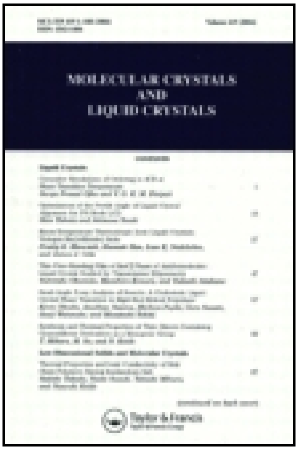

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Modelling Smectic Structures Using Neutron Scattering

L. Rosta [a], N. Kroó [a], GY. Török [b] & G. Pépy [c]

[a] Central Research Institute for Physics, H-1525, Budapest, P.O.B. 49, Hungary

[b] Joint Institute for Nuclear Research, Dubna, 101000, Moscow, P.O.B. 79, USSR

[c] Laboratoire Leon Brillouin, CEN Saclay, 91191, Gif sur Yvette, Cedex, France

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Modelling Smectic Structures Using Neutron Scattering

L. ROSTA and N. KROÓ
Central Research Institute for Physics, H-1525 Budapest, P.O.B. 49, Hungary

and

GY. TÖRÖK
Joint Institute for Nuclear Research, Dubna, 101000, Moscow, P.O.B. 79, USSR

and

G. PÉPY
Laboratoire Léon Brillouin, CEN Saclay, 91191 Gif sur Yvette Cedex, France

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A new approach for describing smectic structures is proposed based on neutron scattering experiments involving fast-cooled liquid crystals. As an example, a comprehensive study of the structure of the MBBA solid modifications (noncrystalline and crystalline phases) is demonstrated.

Neutron diffraction measurements were carried out on four samples with different deuterium/hydrogen contents. By model fitting to the experimental data the structure of the crystalline phases could be characterized by a monoclinic lattice thereby enabling molecular packing model to be proposed.

Information on the structure of the non-crystalline phases was gained from small angle neutrons scattering data. On the one hand smectic-type layers were observed, on the other hand the existence of the theoretically predicted anisotropic density domains was proved. These results together with the molecular pacing model generalized from the crystal phase structure led to classification of nematic, smectic A and tilt smectic-type solid mesophases. The medium range ordering and the local molecular packing are described for these phases.

A procedure for modelling the molecular structure in liquid crystals is proposed based on scattering experiments using the intermediate fast-cooled state.

Keywords: fast-cooling, MBBA, model, smectics, neutron scattering

I. INTRODUCTION

Smectics remain one of the most attractive fields of liquid crystal research. Considerable effort has been made to characterize the microscopic structure of the smectic state, and a large number of papers have been published[1,2] describing the molecular arrangement of different substances with smectic mesophase(s). Most of these structural results were gained from diffraction experiments, usually X-ray[2] measurements, however neutron diffraction studies[3] have also been reported. Besides describing particular structures quite a number of general models of smectic structures have been suggested.[4] Despite these investigations many questions concerning the microscopic description of smectic structures are still open, such as the layer thickness-molecular length relation, molecular tilting relative to the director, correlation distances, etc.

In this paper we propose a new approach to describe the molecular arrangement of liquid crystals, in particular, smectics, based on neutron scattering investigations of fast-cooled liquid crystals. Several papers[5] concern mesogenic substances which have the ability to form a glassy solid phase (termed glassy liquid crystal–GLC) when they are rapidly cooled from the liquid mesophase. The GLC state nearly conserves to a large extent the structural properties of the starting liquid crystal phase—as has been proved in many cases.[5] In view of this it seems reasonable to use information gained from the study of frozen-in liquid crystal structures at low temperatures for modelling the molecular packing in real smectic liquid crystals. N-p-methoxybenzylidene-p-n-butyliniline (MBBA) is the most intensively studied liquid crystal (LC) compound as far as the glassy state and solid polymorphism are concerned. A comprehensive investigation of MBBA by different neutron scattering methods may provide a good example for the present procedure of constructing a molecular packing model of a smectic liquid crystal starting from an analysis of the solid phase structures.

II. SOLID MESOPHASES OF MBBA

MBBA can easily be transformed, by fast cooling (at least 40K/min) from the room temperature nematic phase to liquid N_2 temperature, into a glassy state (labelled C_0 in the case of this substance). During reheating a sequence of polymorphic modifications can be observed. The structure of these states was studied by simultaneous neutron diffraction and Raman-scattering and a phase diagram of MBBA was established.[6] The glassy state (C_0) is followed in the irreversible series of heating transitions first by two modifications (C_1 and C_2) considered as relaxed amorphous structures, then by two metastable crystalline phases (C_3 and C_4). The C_5, C_6 crystalline phases can be produced by slow cooling. The conditions for phase formation and stability as well as the phase transition scheme are given in papers.[6,7]

