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Geometrical Averaging of AFLC Dielectric Tensors*

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The optical transmission of antiferroelectric liquid crystal layers is non-trivial. For optical wavelengths we average the dielectric tensors. The aim is to provide a geometrical way for this averaging. By a thorough mathematical analysis, we are able to construct the representation ellipsoid for the final ε-tensor in most cases. In this way, we can easily predict the axes and indices of refraction of the structure. Especially the molecular states that occur during the hysteresis switching behaviour are studied.

Keywords: Antiferroelectric liquid crystal; birefringence; ray ellipsoid

1. INTRODUCTION

As already indicated in an earlier publication [1], the transmission of electromagnetic waves through antiferroelectric liquid crystal displays leads to grating diffraction and therefore strongly depends on the wavelength. For visible light, the situation is very simple: only the zeroth order of diffraction is of importance. In other words, the alternating structure should be averaged. More precisely, for the determination of the birefringence, one

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should calculate the arithmetic average of the two dielectric ε-tensors, related to the molecular orientation in both of the alternating layers. Remark that suggestions of averaging the molecular positions in the two layers or averaging the optical transmission of both layers are wrong.

Furthermore, it should be clear that, throughout this article, we are dealing with ε-values at optical frequencies, from which the indices of refraction are calculated ($n = \sqrt{\varepsilon}$). These values are different from the values that are needed for electric field calculations at low frequencies.

Numerically, the situation does not need very much comment: starting with the tensors $\bar{\varepsilon}_1$ and $\bar{\varepsilon}_2$, the resulting tensor can be calculated through $\bar{\varepsilon}_3 = (1/2)(\bar{\varepsilon}_1 + \bar{\varepsilon}_2)$. Diagonalisation leads to the principal axes and the indices of refraction.

The purpose of this article is to develop a shortcut: it would be nice to conclude from the position of the molecules on the smectic cone how the axes of birefringence are oriented. Therefore, we consider the geometrical representation of the dielectric tensor by an ellipsoid. Having two ellipsoids, the problem boils down to the geometrical construction of the 'average' of two ellipsoids. The situation is clarified in Figure 1.

First of all, we should specify what we mean by geometrical representation. Let us consider the quadric (ellipsoid) with the following cartesian equation:

$$(x\ y\ z) \cdot \bar{R} \cdot \begin{pmatrix} m_1 & 0 & 0 \\ 0 & m_2 & 0 \\ 0 & 0 & m_3 \end{pmatrix} \cdot \bar{R}^T \cdot \begin{pmatrix} x \\ y \\ z \end{pmatrix} = 1 \qquad (1)$$

$\bar{R}$ denotes a rotation matrix (orthogonal, so that $\bar{R}^{-1} = \bar{R}^T$). If $\vec{u}_x$, $\vec{u}_y$ and $\vec{u}_z$ are the unit vectors in the cartesian frame, $\bar{R}\vec{u}_x$, $\bar{R}\vec{u}_y$ and $\bar{R}\vec{u}_z$ are

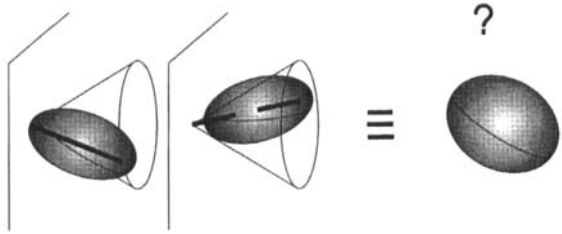

FIGURE 1 Considering the geometrical representation for the dielectric tensors of the alternating smectic layers, we want to 'construct' the resulting tensor for the averaged structure.

eigenvectors of the matrix of coefficients

$$\bar{R} \cdot \begin{pmatrix} m_1 & 0 & 0 \\ 0 & m_2 & 0 \\ 0 & 0 & m_3 \end{pmatrix} \cdot \bar{R}^T.$$

These eigenvectors indicate the principal axes of the ellipsoid. Their eigenvalues are m_1, m_2 and m_3 respectively. The lengths of the ellipsoid's main axes are given by $1/\sqrt{m_1}$, $1/\sqrt{m_2}$ and $1/\sqrt{m_3}$. Now, if one takes $m_i = \varepsilon_i (i = 1, 2, 3)$ the quadric is called the *ray ellipsoid* of the (liquid) crystal [2]. The alternative $m_i = (1/\varepsilon_i)$ gives us the *ellipsoid of wave normals* or *optical indicatrix*. Here, we will use the first option: in this case only, manipulations on the tensor ε directly lead to equivalent transformations of the coefficient matrix. At all instances one can switch to the alternative representation by inverting the coefficient matrix.

