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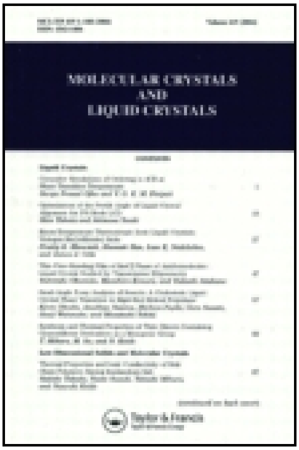

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Effective Mass of a Charge Carrier in Nematic Liquid Crystals

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Effective Mass of a Charge Carrier in Nematic Liquid Crystals

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The estimates of charge carrier mobility in the nematic phase of a liquid crystal (NLC), which were derived from those of viscous friction for a molecular-size Stokes sphere, give much higher values compared with relevant experimental data.[1] One of the possible reasons for such discrepancy may be an increase of the effective mass of an ion due to formation of a polarization coat moving together with the ion.

Keywords: effective mass, charge carrier, nematic liquid crystal

In the present study we calculate the effective mass disregarding the solvation effect since we are particular, first of all, about liquid-crystal properties. Furthermore, the calculations are carried out within the continual approximation which applies because of a large size of the deformation coat. ($R \geqslant 100$ Å).[2]

As shown earlier, along with an ion traveling in a liquid crystal, there also moves a director deformation field linked with the Coulomb field of this ion. Thus, an ion moving inside NLC has the kinetic energy

$$E = \frac{mu^2}{2} \tag{1}$$

that of the deformation coat[1]

$$F_{\mathrm{LC}} = \frac{1}{2}\int d\vec{\tau}\left\{K(\nabla\vec{n})^2 - \frac{\rho_\alpha}{4\pi}(\vec{n}\cdot\vec{D})^2\right\} \tag{2}$$

where K is the Franck constant (in our considerations we employ the single-constant approximation),

$$\rho_\alpha \overset{\mathrm{def}}{=} \frac{1}{\varepsilon_\parallel} - \frac{1}{\varepsilon_\perp} \tag{3}$$

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with $\varepsilon_{\|}$ and $\varepsilon_{\perp}$ being the longitudinal and transverse components of the dielectric permittivity tensor, $\vec{D}$ being the electric induction vector; the same ion is also specified by the kinetic energy of rotation of long molecular axes

$$F_{\tau} = \frac{1}{2}\int \vartheta\left(\frac{d\vec{n}}{dt}\right)^2 d\vec{\tau} \tag{4}$$

where ϑ is the density of the NLC moment of inertia.

We assume that the deformation coat adiabatically follows a moving ion; a similar assumption was used by Pekar in constructing the polaron theory.[13] In this connection, it should be noted that the assumption used implies the following restriction on velocity of the ion, i.e.

$$u < RT \tag{5}$$

where u is the ion velocity, R is a specific size of the deformation coat and T is a time interval during which the director transition to a steady state takes place; relevant estimates of R will be given below.

In the framework of the conception of the deformation coat, the director distribution around an ion can be naturally determined as

$$\vec{n} = \vec{n}(\vec{\tau} - \int \vec{u}(t)dt) \tag{6}$$

With u = const, Equation (6) transforms into

$$\vec{n} = \vec{n}(\vec{\tau} - \vec{u}t) \tag{7}$$

Note that the relation (2) is invariant with respect ot the substitution

$$\vec{\tau} \rightarrow \vec{\tau} - \int \vec{u}(t)dt \tag{8}$$

whereas (4) becomes

$$F_{\tau} = \frac{\vartheta}{2}\int d\vec{\tau}\left\{u_x^2\left(\frac{\partial\vec{n}}{\partial x}\right)^2 + u_y^2\left(\frac{\partial\vec{n}}{\partial y}\right)^2 + u_z^2\left(\frac{\partial\vec{n}}{\partial z}\right)^2\right\} \tag{9}$$

We choose the coordinate system in which $\vec{n}_0$ 110 z, where $\vec{n}_0$ is the direction in the absence of an ion. In this coordinate system Equation (9) leads to

$$F_{\tau} = \frac{\vartheta}{2}\int d\vec{\tau}\left\{u_{\perp}^2\left[\left(\frac{\partial\vec{n}}{\partial x}\right)^2 + \left(\frac{\partial\vec{n}}{\partial y}\right)^2\right] + u_{\|}^2\left(\frac{\partial\vec{n}}{\partial z}\right)^2\right\} \tag{10}$$

and, hence, according to the conventional definition of the effective mass we get

$$m_{\text{ef}}^{\perp} \overset{\text{def}}{=} m + \vartheta \int d\vec{\tau} \left[\left(\frac{\partial \vec{n}}{\partial x} \right)^2 + \left(\frac{\partial \vec{n}}{\partial y} \right)^2 \right] \tag{11}$$

$$m_{\text{ef}}^{\parallel} \overset{\text{def}}{=} m + \vartheta \int d\vec{\tau} \left(\frac{\partial \vec{n}}{\partial z} \right)^2 \tag{12}$$

Numerical estimates of the effective mass can be obtained if one knows the director distribution around a moving ion, the latter may be derived from the minimum of the functional

$$F = F_{\text{LC}} + F_{\tau} \tag{13}$$

However, if we confine our consideration to the adiabatic approximation, the requirement for F_{LC} to bc minimal becomes a sufficient condition for the director distribution to be figured out, i.e. we may calculate the sought distribution around a fixed ion.