It was explained[8] that the set of phases $C_0 \rightarrow C_1 \rightarrow C_2 \rightarrow C_3$ corresponds to different stages of a gradual disorder → order structural transition and the change of the medium range order plays an important role. There is a striking analogy of this phase sequence—on a reversed temperature scale—with the smectic polymorphism of liquid crystals, where the lowering of the temperature leads to smectic phases with increasingly more ordered structures (nematic → SmA → SmB → . . .SmH → crystal). Therefore a special study of medium size structural units (several nanometers) such as density domains and smectic layers was carried out by small angle scattering (SAS) of neutrons.[9] Figure 1 shows neutron diffraction patterns recorded on a small angle scattering (SAS) spectrometer at the Saclay Orphée reactor. The scattering intensity is presented for the C_0, C_1 and C_2 phases of the oriented (by magnetic field H in the scattering plane) MBBA sample. The three-dimensional illustration of the intensity distribution over the 128 × 128 cells area of the *XY* multidetector is presented. Example of treatments of these data is shown in Figure 1.b. For C_0 no peak was observed in the $Q < 10$ nm^{-1} interval ($Q = 4\pi \sin\theta/\lambda$ – scattering vector, where λ is the neutron wavelength and θ is the scattering angle). In the case of the C_1 phase a single peak was recorded at $Q = 3.7$ nm^{-1}. The splitting of this peak was observed in phase C_2 at a slightly different position ($Q = 3.9$ nm^{-1}) and in addition the corresponding higher order reflexions appeared, too. In the higher index phases (C_3–C_6) other peaks can be detected and these modifications can be assumed to be crystalline.

Since no maximum was found in the C_0 phase pattern at $Q < 10$ nm^{-1}, its structure may be assumed to be nematic-type. The relatively sharp single peak at $Q_x = 3.7$ nm^{-1} in the C_1 phase is connected with structural units of 1.7 nm, meaning that the molecules are grouped in layers with 1.7 nm thickness and this phase can be classified as an orthogonal smectic-type modification. The splitting of the peak in the C_2 phase means that the layers of 1.56 nm thickness have a tilt angle relative to the ordering direction: $\alpha = 14°$ $[tg\alpha = (Q_{x1} - Q_{x0})/(Q_{y1} - Q_{y0})]$. Consequently, the C_2 phase has a tilt smectic-type structure.

The structure of the crystalline phases (C_3–C_6) was studied by

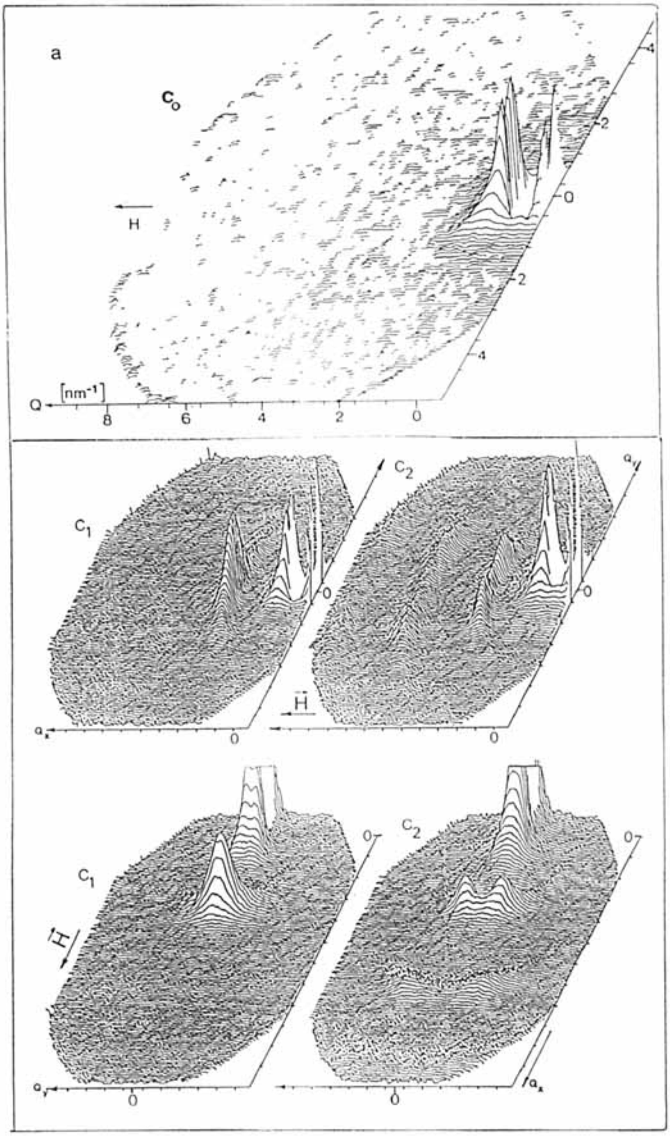

FIGURE 1.a Neutron small angle scattering intensities over the 128 × 128 cells area of the *XY*-detector for the MBBA D_{20} sample in the C_0 and C_1, C_2 phases (two different perspective views of these latter), measured at $\lambda = 0.312\ \mathrm{nm}^{-1}$ wavelength and T = 80K temperature.

