shape the nematic permittivity components in the following form, which is straightforward generalization of the Onsager expression **18**.

$$\varepsilon_{\parallel} - 1 = \frac{NhF}{\varepsilon_0}\left(\bar{\alpha} + \frac{2}{3}\delta\alpha S + \frac{F}{3kT}\left[\mu_1^2(1+2S) + \mu_t^2(1-S)\right]\right) \tag{27}$$

$$\varepsilon_{\perp} - 1 = \frac{NhF}{\varepsilon_0}\left(\bar{\varepsilon} - \frac{1}{3}\delta\alpha S + \frac{F}{3kT}\left[\mu_1^2(1-S) + \mu_t^2(1-\frac{1}{2}S)\right]\right) \tag{28}$$

The mean polarizability α and the anisotropy of polarizability Δα are denoted by:

$$\bar{\varepsilon} = \frac{\alpha_1 + 2\alpha_t}{3}$$

and

$$\Delta\alpha = \alpha_1 - \alpha_t$$

If we use the fact that $\mu_1 = \mu \cos\beta$ and $\mu_t = \mu \sin\beta$(see Figure **1**) from the expression **27** and **28** can easily yield the standard expression for the dielectric anisotropy

$$\Delta\varepsilon = \frac{NhF}{\varepsilon_0}\left(\Delta\alpha + \frac{F}{2kT}\mu^2(1-3\cos^2\beta)\right)S \tag{29}$$

Where β is the angle between the dipole moment μ and the director.

FREQUENCY DEPENDENCE OF THE DIELECTRIC PERMITTIVITY:

When the dielectric is subjected to an alternating electric field there are two possibilities, which depend on the frequency of the field, the temperature and the kind of material. In some cases there is no measurable phase difference between D and E. The polarization is in phase with the alternating field. Then the relation D = εE is also valid for the alternating field and if the dielectric is placed between the plates of the condenser to which an alternating voltage of the appropriate frequency is applied, no possible phase difference between the potential and the true charge of the condenser plates is noticed. In the other case, there is a noticeable phase difference between D and E. Then the relation D = εE is not valid and the phase difference between the potential and the true charge of the condenser makes it impossible to use the formula $C = \varepsilon C_0$ for the capacity of the condenser. In the case of a phase difference between D and E, it is usual to describe the relationship between the scalars D and E with the aid of complex notation: we introduce the complex quantity E^*, given by:

$$E^* = E_0 e^{i\omega t} \quad \textbf{(30)}$$

Where $i = (-1)^{1/2}$, E_0 is the magnitude of E^* and ω is the alternating field frequency. So we write, the electric displacement vector D^* is of the form:

$$D^* = D_0\, e^{(i\omega t-\delta)} \quad \textbf{(31)}$$

Where δ is the phase difference between E^* and D^*.When δ is independent of E, the ratio between the complex quantities D^* and E^* is given, according to **Equations 19** and **20**, by constant complex quantity ε*:

$$\hat{D} = \varepsilon * \hat{E} \quad \textbf{(32)}$$

with

$$\varepsilon * = \frac{D_0}{E_0} e^{-i\delta} \quad \textbf{(33)}$$

Therefore, formally, a complex dielectric constant can be introduced. The introduction of the complex quantities D^* and E^* is a formal description, leading to the complex quantity ε* which turns into the real dielectric constant ε when the phase difference δ equal to zero. Generally ε* is split into two (real and imaginary) parts denoted by ε' and ε":

$$\varepsilon * = \varepsilon' - i\varepsilon'' \quad \textbf{(34)}$$

Writing **Equation 33** in the form:

$$\varepsilon^* = \frac{D_0}{E_0}(\cos\delta - i\sin\delta) \tag{35}$$

Comparing **Equations34** and **35** we get:

$$\varepsilon' = \frac{D_0}{E_0}\cos\delta \tag{36}$$

$$\varepsilon'' = \frac{D_0}{E_0}\sin\delta \tag{37}$$

From these two equations we get:

$$\tan\delta = \frac{\varepsilon''}{\varepsilon'} \tag{38}$$

Now we start from the case where the frequency equals to zero. Then we have:

$$P_s = \varepsilon_s E$$

Where the suffix s indicates that the field is static.

So,

$$P_s = D - \varepsilon_0 E$$

We can divide P_s into two parts:

$$P_s = P_\infty + (P_s)_D \tag{39}$$

Where $(P_s)_D$ indicates that the part of P_s due to permanent dipoles and P_∞ the part due to the polarizability of the particles. From this definition

$$P_\infty = (\varepsilon_\infty - 1)\varepsilon_0 E$$

The time which the permanent dipoles need to reach the equilibrium distribution subsequent to the application of a static external field, then the part $(P_s)_D$ of P_s "built up" and P increases from P_∞ to P_s.