Before we get started, another important characteristic of our structure should be noted: the tensors ε_1 and ε_2 are related through a simple rotation (the two ellipsoids in Fig. 1 are therefore congruent).

2. MATHEMATICAL RESULTS

2.1. The Geometrical Parameters

So, we consider an ellipsoid $\mathcal{E}_1$ with its axes along x, y and z, and its image $\mathcal{E}_2$ by rotation (about an axis through its center point). In Figure 2 the first

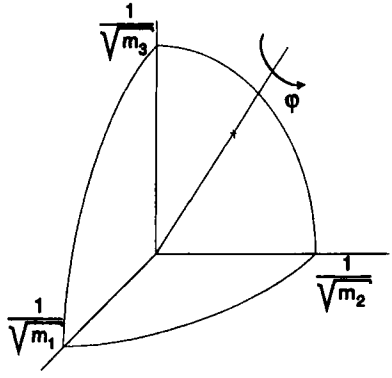

FIGURE 2 The relative magnitudes of the axes, the orientation of the rotation axis and the rotation angle itself are determining whether the shape and/or orientation of the resulting ellipsoid can be predicted.

ellipsoid and the position of the rotation axis are indicated. We have investigated in what cases we can generally predict the shape and/or the orientation of the resulting ellipsoid $\mathcal{E}_3$ (after averaging the coefficient matrices).

The important geometrical parameters are the relative lengths of the ellipsoid's axes ($1/\sqrt{m_1}$, $1/\sqrt{m_2}$ and $1/\sqrt{m_3}$), the orientation of the rotation axis ($a\vec{u}_x + b\vec{u}_y + c\vec{u}_z$) and the angle of rotation φ.

2.2. The Intersection Curves

It is very instructive to look at the intersection between the two ellipsoids $\mathcal{E}_1$ and $\mathcal{E}_2$. We have searched for the condition which guarantees the intersection curves to be planar. In general, they are not, as illustrated in Figure 3. The search for a degenerate quadric in the family of quadrics $(\mathcal{E}_1, \mathcal{E}_2)$ that is generated by $\mathcal{E}_1$ and $\mathcal{E}_2$, leads to the following condition:

$$\sin\varphi(1 - \cos\varphi)\, abc(m_1 - m_2)\,(m_2 - m_3)\,(m_3 - m_1) = 0 \qquad (2)$$

Naturally, this condition leads to a classification of cases. The case $\varphi = 0$ is trivial.

- rotation with a special angle: $\varphi = \pi$
- rotation about a special axis: $a = 0$ or $b = 0$ or $c = 0$
- the ellipsoid has an axis of revolution: $m_1 = m_2$ or $m_2 = m_3$ or $m_3 = m_1$
- the geometry has none of these special features.

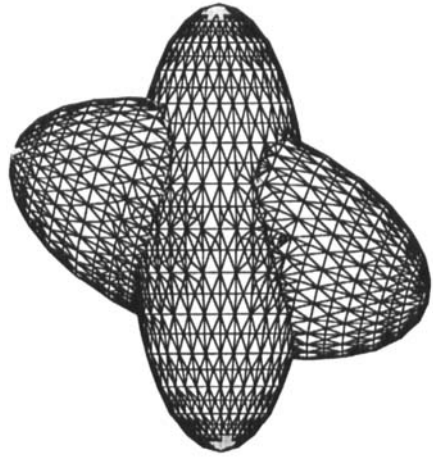

FIGURE 3 The intersection between two congruent ellipsoids is generally non-planar.

It is clear that the resulting ellipsoid ($\mathcal{E}_3 = (1/2)(\mathcal{E}_1 + \mathcal{E}_2)$) is a member of the family ($\mathcal{E}_1$, $\mathcal{E}_2$). So the intersection curve ($\mathcal{E}_1 \cap \mathcal{E}_2$) is always lying on the surface of $\mathcal{E}_3$.

$\bar{\varepsilon}_1$ and $\bar{\varepsilon}_2$ have the same eigenvalues, so a fortiori the same sum of eigenvalues: $\mathrm{Tr}(\bar{\varepsilon}_1) = \mathrm{Tr}(\bar{\varepsilon}_2)$. This sum of eigenvalues remains unchanged through the averaging.

