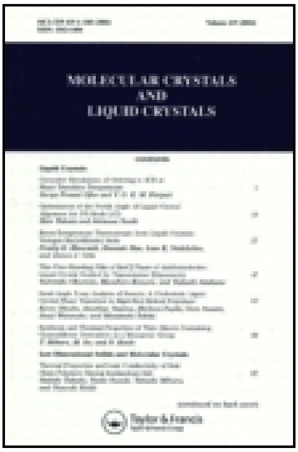

Molecular Crystals and Liquid Crystals Science and Technology. Section A. Molecular Crystals and Liquid Crystals
Publication details, including instructions for authors and subscription information:
http://www.tandfonline.com/loi/gmcl19

Modelling Nematic Liquid Crystal Alignment on Asymmetric Surface Grating Structures

Carl V. Brown [a], Guy P. Bryan-brown [a] & Victor C. Hui [a]
[a] Liquid Crystal Group, DRA Malvern, Great Malvern, Worcs, WR14 3PS, UK

Version of record first published: 04 Oct 2006

Mol. Cryst. Liq. Cryst., 1997, Vol. 301, pp. 163–168
Reprints available directly from the publisher
Photocopying permitted by license only

MODELLING NEMATIC LIQUID CRYSTAL ALIGNMENT ON ASYMMETRIC SURFACE GRATING STRUCTURES

CARL V. BROWN, GUY P. BRYAN-BROWN AND VICTOR C. HUI
Liquid Crystal Group, DRA Malvern, Great Malvern, Worcs WR14 3PS, UK.

Abstract Static nematic liquid crystal director configurations have been calculated numerically for alignment over an asymmetric grooved surface profile. The results demonstrate the existence of a low pretilt regime, where the director field follows the contours of the grating, and a high pretilt regime, where the director field shows a characteristic defect structure. The relative energies of the distorted director field have been calculated for the two regimes. The profile of a real surface has been implemented in the model and the predicted values of the pretilt are commensurate with those measured experimentally.

INTRODUCTION

The production of pretilted alignment is very important for practical nematic liquid crystal devices. Using traditional methods it is difficult to combine controllable high pretilts with good uniformity. With the use of grooved surface profiles the basic mechanism of alignment over the grooves is a result of the surface topology. This has been described previously for a symmetrical sinusoidal surface profile using the formalism of macroscopic continuum theory[1]. Results are presented here from a numerical model showing how the production of pretilted alignment states depends solely on the shape and physical parameters of an asymmetric grooved surface.

THEORY

The elastic deformation energy[2,3] in a nematic liquid crystal is given by :

$$2W = K_{11}(\nabla\cdot\mathbf{n})^2 + K_{22}(\mathbf{n}\cdot\nabla\wedge\mathbf{n})^2 + K_{33}(\mathbf{n}\wedge\nabla\wedge\mathbf{n})^2 \tag{1}$$

Where the elastic constants K_{11}, K_{22} and K_{33} correspond to splay, twist and bend deformations respectively, and the director **n** is a unit vector describing the averaged local orientation of the liquid crystal molecules. The director is assumed to vary in 2 dimensions with the orientation throughout the system described by the zenithal angle θ, so that $\mathbf{n} = (\cos\theta, \sin\theta, 0)$ and the term in K_{22} disappears.

The static configuration of **n** is found by minimisation of equation (1) :

$$\left(\frac{\partial W}{\partial \theta}\right) - \nabla \cdot \left(\frac{\partial W}{\partial \nabla \theta}\right) = 0 \tag{2}$$

Equation (2) is approximated by finite differences and solved iteratively on a rectangular mesh by a relaxation method.

MODEL GEOMETRIES

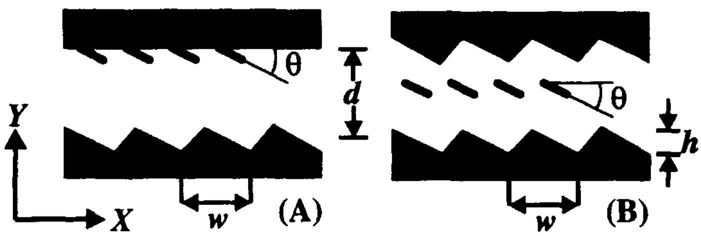

FIGURE 1 The model geometries considered

The geometry of the model used is shown in figure (1a). The grating surface can be conveniently parameterised by :

$$y(x) = \frac{h}{2}\sin\left(\frac{2\pi x}{w} + A\sin\left(\frac{2\pi x}{w}\right)\right) \tag{3}$$

where h and w are the grating amplitude and period respectively and A expresses the degree of asymmetry : $A = 0$ gives a sinusoidal profile ; $0 < A < 0.5$ gives a blazed profile.

At the grooved surface the orientation of the director was fixed at the gradient of the surface. At the upper boundary the angle θ is fixed. The torque balance equation (2) is solved with periodic boundary conditions at $x = 0$ and $x = Nw$ where N is an integer. The total elastic energy is then calculated from the resulting director configuration. The value of θ which gives the minimum elastic energy is then defined as the pretilt angle θ_p.