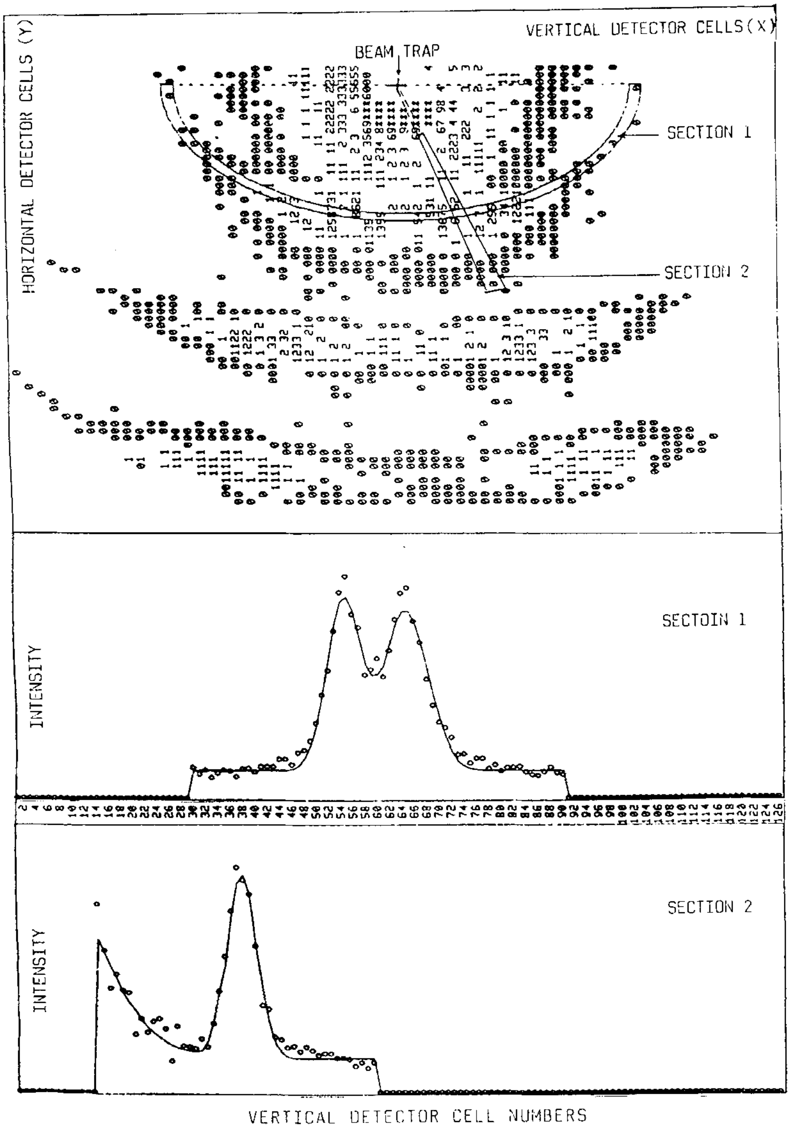

FIGURE 1.b Neutron intensity map of the small angle scattering over the *XY* detector for the C_2 phase (upper part). 20 isointensity levels are marked as: blank, 0, blank, 1, blank, 2. . . with increasing intensity values. Lower curves represent intensities in the sections perpendicular to the map-plane integrated in the areas marked by arrows as function of vertical detector numbers.

neutron diffraction in the $Q < 30\ \mathrm{nm}^{-1}$ momentum transfer range. Most of the results were obtained by time-of-flight diffraction method at the Dubna IBR-2 pulsed reactor.[14] Figure 2 gives an illustration of the measured diffraction patterns in each phase of MBBA and compares samples with different H and D contents (D_0—all hydro-