2.3. A Special Rotation Angle $\varphi = \pi$

The case is illustrated in Figure 4.

One can prove that the two *perpendicular* planes of intersection are given by

$$\begin{cases} ax + by + cz = 0 \\ sx + ty + uz = 0 \end{cases}$$

where a, b and c are the coordinates of the rotation axis and

$$\begin{cases} s = a(a^2 m_1 + b^2 m_2 + c^2 m_3 - m_1) \\ t = b(a^2 m_1 + b^2 m_2 + c^2 m_3 - m_2) \\ u = c(a^2 m_1 + b^2 m_2 + c^2 m_3 - m_3) \end{cases}$$

The only eigenvector, or principal axis of the resulting ellipsoid that is independent of the specific values of the starting eigenvalues is the *rotation axis* itself.

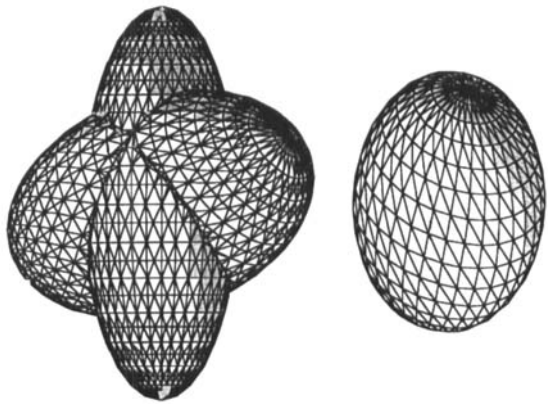

FIGURE 4 The geometry in case of a rotation about the (1, 1, 1)-axis with $\varphi = \pi$: at the left we draw the intersection of the starting ellipsoids (axis lengths 2, 3, 5), at the right the resulting ellipsoid (axis lengths 2.735, 2.262 and 3.726).

The eigenvalue is $a^2m_1 + b^2m_2 + c^2m_3$. (The corresponding 'top' of $\mathcal{E}_3$ is the intersection point between the rotation axis and $\mathcal{E}_1$).

2.4. A Special Rotation Axis

As soon as the rotation axis lies in a mirror plane of $\mathcal{E}_1$, we can be sure (according to Eq. 2) that the intersection $(\mathcal{E}_1 \cap \mathcal{E}_2)$ is planar again. There is a strong analogy with the previous case. Now, the two perpendicular planes are described by:

$$\begin{cases} kx + ly + mz = 0 \\ sx + ty + uz = 0 \end{cases}$$

$$\begin{cases} s = k(k^2m_1 + l^2m_2 + m^2m_3 - m_1) \\ t = l(k^2m_1 + l^2m_2 + m^2m_3 - m_2) \\ u = m(k^2m_1 + l^2m_2 + m^2m_3 - m_3) \end{cases}$$

The vector $k\vec{u}_x + l\vec{u}_y + m\vec{u}_z$ is now different from the rotation vector (actually, it is perpendicular to it). It is the bisector between the main axes of $\mathcal{E}_1$ and $\mathcal{E}_2$ both of which are perpendicular to the rotation axis. This situation is rather important for the antiferroelectric liquid crystals as we will show later on. We therefore illustrate the geometrical configuration in Figure 5.

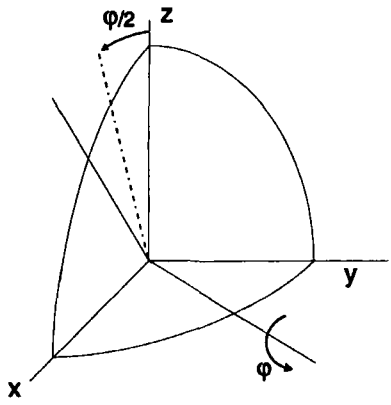

FIGURE 5 When the rotation axis lies in one of the mirror planes of the ellipsoid (e.g., the *xy*-plane), the third axis (e.g., the *z*-axis) of the ellipsoid, perpendicular to the mirror plane is important. The bisector between this axis and its rotated image becomes one of the main axes of the resulting ellipsoid $\mathcal{E}_3$.

In the figure we took $c = 0$, so the rotation axis has coordinates $(a, b, 0)$. In that case $(k, l, m) = (b \sin(\varphi/2), -a \sin(\varphi/2), \cos(\varphi/2))$.