RESULTS FROM THE MODEL

Two distinct alignment regimes are found to occur depending on the value of the tilt angle fixed at the upper boundary. These are shown in figure (2) where a blazed surface grating defined by equation (3) with $A = 0.5$ and $h/w = 0.6$ was used. For $\theta \leq 30°$ the typical resulting director configuration is shown in figure (2a). Here the orientation of the liquid crystal follows the contours of the surface close to the lower boundary and this elastic distortion decays smoothly through the bulk of the cell to the uniform value at the upper surface. This is a near-planar alignment regime since the minimum energy configuration gives a low or zero pretilt.

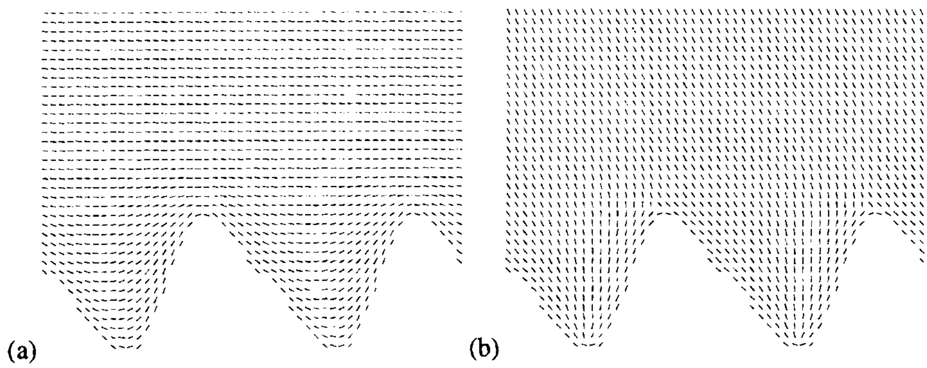

FIGURE 2 Different alignment regimes on a blazed surface grating

For $\theta \geq 50°$ the resulting director configuration is as shown in figure (2b). This is an alignment regime that gives rise to a high pretilt and is characterised by structures that resemble nematic defects[3] in the regions around the peaks and troughs in the grating surface. At the peak in the surface profile the orientation of the director field resembles a nematic -½ defect and at the trough in the surface the structure resembles a +½ defect. The exact position where the defect structures occur is very sensitive to the shape of the surface grating. They occur regardless of the resolution of the mesh and so they are not simply an artefact of the discrete nature of the model. Similar low and high pretilted alignment regimes were suggested by Guyon and co-workers[4] in 1973 to explain the observed bulk orientations of thin layers of nematic liquid crystals on obliquely evaporated silicon oxide films.

Using a surface profile generated by equation (3) with $A = 0.5$ the total elastic energy of the model system has been calculated for h/w varying from 0 to 1. The results are shown in figure (3). The energy for the low pretilt regime rises monotonically from zero as the value of h/w increases. This is expected since in this alignment regime the liquid crystal director follows the contours of the surface profile which costs an increasing amount of elastic strain energy as the amplitude of the grating increases.

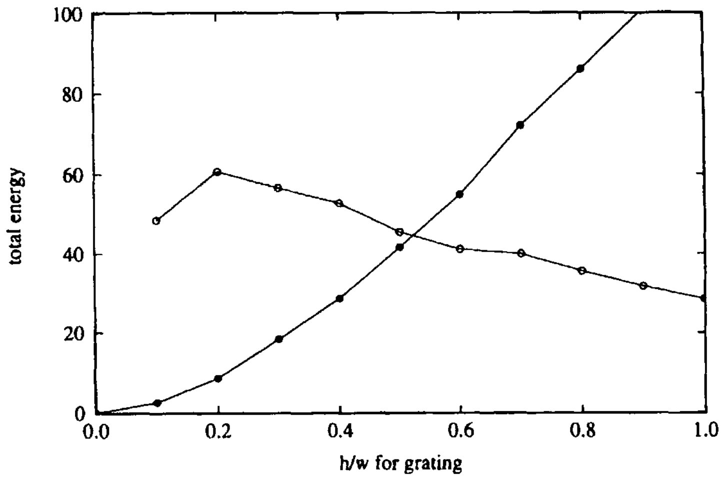

FIGURE 3 Prediction of the relative stability of the low pretilt (filled circles) and high pretilt (open circles) alignment states

The energy for the high pretilt regime rises until $h/w = 0.2$ and then falls monotonically as the value of h/w increases. The fall in energy occurs because the alignment in this regime is closer to homeotropic and so the liquid crystal director tends to 'stand up' in the grating grooves. This obviously costs less energy when the amplitude is increased and the grooves are deeper.

There is a cross over point for the two curves where it is predicted that both alignment regimes would be equally energetically favourable. It should be noted, however, that for the high pretilt configuration the presence of nematic defects would give an additional contribution to the energy. This arises due to the core energy of a defect which is an order parameter effect and can not be taken account of in a continuum description. This extra energy would appear as an offset for the high pretilt state in figure (3) which should be roughly constant as a function of h/w[5].