After a certain time t during this interval we have

$$P(t) = P_\infty + P_D(t)$$

Where $P_D(t)$ is the part of $(P_s)_D$ that has already built up.

As in other relaxation phenomena, e.g. mechanical deformation, we assume that the rate of increase of P_D, $dP_D(t)/dt$ is proportional to the difference between the final value $(P_s)_D$ and the actual value of $P_D(t)$:

$$\frac{dP_D(t)}{dt} = \frac{1}{\tau}\{(P_s)_D - P_D(t)\} \tag{40}$$

where τ is a constant having the dimension of time. Since τ is a measure of time lag, it is called the relaxation time.

In the theory of relaxation time it is generally assumed that the differential **Equation40**is also valid for an alternating field. In that case the quantity $(Ps)_D$ occurring in **Equation 39**is afunction of 't': it represents the value which $P_D(t)$ would finally reach in the static field E(t).

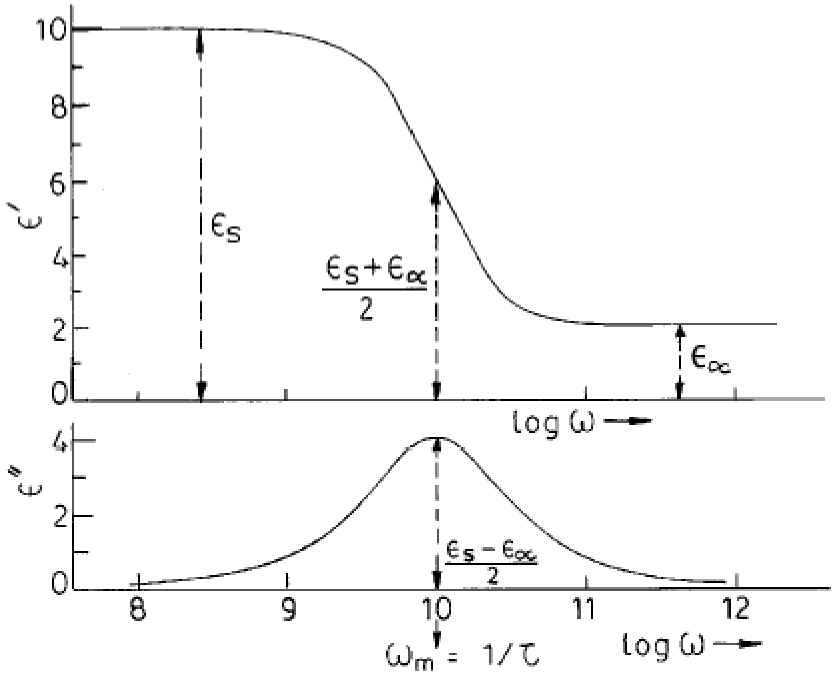

Figure 3: Frequency dependent real and imaginary parts of the dielectric permittivity corresponding to the Debye equation.

$$\tau\frac{dP_D(t)}{dt} + P_D(t) = (\varepsilon_S - \varepsilon_\infty)\varepsilon_0 E(t) \tag{41}$$

The general solution of this equation is:

$$P_D^*(t) = \Pi e^{-\frac{t}{\tau}} + \frac{\varepsilon_s - \varepsilon_\infty}{1 + i\omega\tau} \varepsilon_0 E_0 e^{i\omega t} \qquad \textbf{(42)}$$

where the constant Π characterizes the initial polarization. The first term of the **Equation 42** decays with time, and, therefore, it may be neglected in comparison with the second term. Thus we obtain for the total polarization:

$$P_D^*(t) = \frac{\varepsilon_s - \varepsilon_\infty}{1 + i\omega\tau} \varepsilon_0 E_0 e^{i\omega t} \qquad \textbf{(43)}$$

Therefore the dielectric displacement vector

$$D^* = \varepsilon_0 E^* + P^* = \left[\varepsilon_\infty + \frac{\varepsilon_s - \varepsilon_\infty}{1 + i\omega\tau} \right] \varepsilon_0 E_0 e^{i\omega\tau} \qquad \textbf{(44)}$$

and the complex dielectric permittivity ε* is given by

$$\varepsilon^* = \varepsilon_\infty + \frac{\varepsilon_s - \varepsilon_\infty}{1 + i\omega\tau} \qquad \textbf{(45)}$$