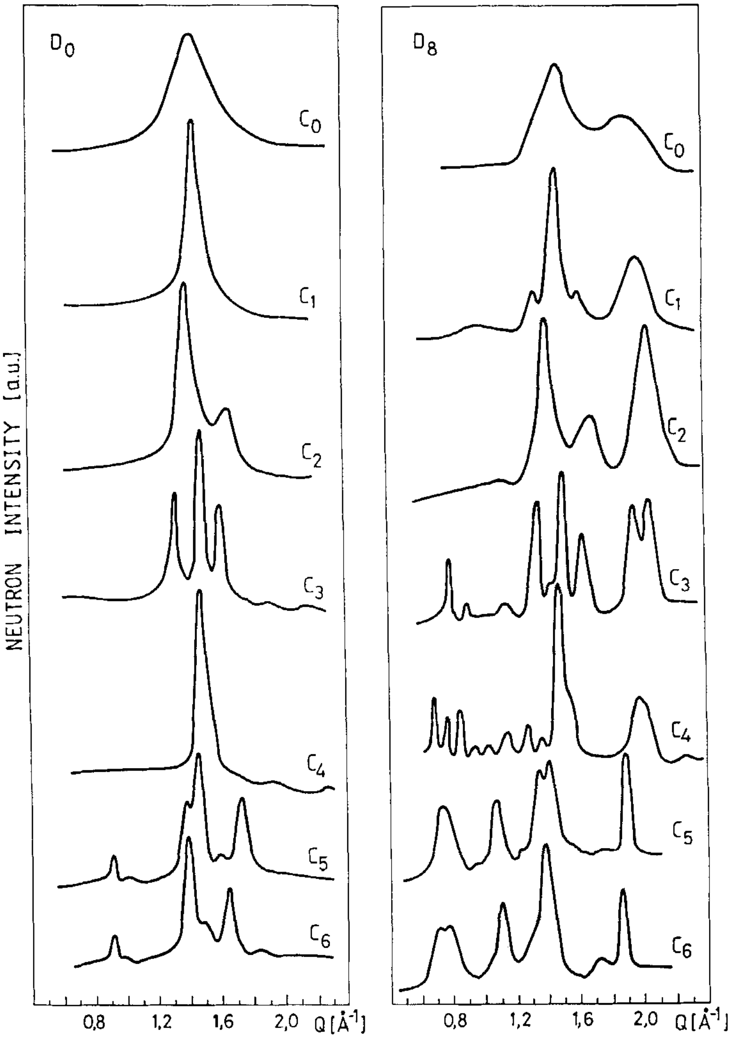

FIGURE 2 Diffraction patterns of different phases for the D_0 and D_8 MBBA samples ($H = 0$, $T = 80$K, $T = 260$K for C_6).

gen, D_8—benzene rings deuterated, D_{12}—end-groups deuterated, D_{20}—benzene rings and end-groups deuterated).

On the basis of these experimental results and model calculations for fitting to the experimental data[10] a rough scheme of molecular packing can be given for the crystalline phases. The most reliable description can be achieved for the D_{20} sample in the C_5 and C_6 phases where the greatest number of peaks could be identified, compared with the lower index phases or samples with lower D-content. As a result of this modelling the crystalline phases can be characterized by a monoclinic lattice with parameters near to the following values:

$$C_5 \ a \cong 0.77 \text{ nm}, \ b \cong 0.53 \text{ nm}, \ c \cong 3.48 \text{ nm}, \ \beta \cong 94.6^\circ$$

$$C_6 \ a = 0.78 \text{ nm}, \ b \cong 0.57 \text{ nm}, \ c \cong 3.35 \text{ nm} \ \beta \cong 94.2^\circ$$

Molecules form long chains with "head to head" arrangements and their long axes are parallel to each other. Two molecules can be considered in the elementary cell. Such a packing scheme is shown in Figure 3 (without H and D atoms). It is supposed that the monoclinic lattice is nearly conserved in each of the crystalline phases, however, the atomic positions could be varied considerably due to the twisting of the benzene rings and/or the reorientation of the end groups.

III. MEDIUM RANGE ORDER

The molecular packing given in the previous section—in spite of the roughness of the model—may well serve to characterize the short range order of the non-crystalline phases of MBBA, too. A more relevant description of the (nearly) amorphous structure of the C_0, C_1, C_2 phases should, however, include information on the medium range ordering.[11] Analysis of the small angle scattering of neutrons in the small Q range ($Q < 1 \text{ nm}^{-1}$) may give the answer to this problem.

The neutron scattering cross-section of nematic liquid crystals has been studied by Skripnik *et al.*[15] theoretically. The coherent elastic scattering can be described by exact formulae, however, simple expressions for comparison with experimental data can be derived

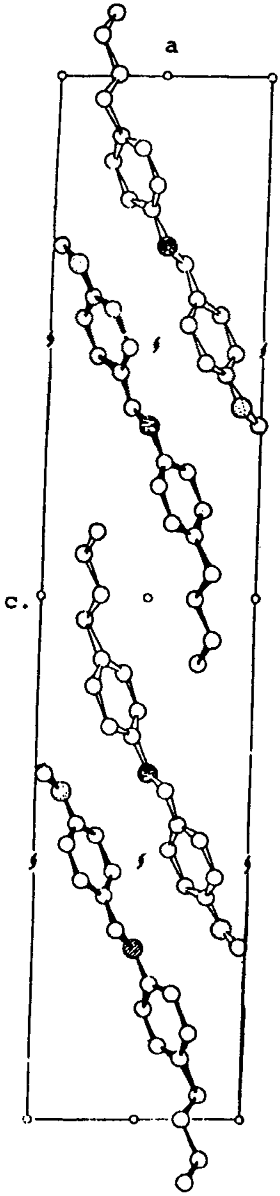

FIGURE 3 Molecular packing scheme in the ac plane of the monoclinic lattice of a crystalline phase of MBBA (without H-atoms).

only in the small and large scattering vector ranges. In order to describe the microstructure of the nematic state on the basis of such a comparison one has to know the structure of the individual molecules (taken, for example, from the crystalline phase packing) and certain macroscopic parameters: density, isothermic compressibility, pressure dependence of the order parameter, Frank-elastic constants.