The eigenvalue of the eigenvector (k, l, m) is $k^2 m_1 + l^2 m_2 + m^2 m_3$.

Generally, this is the only eigenvector that is independent from the shape of the original ellipsoid $\mathcal{E}_1$. However, when one of the main axes of $\mathcal{E}_1$ is the axis of rotation, the problem can be fully solved. In fact, the construciton becomes totally 2-dimensional. This is illustrated in Figure 6.

Suppose x becomes the rotation axis. Then x remains a main axis with eigenvalue m_1. The other eigenvectors are the bisectors of the original main axes. The eigenvalues are $\sin^2(\varphi/2)m_2 + \cos^2(\varphi/2)m_3$ and $\cos^2(\varphi/2)\, m_2 + \sin^2(\varphi/2)m_3$.

2.5. Ellipsoids of Revolution

When two eigenvalues are equal, the intersection between $\mathcal{E}_1$ and $\mathcal{E}_2$ is surely planar. In fact, this could be concluded from the previous case: since all planes through the axis of revolution are mirror planes, all possible rotation axes are lying in a mirror plane of $\mathcal{E}_1$. The situation is illustrated in Figure 7.

The eigenvalue problem for $\bar{\varepsilon}_3$ can always be fully solved. Now the axis of revolution of $\mathcal{E}_1$ is crucial. Supposed $m_1 = m_2$, then $z = (0, 0, 1)$ is the axis of revolution. Let us write (r_1, r_2, r_3) as coordinates for its image (the axis of revolution of $\mathcal{E}_2$). Then the three eigenvectors and eigenvalues are:

$$\begin{cases} (r_1, r_2, r_3 + 1) & \text{eigenvalue} \quad (1/2)(1 - r_3)m_1 + (1/2)(1 + r_3)m_3 \\ (r_1, r_2, r_3 - 1) & \text{eigenvalue} \quad (1/2)(1 + r_3)m_1 + (1/2)(1 - r_3)m_3 \\ (-r_2, r_1, 0) & \text{eigenvalue} \quad m_1 \end{cases} \tag{3}$$

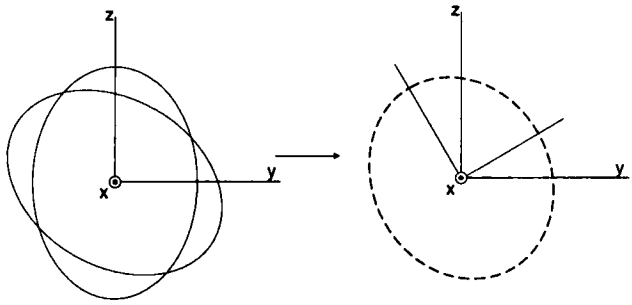

FIGURE 6 If, for instance, the rotation axis is x, then the geometrical construction of the resulting ellipse is straightforward.

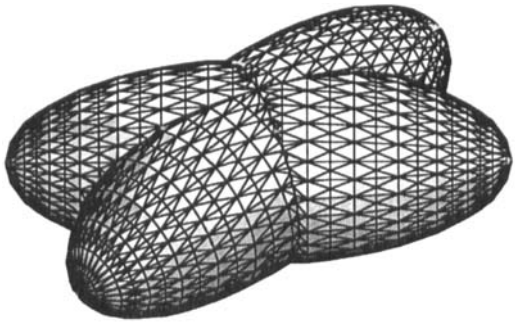

FIGURE 7 The intersection of two ellipsoids of revolution, connected by a simple rotation, is always planar.

The first two vectors are the inner and outer bisectors of the axes of revolution of $\mathcal{E}_1$ and $\mathcal{E}_2$, the last one is orthogonal to them.

2.6. No Special Geometry

In case there is none of the special features that we mentioned above, the intersection $(\mathcal{E}_1 \cap \mathcal{E}_2)$ is non-planar, as already illustrated in Figure 3. The eigenvalue problem of $\bar{\varepsilon}_3$ is dramatic in such a sense that it fully depends on m_1, m_2 and m_3. Therefore, we did not succeed in a general geometrical construction of $\mathcal{E}_3$. It turns out that this most general case is not present in the antiferroelectric structure.