ε* may again be separated into its real (ε') and imaginary (ε") parts **(see Figure 4):**

$$\varepsilon' = \varepsilon_\infty + \frac{\varepsilon_s - \varepsilon_\infty}{1 + \omega^2\tau^2} \qquad \textbf{(46)}$$

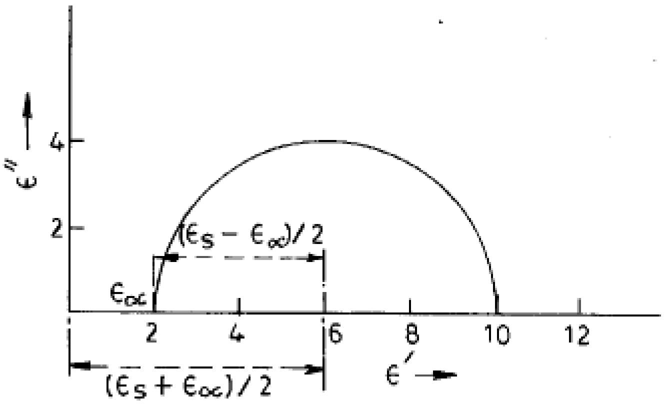

Figure 4: The Debye plot.

$$\left(\varepsilon' - \frac{\varepsilon_S + \varepsilon_\infty}{2}\right)^2 + \left(\varepsilon''\right)^2 = \left(\frac{\varepsilon_S - \varepsilon_\infty}{2}\right)^2 \qquad \textbf{(48)}$$

Thus, the Debye relaxation can be represented by a semicircle (see **Figure 5**), with the center on the abscissa axis and the radius (ε_s - ε_∞)/2.

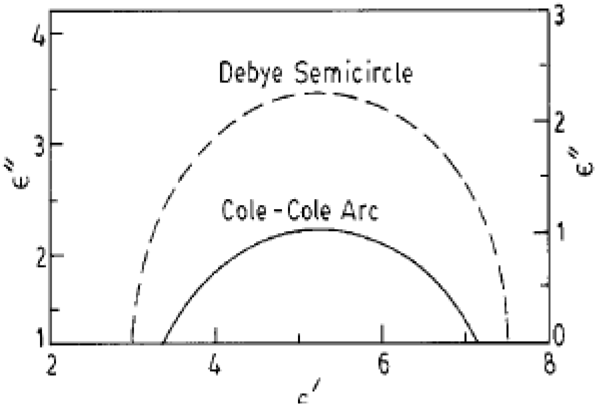

Figure 5: The Debye and Cole-Cole plot.

The **Equations 46**and**47**are known as the Debye equations, since they were first derived by Debye on a molecular basis to describe the orientational polarizability. The Debye theory was the first attempt to relate the relaxation time τ to molecular properties of the media. Later it was extended to the nematic liquid crystals by Maier and Meier [**6**].Progressively increasing quest for synthesizing/designing and characterizing mesogens/mixtures of mesogens with an aim to examine their possible use in devices, has resulted into a large number of theories and models which can effectively help us to understand the underlying mechanism. [**7-13**].

REFERENCES:

[1]. Botscher, C.H.F.; Bordewijk, P. *Theory of Dielectric Polarization*, Elsevier Scientific Publishing 1973, **I**.
[2]. Mossotti, O.F. Bibl. Univ. Modena. 1847, 6, 193.
[3]. Clausius, R. Die Mech. Warmtheorie, Braunschweig 1879, II, 62.
[4]. Onsager, L. J. Am. Chem. Soc. 1936, 58, 1486.
[5]. Maier, W.; Meier, G. Z. Naturforsh. 1961, 16a, 262.
[6]. Cole, K.S.; Cole, R.H. J. Chem. Phys. 1941, 9, 341.
[7]. Chandrashekhar, S., 1992. Liquid Crystals, Cambridge University Press, London.
[8]. de Gennes, P.G., 1993. The Physics of Liquid Crystals, Clarendon Press, Oxford.

[9]. Kumar, S., 1996. Liquid Crystals in the Nineties and Beyond, World Scientific, Singapore.

[10]. Singh, S., 2002. Liquid Crystals: Fundamentals, World Scientific, Singapore.

[11]. Stewart, I.W., 2004. The Static and Dynamic Continuum Theory of Liquid Crystals, CRC Press, London.

[12]. Oswald, P.; Pieranski, P., 2006. Liquid Crystals: Concepts and Physical Properties Illustrated by Experiments. CRC Press, London.

[13]. Jakli, A.; Saupe, A., 2006. One and Two-Dimensional Fluids: Properties of Smectic, Lamellar and columnar Liquid Crystals, CRC Press, London.