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Structure of the hidden interfaces in liquid crystal electro-optical cell studied by X-ray scattering and atomic force microscopy

Y. O. Volkov[+*1)], *B. S. Roshchin*[+], *A. D. Nuzhdin*[+], *A. A. Zhukovich-Gordeeva*[×], *E. P. Pozhidaev*[×], *R. V. Gainutdinov*[+], *V. E. Asadchikov*[+], *B. I. Ostrovskii*[+*]

[+]*National Research Center "Kurchatov Institute", 119333 Moscow, Russia*

[*]*Y. A. Osipyan Institute of Solid State Physics, Russian Academy Sciences, 142432 Chernogolovka, Russia*

[×]*P. N. Lebedev Physical Institute, Russian Academy Sciences, 119991 Moscow, Russia*

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The structure of interfacial boundaries in a liquid crystal (LC) cell, composed of sequential layers of a thin-film electrode, an alignment polymer coating, and a ferroelectric LC, was investigated using X-ray scattering and atomic force microscopy. Quantitative parameters describing the structure of transition layers were obtained, along with statistical data on interface roughness and dielectric constant distribution across the film. These data are expected to provide a link between the roughness and anchoring properties of LC materials at interfaces and give an assessment of the structural modifications occurring at each stage of the electro-optical cell assembly.

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Liquid crystals (LCs) play a significant role in display technologies, photonics, sensors, communication systems, and data processing applications [1, 2]. To date, most industrial applications have relied on nematic LCs in combination with an active matrix, which is sufficient to maintain the required frame refresh rates of approximately 60–80 Hz. However, certain advanced applications, including high-speed optical modulators, field sequential color displays, and three-dimensional television, require response times that are several orders of magnitude shorter. A promising approach to achieving such high-speed electro-optical switching involves ferroelectric LC (FLC) materials [3–5].

Here we report on the structure of transition layers in an electro-optical LC cell composed of a transparent indium tin oxide (ITO) electrode deposited on an optical glass substrate, an aligning polymer coating (PMDA-ODA), and a ferroelectric liquid crystal (FLC-497). Previous studies have indicated that the anisotropy of surface energy, determining the domain structure and contrast ratio of the ferroelectric LC cell, is closely related to the roughness of successive interfaces within the cell [6, 7]. To investigate the internal layer structure of the LC cell, we applied X-ray scattering (XRS) in the grazing incidence geometry [8, 9] complemented by atomic force microscopy (AFM) studies of the surface morphology of the sequential layers. To the best of our knowledge, such an in-depth characterization and analysis of the sequential interface evolution in a LC cell have not yet been reported in the relevant literature.

The X-ray experiments were performed using a laboratory multipurpose X-ray diffractometer equipped with a movable source-detector system [10]. Diffuse scattering distributions (Fig. 1) were obtained in a so-called detector scan setup, where the incident X-ray beam was set at a fixed grazing angle $\alpha = \alpha_0$ relative to the sample surface [11]. The AFM measurements were performed on the surfaces of samples with deposited ITO and PMDA-ODA layers using NTEGRA Prima scanning probe microscope (NT-MDT Spectrum Instruments, Zelenograd).

The analysis on specular reflectivity from the sequential layers of the LC cell was reported by us earlier [12]. The analysis on grazing-incidence diffuse scattering data from a structure with $N > 1$ interfaces was performed in the framework of the first-order perturbation theory, using a formalism developed in the papers [13, 14]. This approach evaluates the statistical characteristics of roughness represented by the one-dimensional power spectral density function $\mathrm{PSD}_j(\nu)$ for the j-th interface. It determines the spatial autocorrelations of the stochastic surface heights profile, $\zeta(u = x, y)$, across the illuminated area S of the interface plane. Other important parameters used in the