In calculating the latter distribution, the following pertinent arguments may be employed. The strong field around an ion lines up the director in a "hedgehog" configuration. In the absence of a disordering effect of thermal fluctuations, of the external field etc., the hedgehog configuration takes up a large spatial region, far away from the ion. On the other hand, the external field influences the director at a large distance from an ion; boundaries bring a similar effect, too. Assuming the vector $\vec{n}_0$ to be set along the field $\vec{D}_u + \vec{D}_0$, where $\vec{D}_u$ is the field of an ion and $\vec{D}_0$ is the external field, we arrive at a rigorous description of director's behavior both in the vicinity of the ion and fairly far away from it. To describe it properly in an intermediate region, we make use of the fact that at small distance this field is strong enough and decreases as $1/\tau^2$. The director, considered as a coordinate function, changes markedly at a distance of the order of magnitude of the correlation radius η^{-1}. As regards the region $\tau < \eta^{-1}$, the field of an ion may be taken into account by introducing a boundary condition at the ion radius.

The above-mentioned makes it possible to substitute a certain effective value of the induction

$$\vec{D}_{\text{ef}} = \frac{e}{\tau_0^2} \frac{\vec{\tau}}{\tau} \exp[-\eta(\tau - \tau_0)] \tag{14}$$

describing properly, the coordinate dependence of $\vec{D}_u$ both near an ion and far away from it, for the actual value of the induction specified by the ion charge.

Assuming the trial solution for the director $\vec{n}_0(\tau)$ to be given by the expression

$$\vec{n}_0 = \frac{\vec{D}_{\text{ef}} + \vec{D}_0}{|\vec{D}_{\text{ef}} + \vec{D}_0|} \tag{15}$$

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we can calculate the correlation radius η^{-1} as a variational parameter of the minimum of the free energy F_{LC}

$$\eta^{-1} = \left(\frac{4\pi K\tau_0^4}{\rho_\alpha e^2}\right)^{1/2} \tag{16}$$

In the final analysis the external field may be set equal to zero as it is a custom with calculations of quasi-average values. The coordinate dependence of the director, given by (15), applies to all distances. Note that with strong external fields the range, where the ion charge brings an essential effect, is approximately equal to $R_1 \sim (ze/D_0)^{1/2}$.

We have already mentioned that the "hedgehog" size may be also determined by a disordering effect of thermal fluctuations. Such being the case, the characteristic length proves to be $R_2 \sim ze/\varepsilon_{\perp K}T$. Naturally, the "hedgehog" size is governed by the smaller value of the both ones considered above.

It should be also pointed out that in the vicinity of the point $\vec{D}_{ef} = -\vec{D}_0$ the director exhibits a singular behavior resulting in a logarithmic discontinuity of the elastic energy. This fact may be neglected, however, in estimating the lower bounds of the effective mass since integration of the free energy density may be carried out over a semispace without this singular point.

Using the relations (14) – (16), we arrive at the following expression of the effective mass

$$m_{ef}^{\perp} = m + \frac{8}{3}\frac{\vartheta}{K}\frac{|\rho_\alpha| ze^2}{\tau_0}\left(\frac{R}{\tau_0} - 1\right) \tag{17}$$

$$m_{ef}^{\parallel} = m + \frac{4}{3}\frac{\vartheta}{K}\frac{|\rho_\alpha| ze^2}{\tau_0}\left(\frac{R}{\tau_0} - 1\right) \tag{18}$$

Employing the values of parameters reported for such a typical LNC as MBBA,[4] we obtain the estimate

$$m_{ef} \simeq 10\, m \tag{19}$$

which fits known experimental data.

It should be noted in conclusion that the suggested approach to calculations of the effective mass differs from that advanced in Reference 1 where by analogy with the polaron theory wave equations were applied to description of the director. Yet, the present study implies that existence of vibrational modes should not be regarded as an obligatory condition for the effective mass to be an applicable notion and, therefore, it essentially extends the validity domain of this conception. Thus, it becomes possible to attribute a decrease of ion mobility, observed under the transformation into the nematic phase, to the polarization coating effect and, consequently, to the increasing effective mass of an ion.

Here we have made use of the continual approximation, applicable to systems with long-range forces (such as an ion in a polarizing medium); yet, the idea about existence of a polarization coat (and the effective mass) is likely to apply to systems with shorter interactions. For example, mobility of impurity molecules was shown to become almost 5 times lower in the ordered NLC phase.[5] This observation is supposedly also related to an increase of the effective mass of an impurity molecule, however, such particular calculations should be carried out without the continual approximation.

In conclusion, the authors thank O. V. Jarotschuk listed in Reference 5.

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