Alignment of liquid crystals using submicrometer periodicity gratings[a)]

D. C. Flanders,[b)] D. C. Shaver,[b)] and Henry I. Smith[b)]

Lincoln Laboratory, Massachusetts Institute of Technology, Lexington, Massachusetts 02173

(Received 3 January 1978; accepted for publication 6 March 1978)

Square-wave gratings of 320-nm spatial period fabricated on amorphous SiO_2 substrates were used to produce uniform alignment of the director in nematic and smectic liquid-crystal layers. This demonstrates that molecular alignment can be achieved using surface structures fabricated by a planar process. A novel method of producing twisted-nematic liquid-crystal displays using surface gratings is described.

PACS numbers: 61.30.Gd, 42.80.Fn, 68.55.+b, 85.60.Me

Several researchers have demonstrated that surfaces which have been made anisotropic by rubbing with abrasives,[1] by directed oblique evaporation of silicon monoxide,[2] or by dipping in surfactants[3] will align nematic liquid crystals. It is believed that such alignment minimizes the free energy associated with elastic deformation of the liquid crystal. In particular, if the long axes of the liquid-crystal molecules are constrained to lie in, or at a small tilt angle to, the plane of a smooth surface, then one expects a grating structure on that same surface to induce alignment of the nematic director along the groove direction. Berreman[4,5] has proposed a detailed model which supports this idea.

Oblique evaporation and rubbing techniques produce surfaces with a topography that is largely uncontrolled and thus difficult to reproduce or quantify exactly. We demonstrate here that liquid crystals can be aligned on gratings whose topography is directly controlled. It is significant that the spatial period of the gratings used was 320 nm, which is much larger than the size of the molecules (≈2 nm) being aligned. We expect the forces which favor alignment to increase with gratings of higher spatial frequency.

The gratings for the following experiments were fabricated in SiO_2 by reactive ion etching in CHF_3 gas using a mask of 100-Å-thick chromium. The chromium grating was produced by a liftoff process from a grating pattern exposed in PMMA using Cu_L soft x-ray lithography.[6] Holographic lithography was used as the pattern generation step in producing the x-ray mask. The etch depth of our SiO_2 gratings was about 25 nm. Recent measurements in a transmission electron microscope on gratings fabricated by this process indicate that the sidewalls are within 6° of the vertical, and that the radius of curvature at the top and bottom corners of the sidewalls is less than 5 nm. Gratings were fabricated over a 1.25×1.25-cm area on two highly polished fused quartz substrates.[7] The two substrates were assembled into a sandwich with 50-μm-thick Teflon spacers holding them apart. The gratings were on the inside of the sandwich and faced each other with their groove directions parallel. A high degree of parallelism is easily obtained by first roughly aligning the gratings so that a beam of light incident on them is simultaneously diffracted from both gratings towards an observer; then, fine adjustments in the alignement can be made while observing moiré interference fringe patterns in the overlapping diffracted beams.

After alignment of the gratings, the sandwich was heated above the nematic-isotropic transition temperature of MBBA (*N*-(*p*-methoxybenzilidene)-*p*-butylaniline) and the liquid crystal was introduced into the sandwich by capillary action. The sandwich was allowed to cool to room temperature where MBBA is nematic and was observed in transmission in a microscope between crossed polarizers. The incident polarized light was normal to the thin liquid-crystal layer, and the entire sandwich could be rotated in the plane of the layer.

An aligned liquid crystal behaves as an optically uniaxial medium with its optic axis in the direction of the nematic director. When a linearly polarized beam of light is normally incident on a uniaxial slab of arbitrary thickness, it will remain linearly polarized after passing through the medium only if the polarization is perpendicular to the optic axis or parallel to the projection of the optic axis on the slab. In the area between the two gratings, distinct peaks and nulls in the light transmission were observed as the sandwich was rotated, the nulls occurring every 90°. Furthermore, the entire liquid-crystal layer in the grating area had a uniform brightness, with nulls in the light transmission occurring simultaneously across the entire field of view. Our interpretation is that the nematic director is not perpendicular to the substrates and that it is uniformly oriented in the grating area. The liquid-crystal layer had a distinctly different appearance in the region outside the grating area where it was confined between two smooth surfaces. It did not appear uniform, and many small domains were visible, indicating that the direction of the nematic director varies randomly in this region. The light transmission in the grating area went through a null when the incident polarization was along the groove direction, to within the experimental error of our apparatus (~0.5°). This indicates that the projection of the nematic director was aligned along the groove direction or perpendicular to it. In order to distinguish these two possibilities, we doped the MBBA with the dye DODCI (3, 3′ diethyloxadi-

---

[a)] Work sponsored by the Defense Advanced Research Projects Agency.

[b)] Also, Department of Electrical Engineering and Computer Science, Massachusetts Institute of Technology, Cambridge, Mass. 02139.

carbocyanine iodide), which aligns with the nematic director and absorbs most strongly light that is polarized in the direction of alignment. In this way, we established that the nematic director projection was along the groove direction.