3. CONSTRUCTION OF $\mathcal{E}_3$ FOR THE AFLC STRUCTURE

In Figure 8, we recall the coordinate system of the smectic cone, with half cone angle θ. The molecular long axis is indicated by the vector $\vec{n}$. The vector $\vec{p}$ gives the direction of the polarisation. It is always lying in the smectic plane and tangent to the cone.

Remark that the vector $\vec{q}$ is not lying in the smectic plane and is therefore not lying in the plane of the drawing at the right hand side. This has been indicated by the dotted line. The ellipsoid $\mathcal{E}_1$ has main axes *qpn*, indicated by an angle φ_1. The same kind of drawing could be made for molecules in the adjacent layer, with ellipsoid $\mathcal{E}_2$, and angle φ_2. $\mathcal{E}_1$ and $\mathcal{E}_2$ are connected with each other through a pure rotation about $\vec{k}$ with an angle $\phi = \varphi_2 - \varphi_1$.

Now, according to our extensive mathematical discussion, it is important to analyze the relationship between the rotation axis and the ellipsoid. Since

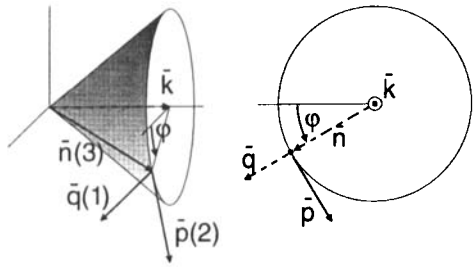

FIGURE 8 The smectic cone seen in perspective and in the direction $\vec{k}$.

$\vec{k}$ is always lying in the qn-plane, we are in a special case (see subsection 2.4). Therefore, we can always conclude that the bisector between $\vec{p}_1$ and $\vec{p}_2$ is a main axis of $\mathcal{E}_3$ (and hence an axis of birefringence for the antiferroelectric structure) with eigenvalue $\sin^2(\phi/2)\cos^2(\theta)\,\varepsilon_1 + \cos^2(\phi/2)\,\varepsilon_2 + \sin^2(\phi/2)\sin^2(\theta)\,\varepsilon_3$. The numbering 1, 2, 3 corresponds with the order q, p, n.

In case we are dealing with a uniaxial anisotropy where $\varepsilon_1 = \varepsilon_2$, all three axes can be constructed according to the rules of subsection 2.5. Additional to the bisector of the two $\vec{p}$ vectors ($\vec{P}$), we now have the bisector $\vec{N}$ of the two $\vec{n}$ vectors. The third one completes the orthogonal axes frame. The construction is illustrated in Figure 9 (left hand side). Remark that the whole structure behaves in a biaxial way, since the three eigenvalues of the averaged tensor in general will be different.

For the case where $\phi = \pi$, i.e. when the polarisation of adjacent layers is opposite (as in the normal stable state), the geometry can be fully solved

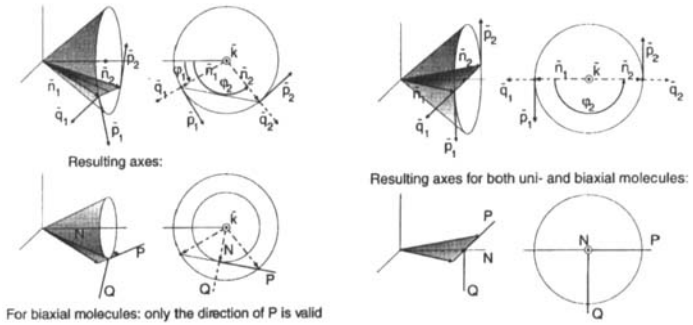

FIGURE 9 **left**: Starting from two arbitrary positions of the uniaxial antiferroelectric molecules, the resulting birefringent axes can be constructed as shown. In case the molecules are biaxial, only the construction of the $\vec{P}$ axis remains valid. The orientation of $\vec{N}$ and $\vec{Q}$ for biaxial molecules depends on the relative magnitudes of ε_1, ε_2 and ε_3. **right**: For the normal antiferroelectric state the geometrical problem can be fully solved without the hypothesis of uniaxiality.

again. One either considers the rotation about $\vec{k}$ with an angle π (case 2.3), or the rotation about $\vec{p}$ with an angle -2θ (case 2.4).

The last interpretation shows that we are in fact dealing with a two-dimensional problem. The construction is illustrated in Figure 9 (right hand side). Remark that the condition of uniaxiality is not needed here in order to fully solve the problem.