The scattering cross-section can be presented as a series by even powers of Q if terms higher than Q^2 for the small Q range are neglected:

$$\frac{d\sigma}{d\Omega} = nVB_\nu^2 k_B T \left\{ \left(\frac{\partial n}{\partial p}\right) + Q^2 \left[-\left(\frac{\partial n}{\partial p}\right)_T \left(r_\parallel^2 \cos^2\phi + r_\perp^2 \sin^2\phi \right) - 2a^2 \left(\frac{\partial n S_{20}}{\partial p}\right)_T P_2(\cos\phi) + \frac{9n\, S_{20}^2 a^4 \sin^2\phi \cos^2\phi}{K_{33}\cos^2\phi + K_{11}\sin^2\phi} \right] \right\} \tag{1}$$

$$B_\nu = \sum_{\nu=1}^{N} b_\nu^c, \quad a^2 = \frac{\sqrt{20\pi}}{15B_\nu} \sum_{\nu=1}^{N} b_\nu^c u_\nu^2 Y_{20}(\mathbf{u}_\nu)$$

here n–density; V–scattering volume; ϕ–the angle of the nematic director $\mathbf{n}$ and the scattering vector $\mathbf{Q}$; k_B–Boltzmann's constant; T–temperature; P_L–orientational order parameter; S_{LM}–the coefficients of the order parameter; b_ν^c–the coherent atomic scattering amplitudes; N–the number of atoms; $\mathbf{u}$–radius-vector of an atom in the molecule, $r_\perp$ and $r_\parallel$–correlation lengths of the density domains perpendicular or parallel to the director; K_{ii}–elastic constants. For a simplified analysis of the scattering cross-section (since some macroscopic parameters are unknown in the case of the fast-cooled MBBA) expression (1) can be written in the form:

$$\frac{d\sigma}{d\Omega} = AT + Q^2 T \left[-B(r_\parallel^2 \cdot \cos^2\phi + r_\perp^2 \cdot \sin^2\phi) - CP_2(\cos\phi) + D\frac{\sin^2\phi \cdot \cos^2\phi}{K_{33}\cos^2\phi + K_{11}\sin^2\phi} \right] \tag{2}$$

where $P_2(\cos\phi)$—orientational order parameter, K_{11} and K_{33}—elastic constants, A,B,C,D—coefficients containing density, atomic scattering and other parameters.

The constant term is due to macroscopic fluctuations of density, the quadratic term includes angular dependent terms of different nature. Here the first part is connected with the dispersion of density fluctuations; the second one with the correlation between density fluctuations and the order parameter; while the third with the fluctuations of the director.

The situation is very similar in the case of a frozen-in nematic substance such as the C_0 phase in MBBA. The scattering mechanisms defined in (2) are more unambiguous in fast-cooled liquid crystal state then in the liquid crystal one. This is due to the freezing-in of some degrees of freedom and of fixing of density fluctuation and director fluctuation in a given state. In addition to this, the measurements are conducted at low temperature, smearing out effects are decreased. Measurements on *oriented* sample with anisotropic domains defined by their correlation lengths $r_\perp$ and $r_\parallel$ and the direction of molecules established by the order parameter and director fluctuations cause an anisotropic, direction dependent distribution of the small angle neutron scattering intensity.

The left hand patterns of Figure 4 show the intensity–momentum transfer dependence of the C_0 and C_1 phases. On the vertical axis those components of Q are plotted which are perpendicular to the director $Q_\perp = Q_y$; on the horizontal axis the $Q_\parallel = Q_x$ ($\mathbf{n} \parallel Q_x$) component, while the lines proceed on equal levels of intensity, i.e. they are iso-intensity contours. It can be established that the star-from picture indicates anisotropic scattering as predicted by theory. On the basis of these measurements data on the medium range order of the examined phases can be obtained if simple, logical postulations are used, even if several parameters (elastic constants, compressibility, etc.) remain unknown.

Figure 5 shows intensity-angular distribution curves representing different Q values (Q_x at $\phi = 0$, Q_y at $\phi = 90°$), as the scattering components given in the cross-section (2). In accordance with this, the intensity can be expressed as follows:

$$I(\phi) = 1 - Q^2(r_\parallel^2 \cos^2\phi + r_\perp^2 \sin^2\phi) - Q^2 S(\cos\phi) + Q^2 K \frac{\cos^2\phi \sin^2\phi}{K_1 \sin^2\phi + K_3 \cos^2\phi} \quad (3)$$

In this case $I(\phi)$, $S(\cos\phi)$, and K are intensity reduced constants and coefficients of terms containing order parameter fluctuations, and of