[1)]e-mail: volkov.y@crys.ras.ru

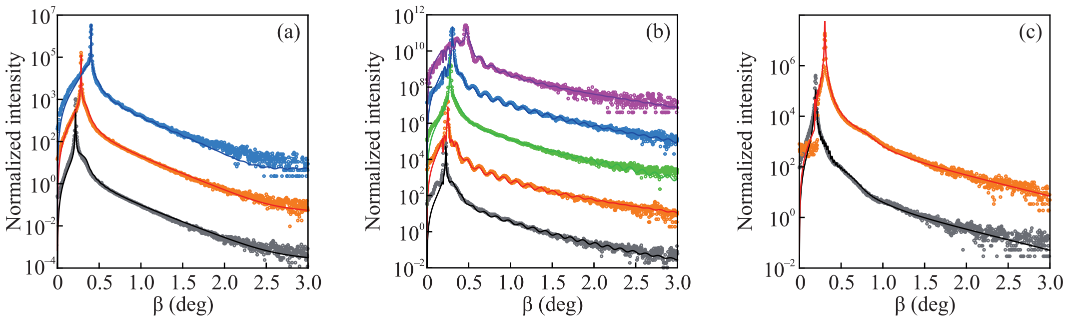

Fig. 1. (Color online) Normalized scattering intensity (symbols) versus scattering angle, measured under different incident angles α_0, for succession of samples (a)–(c). (a) – ITO film on a glass substrate, at $\alpha_0 = 0.217°$, $0.283°$ and $0.403°$; (b) – ITO + PMDA-ODA film, at $\alpha_0 = 0.226°$, $0.25°$, $0.278°$, $0.305°$ and $0.47°$; (c) – ITO + PMDA-ODA + FLC film, at $\alpha_0 = 0.2°$ and $0.31°$. The solid curves represent the scattering distributions calculated using theoretical formalism. For clarity the curves in (a)–(c) corresponding to different incident angles are shifted vertically by a factor of 100. The sharp peaks at $\beta = \alpha$ correspond to the specular reflected beam

theory are $K_c \in \{-1, 1\}$ defining the cross-correlation coefficients between the roughness spectra for each pair of interfaces $\mathrm{PSD}_{i,j}$, and the fractal parameter h that determines self-affinity of the surface profile under linear scaling [15, 16]. Since a set of samples with sequentially deposited layers was available, a detailed analysis was conducted starting from the simplest one (an ITO film on glass substrate), and continued for samples containing PMDA-ODA and PMDA-ODA + FLC layers.

The effective roughness heights, σ_{eff}, are summarized in Table 1. Evaluated effective roughness height of the initial glass substrate is found within 0.9 nm. In turn, the effective roughness height, σ_{eff}, of the ITO surface reaches 1.4 nm, while the cross-correlation parameter against the substrate $K_c^0 = 0.85$. Compared to the graded interface width, $\sigma_s \approx 5.1$ nm, it is atypical for the data on such ITO films reported in literature [17, 18], and suggest additional post-synthesis low-temperature annealing [19, 20]. The roughness height of the PMDA-ODA surface and the PMDA-ODA/LC interface is approximately 4.6 nm with cross-correlation factor against the underlying ITO surface $K_c^1 = 0.28$, which is likely a result of the island-like polymer growth mechanism.

Table 1. Main calculated parameters of PSD functions characterizing the top interfaces of each layer within the studied LC cell

	Substrate	ITO	PMDA	LC
σ_{eff}, nm	0.87	1.36	$\simeq 4.6$	≥ 8.5
h	1.24	1.32	1.21	—
K_c	—	0.85	0.28	—

Additional PSD functions calculated directly from the $9 \times 9\,\mu$m AFM topography scans $\zeta(x, y)$, measured for various interfaces, were compared against the results of X-ray measurements. The good agreement between the results from these two independent methods validates the accuracy and reliability of the extracted structural parameters (see also [21, 22]).

To conclude, the quantitative parameters of the transition layers structure, as well as the statistical properties of roughness at interfaces, have been determined for the prototype of a LC cell based on ferroelectric LC. At present, a comprehensive theoretical framework linking the statistical characteristics of substrate roughness to the anchoring energy of LCs is lacking [1, 2, 7]. Nonetheless, numerous experimental studies have demonstrated that spatial correlations in surface roughness significantly influence the anisotropy of the substrate's surface energy, and thereby affect the anchoring strength and the alignment quality of LCs [6, 23]. The findings presented in this work are expected to provide valuable insights toward the development of such a theoretical model and may aid in the optimization of LC cell performance, particularly for systems incorporating ferroelectric LCs.

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Conflict of interest. The authors of this work declare that they have no conflicts of interest.

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