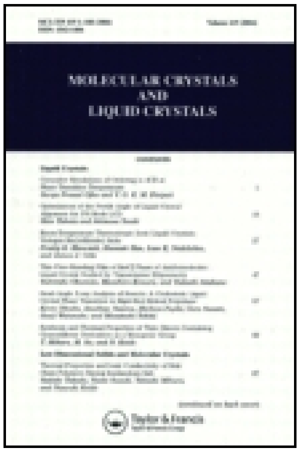

Molecular Crystals and Liquid Crystals Science and Technology. Section A. Molecular Crystals and Liquid Crystals
Publication details, including instructions for authors and subscription information:
http://www.tandfonline.com/loi/gmcl19

# A Flexoelectric Mechanism: The Quadrupole Surfing

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To cite this article: J. F. Palierne (1992): A Flexoelectric Mechanism: The Quadrupole Surfing, Molecular Crystals and Liquid Crystals Science and Technology. Section A. Molecular Crystals and Liquid Crystals, 222:1, 215-218

To link to this article: http://dx.doi.org/10.1080/15421409208048695

*Mol. Cryst. Liq. Cryst.* 1992, Vol. 222, pp. 215–218
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Printed in the United States of America

# A FLEXOELECTRIC MECHANISM: THE QUADRUPOLE SURFING

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*(Received October 7, 1991)*

Abstract A flexoelectric polarization proportional to the splay deformation is expected in phases with local smectic order, because the alternation of highly polarizable molecular cores with paraffinic tails of lower polarizability produces a spatial modulation of electric fields applied normal to the layers, and the locally inhomogeneous field pushes the permanent quadrupole moment of the core along the field direction, coupling with the splay deformations.

Most nematogenic molecules are made with a rigid core of high electric polarizability, prolonged by one or two flexible tails of lower polarizability. Smectic planes thus have in their middle a layer of high dielectric constant, which contains the cores, bordered on each side by layers of low dielectric constant, containing the tails. The simplest model for the dielectric behaviour of smectics can be based on a periodic local dielectric constant

$$\varepsilon\left(z+l_s\right) = \varepsilon(z) \tag{1}$$

where $l_s$ is the thickness of the smectic planes, and the z-axis is parallel to the local director $\vec{n}$ and perpendicular to the layers. Let us now consider the effect of an electric field applied parallel to the director, of magnitude $E = \vec{E}.\vec{n}$. This macroscopic field is the average of the microscopic field $\vec{e}$ over a small but macroscopic region, therefore, it is smooth at the molecular scale. It is related to the macroscopic induction $\vec{D} = \vec{n}D$ by the macroscopic dielectric tensor, which zz-eigenvalue will be denoted $\bar{\varepsilon}$ and satisfies

$$E = \bar{\varepsilon}^{-1}D \tag{2}$$

As the induction is uniform, the z-component of the local field reads

$$e(z) = \varepsilon^{-1}(z)\,D = \frac{\bar{\varepsilon}}{\varepsilon(z)}\,E \tag{3}$$

The effect of the layered dielectric constant is thus a modulation of the macroscopic electric field at the molecular scale. In addition to the dipoles induced by the electric field, the core carries a permanent quadrupole moment of zz+component $\theta$ [1], which undergoes a force due to the induced field

$$f_E = \theta\,\partial_z^2 e = \theta\, l_E^{-2}\,E \tag{4}$$

where the quantity

$$l_E = \left[\bar{\varepsilon}\,\partial_z^2 \varepsilon(z)^{-1}\right]^{-1/2}_{z=z_c} \tag{5}$$

has the dimension of a length, and compares with the layer thickness $l_s$. Since the position $z_C$ of the core corresponds to a maximum of $\varepsilon(z)$, the term between brackets in eq. (5) is positive. The core is then pushed by the local field as if it were carrying a 'pseudo charge' $q = \theta\, l_E^{-2}$, acted upon by the macroscopic field.