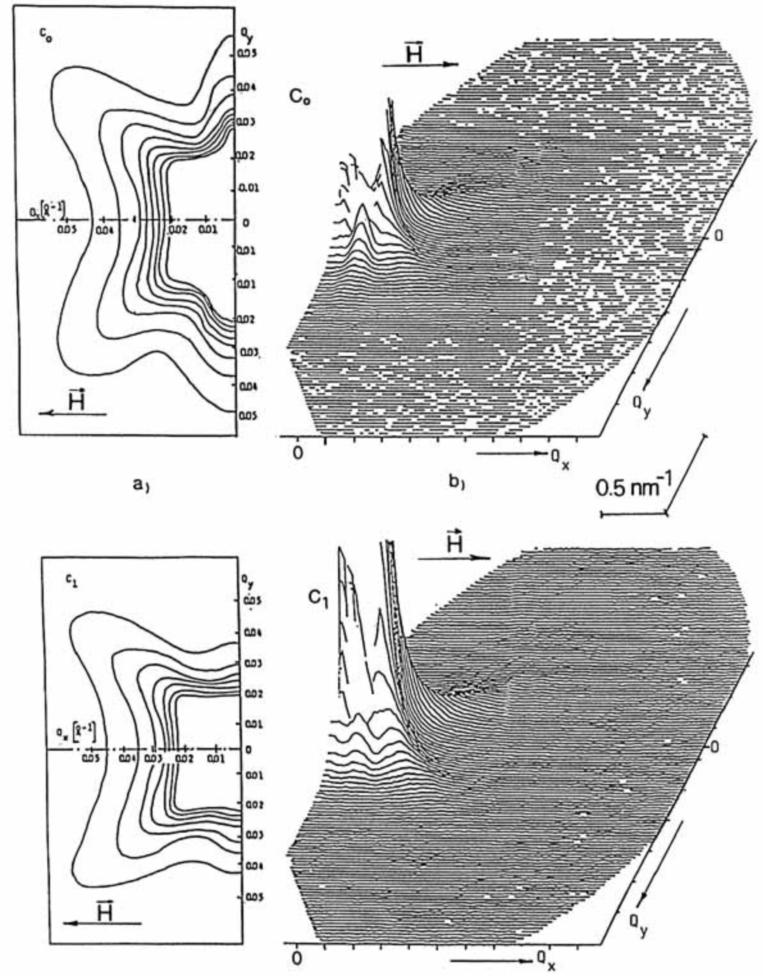

FIGURE 4 Neutron small angle scattering intensities at $\lambda = 1.5$ nm wavelength for the C_0 and C_1 phases of MBBA. Figures a) represent iso-intensity-lines, and pictures b) perspective views of the intensity distribution over the XY-detector.

the term connected with director fluctuations, respectively. In the direction parallel to the ordering direction ($\phi = 0$), the intensity value is

$$I(0) = 1 - Q^2[r_{\parallel}^2 + S(0)] \tag{4}$$

The empirical analysis of the components in (3) suggests that the third and fourth terms by the minimum of the intensity can be neglected

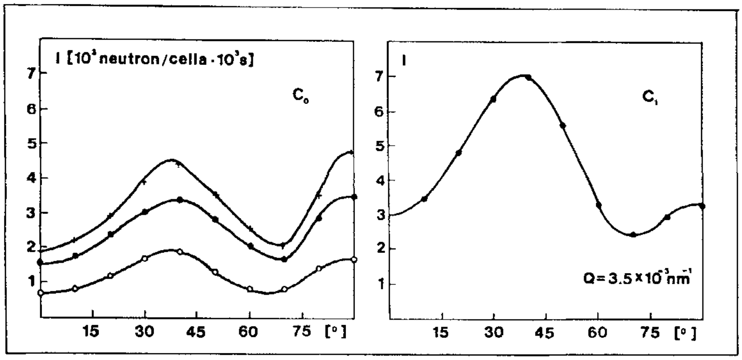

FIGURE 5 Intensity distribution of small angle scattering with respect to the angle of the orientation direction H, at different Q values. ●—Q = 3.5 nm^{-1}, + —Q = 3 nm^{-1}, ○—Q = 4 nm^{-1}.

since they are functions tending to 0 by increasing ϕ, so the intensity of the minimum position can be written as:

$$I(\phi_{\min}) = 1 - Q^2(r_{\parallel}^2 \cos^2\phi_{\min} + r_{\perp}^2 \sin^2\phi_{\min}) \tag{5}$$

The intensity measured in the direction perpendicular to the director ($\phi = 90°$) is:

$$I\left(\frac{\pi}{2}\right) = 1 - Q^2 r_{\perp}^2 - Q^2 S\left(\frac{\pi}{2}\right) \tag{6}$$

It can be obtained from the curves of Figure 5:

$$I(0) \simeq I(\phi_{\min}) \tag{7}$$

If we place the intensities measured at different Q values into (7) and solve the equation system (3–7), we obtain:

$$r_{\parallel} = \sqrt{\frac{I_1(\pi/2) - I_2(\pi/2)}{(Q_2^2 - Q_1^2)\cos^2\phi_{\min}} - r_{\perp} tg^2\, \phi_{\min}} \tag{8}$$

where I_1 ($\pi/2$) and I_2 ($\pi/2$) are the absolute intensities measured at Q_1 and Q_2 when $\phi = 90°$. These values can be read from Figure 4 for the C_0 phase, and $\phi_{\min} = 68°$ can also be obtained. It has been shown[8] that from Hoseman's model the width ΔQ = 2.39 nm^{-1} of the diffraction maximum at $Q = 14.7\ \text{nm}^{-1}$ determines the value of $r_\perp = 4.2$ nm. In this way we get from (8) $r_\| = 2.5$ nm.

Thus we can state that the density ranges, i.e. medium range correlation, can be characterized parallel or perpendicular to the direction of ordering by a 2.5 nm and 4.2 nm length, respectively. Diffraction measurements[8] show that there is an increase in phase C_1 – $r_\perp \simeq 12$ nm, and the system is ordered to a greater extent. This is supported by measuring the angular distribution of the main diffraction peak (rocking curve–relating to the mosaisity) which has a width of 38° in the phase C_0. When passing to phase C_1 this width reduces to ~10°.