COMPARISON WITH EXPERIMENTAL RESULTS

For the geometry considered so far the liquid crystal director is forced to lie along the direction of the tangent to the surface across the grating grooves. This corresponds to locally planar alignment at the grating surface. In reality it is more energetically favourable for the director to twist round and lie in the plane along the grooves. The director can be forced to lie across the grooves with another set of grooves forming a bigrating structure. In this geometry the current 2 dimensional model is no longer valid.

With a homeotropic surfactant treatment the orientation of the director at the grating surface is perpendicular to the local gradient of the blazed profile. The elastic distortion then occurs in the plane normal to the grating rather than along the grating grooves. Using the geometry depicted in figure (1b) it is then possible to make a direct comparison between the model and an experimentally realisable geometry.

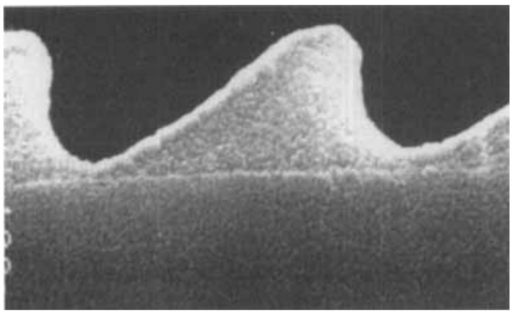

FIGURE 4 A scanning electron microscope image of an experimental blazed grating surface

In figure (4) an S.E.M. image is shown of an experimental surface grating structure. This is highly blazed profile with a near vertical slope on the right hand facet. A cell was assembled with this grating structure on both the upper and lower bounding plates. The surfaces had been treated with a homeotropic surfactant and the cell was filled with the nematic material E7. Upon cooling from the isotropic phase into the nematic two distinct light and dark alignment domains were visible between crossed polarisers. Measurements of the pretilt using a sample rotation method showed that the dark state corresponded to near homeotropic alignment where the liquid crystal director was at an angle close to 90°. The light state was tilted homeotropic alignment where the liquid crystal director is tilted at 60° relative to the plane of the surface.

In figure (5) two calculated director configurations are shown where the experimental surface from figure (4) was used directly in the model. The director profiles were calculated using the geometry shown in figure (5). In these calculations extra positions on the solution grid were added at the grating surface in order to reproduce the shape of the surface as closely as possible. The profile in figure (5a) gave a value of 92.2° for the pretilt in the centre of the cell and the pretilt for the director profile in (5b) was 64.7°. This is in good agreement with the experimental results.

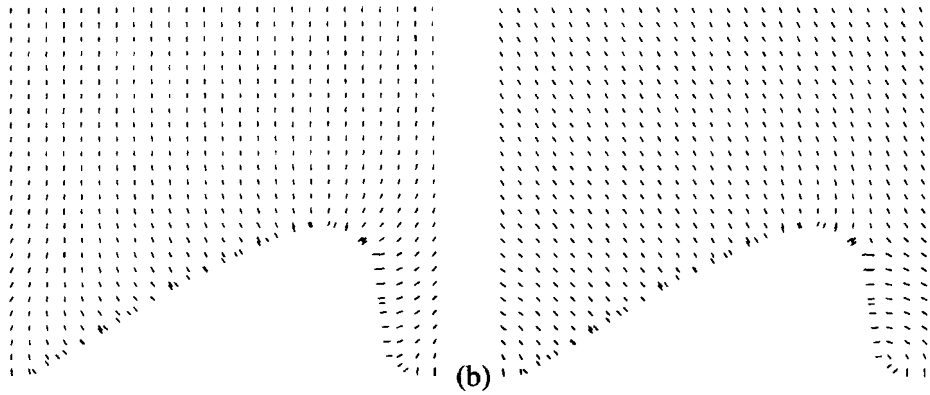
(a) (b)

FIGURE 5 Calculated director configurations for homeotropic alignment on the grating profile shown in figure (4)

CONCLUSIONS

Continuum modelling has allowed a quantitative understanding of the links between the surface properties and the pretilted alignment of nematic liquid crystals over asymmetric grooved surface profiles.

ACKNOWLEDGEMENTS

We gratefully acknowledge Dr. M.J. Towler, Prof. F.M. Leslie and Prof. J.R. Sambles for stimulating discussions and Prof. D.G. McDonnell for initiating the work.

REFERENCES

[1] D.W. Berreman, Phys. Rev. Lett, 28, 1683 (1972)
[2] C.W. Oseen, Trans. Faraday. Soc, 29, 883 (1933). H. Zöcher, Trans. Faraday. Soc, 29, 945 (1933).
[3] F.C. Frank, Disc. Faraday. Soc, 25, 19 (1958).
[4] E. Guyon, P. Pieranski and M. Boix, Lett. in Appl. and Eng. Sci, 1, 19 (1973)
[5] V.C. Hui, in preparation for publication.