The angle between the nematic director and the plane of the substrate was estimated by measuring the difference between the refractive index for the ordinary wave and the extraordinary wave with light normally incident on the substrate. The extraordinary index varies with the angle between the incident ray and the optic axis. To make the measurement, one of the Teflon spacers was removed, thereby introducing a known tilt between the two quartz substrates. When viewed at normal incidence in monochromatic light (589 nm) between crossed polarizers, distinct dark and light bands were visible due to the linear variation in thickness of the birefringent medium. The dark bands occur when the relative phase shift between ordinary and extraordinary waves is an integral number of cycles. Knowing the tilt between the two substrates, the difference in index of refraction can be calculated from the spacing of the bands.[8] We measured an index difference of 0.18 ± 10%. This corresponds to a nominal tilt of 23° between the nematic director and the substrate plane; this was the same inside and outside the grating area. For the tilt calculation we used the value of 0.225 (± 0.006) for the birefringence of MBBA at 25 °C, which is correct if the nematic-isotropic transition temperature is 41–45 °C.[8] The transition temperature is sensitive to the purity of the liquid crystal and typically drops slowly when MBBA is first exposed to air, with a corresponding decrease in the birefringence. Though we did not measure it, the transition temperature is usually in the range 41–45 °C. Furthermore, conoscopic examination of our sample confirmed that the nematic director was tilted at least 20° from the substrate plane.

Surface contamination can make the nematic director approach the substrate normal and thus degrade the orienting influence of the grating. Freshly made substrates, and those cleaned in uv-generated ozone[9] or concentrated H_2SO_4, exhibited good alignment, low tilt angle, and consistent results. Both highly polished fused quartz and SiO_2 prepared by thermal oxidation of silicon wafers showed similar results.

We also aligned the liquid-crystal M24 (BDH Chemicals Ltd., 4-cyano-4′-octoxybiphenyl), which has a smectic *A* as well as a nematic phase. We found that M24 in the nematic phase aligned uniformly along the groove direction in the grating area, but it exhibited a slowly varying nematic director outside the grating area where it was not constrained. The effect of the grating was striking when the liquid crystal was cooled to the smectic phase. The liquid crystal in the grating area appeared as a uniform uniaxial slab with the projection of its optic axis parallel to the groove direction; outside the grating area a multitude of striations and fan-shaped defects appeared. No striations were visible in the area confined between two gratings.

Based on the above results, we have constructed a novel type of twisted nematic display using grating technology. Gratings of 100-nm-thick gold lines and 320-nm period were fabricated on a 225-μm-thick Corning 0211 glass substrate using holographic lithography and ion-beam etching. The gold grating lines were interconnected by a continuous gold film which surrounded the grating area. Two of these 0211 glass pieces were assembled into a sandwich using Teflon spacers to maintain a gap between them. The gratings, which were inside the sandwich, were oriented with their groove directions perpendicular to each other. Electrical contact was made to each gold surface. All the elements of a twisted nematic display are present in this structure: (i) the gratings provide two liquid-crystal-aligning surfaces at right angles to one another, (ii) the gratings polarize light and act as crossed polarizers, and (iii) the gratings are highly conductive at dc and form effective conducting parallel plates to align the liquid crystal by means of an electric field. The contrast ratio of the polarizer limits the performance of the display. Contrast ratios of 10 : 1 have been obtained using He-Ne laser light (632.8 nm). Improvements should be obtained with gratings of finer spatial period.

In conclusion, we have demonstrated that square-wave-grating surface-relief structures can be used to align nematic and smectic liquid crystals. Since these structures are well controlled and characterized, they permit quantitative models for alignment of liquid crystals by surfaces to be tested. Finally, surface structures may find wide application in other systems where anisotropic surface interactions are present.

We would like to thank R. Pindak and R. B. Meyer of the Gordon MacKay Laboratories, Harvard University, for their assistance in our early experiments with MBBA. We also wish to thank R. Schaetzing of MIT for his assistance in our experiments with M24.

[1] L. T. Creagh and A. R. Kmetz, Mol. Cryst. Liq. Cryst. **24**, 59 (1973).
[2] J. L. Janning, Appl. Phys. Lett. **21**, 173 (1972).
[3] J. E. Proust, L. Ter-Minassian-Saraga, and E. Guyon, Solid State Commun. **11**, 1227 (1972).
[4] D. W. Berreman, Phys. Rev. Lett. **28**, 1683 (1972).
[5] D. W. Berreman, Mol. Cryst. Liq. Cryst. **23**, 215 (1974).
[6] D. C. Flanders, Henry I. Smith, H. W. Lehmann, R. Widmer, and D. C. Shaver, Appl. Phys. Lett. **32**, 112 (1978).
[7] Optosil 2, Amersil Inc.
[8] Ivan Haller, H. A. Huggins, and M. J. Freiser, Mol. Cryst. Liq. Cryst. **16**, 53 (1972).
[9] J. R. Vig. IEEE Trans. Parts Hybrids Packag. **PHP-12**, 365 (1976).