4. AXES AND INDICES OF REFRACTION DURING THE AFLCD SWITCHING CYCLE

It is possible to treat the switching of AFLCD's in an analytical way [3–5]. In Figure 10 the calculated hysteresis curve is shown schematically (on top).

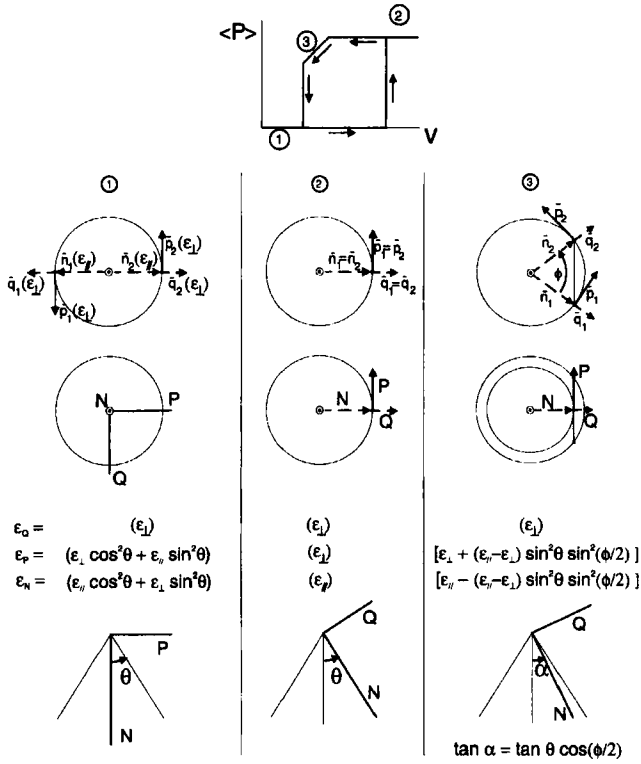

FIGURE 10 For the three states of the AFLCD switching cycle (1 antiferroelectric, 2 ferroelectric and 3 symmetrical) the orientation of the individual molecular axes, as well as the averaged structure axes are indicated on the smectic cone. The bottom row shows the view through the display's glassplates, the orientation of the axes of birefringence with the expressions for the ε-values.

Three important structures occur: (1) the antiferroelectric state, for which the molecules have opposite polarisation, (2) the ferroelectric state, where all molecules have the same orientation, and (3) the symmetric structure, with changing angle between the molecular directors of the adjacent layers. In short circuit, the antiferroelectric LCD is in the antiferroelectric state. When the voltage exceeds a certain threshold, the system switches to the ferroelectric state. In returning, the structure stays ferroelectric until a lower threshold. Instead of returning immediately to the antiferroelectric state, the directors in both layers deviate in a symmetric way from the ferroelectric position. Finally, when the voltage is low enough, the system switches back to its original antiferroelectric situation.

It is important for experimental verifications to be able to calculate the corresponding optical transmission for each of the three structures. We consider the practical case of uniaxiality: the (optical) dielectric constant in the direction parallel with the molecules is called $\varepsilon_{\parallel}$; in both perpendicular directions, the dielectric constant is $\varepsilon_{\perp}$.

The ferroelectric state (2), middle column, is homogeneous and thus needs no special treatment. The antiferroelectric state (1) has to be compared with Figure 9 (right hand side), while the symmetrical structure (3) with uniaxial molecules corresponds with Figure 9 (left hand side). For the calculation of the indices of refraction of this symmetrical structure, one should use formulas (3) (with $r_1 = \sin\theta\cos\theta(\cos\phi - 1)$, $r_2 = \sin\theta\sin\phi$, $r_3 = \sin^2\theta\cos\phi + \cos^2\theta$). The expressions for ε are indicated in Figure 10. The indices of refraction are calculated by $n = \sqrt{\varepsilon}$.

5. CONCLUSIONS

With a thorough mathematical analysis, we were able to construct the axes of birefringence and to calculate the indices of refraction for uniaxial antiferroelectric materials in all positions on the smectic cone. For biaxial materials it is always possible to construct at least one of the main axes. In case the polarisation of the adjacent layers is opposite, all three axes can be constructed.

In this way, we were able to provide a shortcut to make quick conclusions about the optical behaviour of the antiferroelectric material. This is illustrated in the practical case of the geometries that occur during the ALFCD-switching cycle.

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