All the same, only qualitative statements are possible on the basis of data of Figure 4. At $\phi = 0$ the S(0) term diminishes the general increase of intensity caused by macroscopic density fluctuations (due to the constant term in (2)); with greater ϕ angles, however, the increase of $r_\perp$ is dominant (in the case of C_1 $I(0) > I(\pi/2)$ while in C_0 the opposite was true). It thus seems logical to suppose that $r_\|$ did not change to any great extent compared with C_0, and so the medium range order of the C_1 modification can be characterized by the $r_\| \simeq 2.5$ nm correlational lengths.

IV. STRUCTURAL MODEL OF THE SOLID MESOPHASES

We can construct a model describing the structure of phases C_0, C_1 and C_2, i.e. the solid mesophases of MBBA, by summarizing the results of the neutron scattering experiments. The structure of phases C_0 freezed out from a nematic state has a nematic character; that is, the mass centers of the molecules have no long range order. The diffraction measurements made after fast cooling in a magnetic field,[7] show however, an orientational order whose director is parallel to the magnetic field. Analysis of the data of small angle scattering shows that the molecules are ordered into density domains. Such nematic clusters can be described by two correlational lengths; the one parallel to the direction of average ordering, $r_\|$, is approximately 2.5 nm; the one perpendicular to the direction of average ordering, $r_\perp$, approximately 4.2 nm. The short range order within the domains can be described by a molecular order similar to the structure of crystalline modifications[12,13] i.e. the crystal structure scheme shown in Figure 2 can be used, meaning that "head-to-foot" pairs of parallel molecules should be placed into a lattice in such a way that they form chains coupled with their indentical (either —CH_3 or —C_5H_9) end-groups—

as schematically shown in Figure 6. In determining of the packing matrix the following conditions have been also used:

> The average distance between molecules in the direction ||**n** is 0.428 nm—as determined from the diffraction peak position at $Q = 14.7$ nm^{-1} [7]—, i.e. ~10 molecules are in a row to determine the linear size of a domain as $r_\perp \simeq 4.2$ nm.
>
> The maximum in the angular distribution of the SAS intensity connected with the director (see Figure 5), i.e. with the molecular long axis (defined by the rigid core of the benzene rings), within a domain leading to a tilt angle of $\phi = 38°$ as measured rel. the magnetic-field direction used for orienting the sample (see Figure 5).

In this way the nematic-type structure of the C_0 phase is described by a short range order which is determined by a lattice containing on average, one row of 10 molecules, and extending for the neighboring rows as shown in Figure 6a. Inside the lattice, molecular cores are relatively randomly distributed due to the more or less free positions of endgroups, so that the centers of mass of molecules are not correlated (as known for nematics). The macrostructure is formed by these density domains (with characteristic average $r_\perp$ and $r_\parallel$) with slightly fluctuating local directors ensuring a continuous transition between the lattice fragments of the short range order.

V. SMECTIC-TYPE PHASES OF SOLID MBBA

The C_1 phase has been ascertained (see section 2) as belonging to the orthogonal type of smectic structures.

In the classical sense of the word this means that the molecules of the liquid crystals are ordered in planes and within these planes molecular orientation and even the long axis of the molecules form a right angle to the layers. In the case of modification C_1 we were able to define the layer structure by considering the short range packing. From the small angle scattering data the medium range order parameters can be determined as $r_\parallel \simeq 2.5$ nm and $r_\perp \simeq 12.0$ nm. The benzene rings have a tilt angle of about 38°, similarly to phase C_0. The short range order within the domain is similar to that of phase C_0. The peak appearing in the scattering (indicating a layer distance of 1.7 nm) is due to interference of scattered waves on the identically positioned scattering centres of the neighbour molecules as from the orthogonal layer structure. (Figure 6b shows this schematically.) In