This force, which tends to distort the molecule by pushing the core against one tail and away from the other one, is resisted by the mechanical force

$$f_M = -k\left(z_C - z_0\right) \tag{6}$$

due to the tails acting like springs, which tends to bring the core back to its rest position $z_0$ in the middle of the layer. The constant k compares with the stiffness of an entropic chain of b bounds of length $l_b$ : $k \simeq 3k_B T/\left(b l_b^2\right)$. The position $z_0$ is no longer the rest position of the core when a splay imposed to the smectic bends the layers. The tails situated on the convex side are then given more room, whereas on the concave side the tails are compressed. The core then moves towards the convex side by a displacement in the $\vec{n}$ direction, of magnitude

$$z_C - z_0 = \lambda^2\,\mathrm{div}\,\vec{n} \tag{7}$$

The constant $\lambda$, which has the dimension of a length, can be estimated as follows: let S be the section of the molecule projected on the smectic plane. In a bended layer, the surface allowed to the tail on the convex side is increased by $\delta S \simeq S l_s/2 \operatorname{div} \vec{n}$, and reduced by the same amount on the concave side. The variation $\delta v \simeq l_s/2\, \delta S$ of the volume offered to each tail is compensated by a displacement of the core such that $S(z_c - z_0) = \delta v \approx 1/4\, S l_s^2 \operatorname{div} \vec{n}$. From eq. (7) one gets the order of magnitude $\lambda \approx l_s/2 \approx$ tail length. The force which produces the displacement (7) reads

$$f_S = \lambda^2 k \operatorname{div} \vec{n} \tag{8}$$

The total force $f_E + f_M + f_S$ acting on the core derives from the energy

$$w\left(z_C, E, \vec{n}\right) = k/2\left(z_C - z_0\right)^2 - \left(\theta l_E^{-2} E + \lambda^2 k \operatorname{div} \vec{n}\right)\left(z_C - z_0\right) \tag{9}$$

which reaches its minimal value

$$w(E, \vec{n}) = -\frac{1}{2} k \lambda^4 (\operatorname{div} \vec{n})^2 - \frac{1}{2} \theta^2 l_E^{-4} k^{-1} E^2 - \theta l_E^{-2} \lambda^2 E \operatorname{div} \vec{n} \tag{10}$$

at the equilibrium position of the core

$$z_C = z_0 + \theta l_E^{-2} k^{-1} E + \lambda^2 \operatorname{div} \vec{n} \tag{11}$$

corresponding to a zero total force $f_E + f_M + f_S$.

We are now in a position to write down the contribution of the quadrupole surfing to the free energy density of the liquid crystal:

$$F^s\left(\vec{E}, \vec{n}\right) = N w\left(\vec{E}, \vec{n}\right) = -\frac{1}{2} \chi_{//}^{s} \left(\vec{E}, \vec{n}\right)^2 + \frac{1}{2} K_{11}^{s} (\operatorname{div} \vec{n})^2 - e_1^{s}\, \vec{E}.\vec{n} \operatorname{div} \vec{n} \tag{12}$$

where N is the molecule number density, and

$$\chi_{//}^{S} = N \theta^2 l_E^{-4} k^{-1}, \qquad K_{11}^{S} = -N k \lambda^4, \qquad e_1^{S} = N \theta l_E^{-2} \lambda^2 \tag{13}$$

are the surfing contributions to the longitudinal electric polarizability, the Franck splay coefficient and the splay flexocoefficient respectively. The macroscopic electric polarization

$$\vec{P}^{s} = -\frac{\partial F^{s}}{\partial \vec{E}} = \chi^{s}_{//}\left(\vec{E}.\vec{n}\right)\vec{n} + e^{s}_{1}\vec{n}\,\mathrm{div}\,\vec{n} \qquad (14)$$

exhibits both the dielectric and the flexoelectric effect of the quadrupole surfing mechanism.

In contrast with the flexoelectric polarization due to the orientation of the quadrupoles [1], for which the splay and bend flexocoefficients $e_1$ and $e_2$ respectively are identical, the quadrupole surfing mechanism contributes to $e_1$ only. Since the dimensionless group $l_E^{-2}\lambda^2$ is of order unity, the contributions of either the quadrupole surfing and the quadrupole orientation have the same order of magnitude, with opposite signs.

In conclusion, the semiquantitative theory presented here points to the existence of a specific mechanism for splay flexoelectricity, which involves both the nematic order, responsible for the orientation of the molecular quadrupoles along the director, and the smectic order, for the spatial modulation of the local dielectric constant. However, a local smectic-like environment suffices to modulate the electric field acting on a given molecule, provided this order extends over a few molecular lengths. Therefore, the quadrupole surfing can be expected also in the nematic phase, and provides a measure of the fluctuations of the smectic order.

[1] J. Prost, J.P. Marcerou, *J. Physique* **38**, 315 (1977).