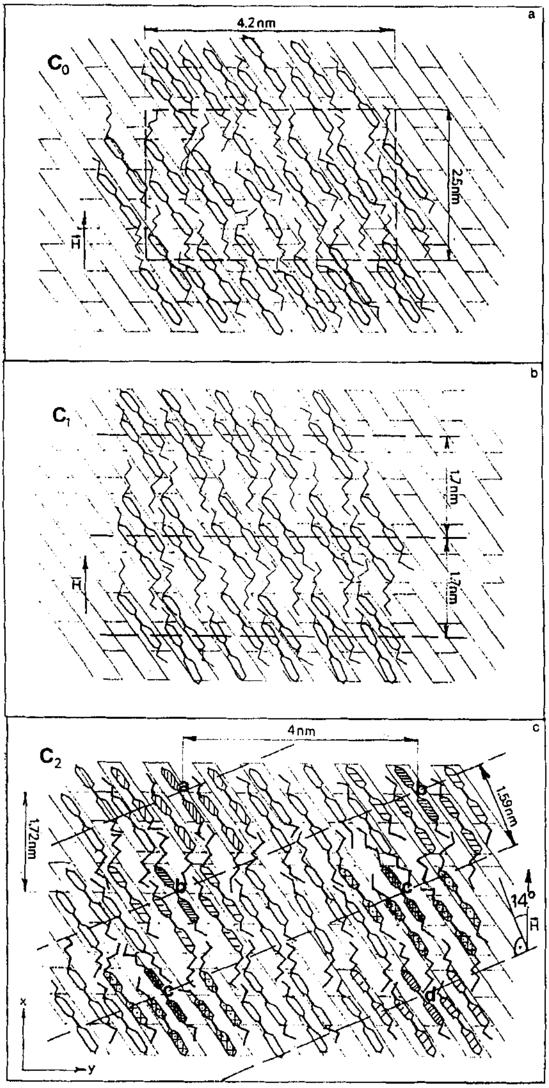

FIGURE 6 Molecular packing scheme of the solid mesophases of MBBA indicating the size of the medium range ordering (for C_0) and the smectic layers (C_1, C_2). The matrix to insert the molecules is taken from the crystalline phase packing (ac plane) as in Figure 3.

these smectic layers not a single row of molecules but head-to-foot pairs of molecules determine the layer distance. There is no long range order within the layers and similarly to phase C_0 mainly due to the relatively free motion of end-chains and the great number of "lattice defects."

From the small angle diffraction diagram of phase C_2 a tilt smectic structure can be determined, i.e. the layers are tilted as compared to the director (direction of macroscopic order), but if we also consider molecular packing we cannot connect the smectic layers to tilt monomolecular layers since the molecules are—in addition—tilted compared to these layers. Figure 6c shows the possible molecular order determining the structure of phase C_2. Because of the density of packing there is no possibility of drastic changes of order during $C_0 \rightarrow C_1 \rightarrow C_2$ transitions. Therefore in phase C_2 the same matrix can be supposed which was used for the crystalline structure and which determines short range order. The position of the molecules may be indicated within this by determining *a*,*b*,*c*,*d*, etc. "lattice points." The distance of these points along axis *x* is equal to the size of a pair of molecules, i.e. 1.7 nm, and along axis *y* it is 10 molecular units, i.e. 4.0 nm. If we suppose that because of the lack of microscopic order the position of points *a*,*b*,*c*,*d* is not identical—and so there is no interference between the scattered by them neutron waves but the *a*-*a*-. . . ,*b*-*b*-. . . ,*c*-*c*-. . . etc. molecular environments have identical positions leading to interference—we are able to lay planes through them; in this way as concluded from the measurements, the thickness of the layers is $d \sim 1.59$ nm and the tilt angle $\alpha = 14°$. Further, it is to be considered when defining molecular packing that in neutron diffraction measurements (e.g. Figure 2) in the greater Q range there are peaks indicating distances of 0.433 nm and 0.397 nm, etc. This means that there is an order within the layers. Figure 6c shows the section in the "ac plane" of the lattice and a fishbone structure can be realized in the third dimension, i.e. perpendicular to the plane of the figure. If we also consider as further information the reflexions of higher order measured in small angle diffraction we can stipulate that the correlation between layers is of relatively long range (this is not true for phase C_1). Thus we can state that modification C_2 tends towards being perfectly ordered, almost crystalline; and, from the point of view of diffraction, a structure which, is reminiscent a highly ordered smectic phase.

VI. CONCLUSION

Neutron scattering experiments (diffraction and small angle scattering have provided information on the structure of the solid phases of MBBA, namely on the molecular arrangement of the oriented non-crystalline solid modifications C_0, C_1 and C_2. They can be described by means of modelling the molecular packing on short and medium range distances. It has been established that phase C_0 is a nematic; phase C_1 is smectic-type structure with orthogonal layers, and phase C_2 is a highly ordered tilt smectic structure. One has to note, however, that in each phase molecules are tilted by an angle ϕ relative to the orientation direction, inside the medium range structural units. It means that the local value of the director, $\mathbf{n}_l$ in a domain ($\mathbf{n}_l$-parallel to the long molecular axis) closes an angle ϕ with the macroscopic director $\mathbf{n} \parallel \mathbf{H}$, the orienting magnetic field (ϕ certainly may have a relatively large spread). This tilting of the molecules in these domains is due to the simultaneous effects of the orientation by the external magnetic field and the short range molecular interaction.

As a conclusion of the results demonstrated on the fast-cooled MBBA one has to consider the molecular arrangement on two levels: at short and at medium range distances, when describing the structure of liquid crystals, especially smectics. Furthermore the procedure followed in this paper can be applied to modelling the structure of any liquid crystal which can be quenched to form a glassy phase, playing the role of the intermediate between the crystal and the LC state. In this way the structure of a liquid crystal can be described as follows:

i. The local arrangement of molecules is nearly that of the crystalline phases.

ii. From this packing one can construct the short range order lattice of the GLC state.

iii. From diffraction and small angle scattering data the parameters of this short range order lattice should be determined (tilt angle, cell dimensions) and the dimensions of medium range order structural units ($r_\perp$, $r_\parallel$ and the thickness d of smectic layers) should also be derived.

To sum up: the use of the neutron scattering method (X-ray scattering can be applied in an analogous way) has been demonstrated for describing the molecular packing of liquid crystals, in particular smectics, by analysing of the structure of the fast-cooled phase as being an intermediate state between the crystal and liquid crystal structure.

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