Supplementary information — "Topographical Changes in Photo-responsive Liquid Crystal films: A Computational Analysis" by Ling Liu and Patrick R. Onck

S1 Light attenuation and isomerization through the thickness

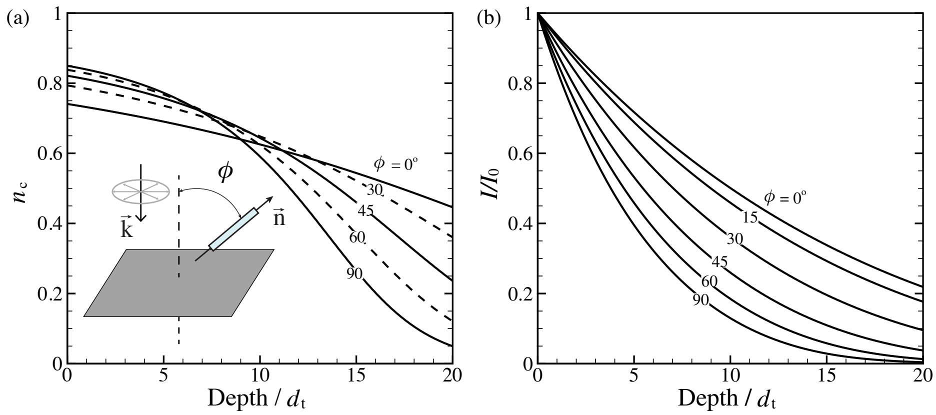

Fig. S1 Volume fraction of the cis-state azobenzene n_c (a) and the reduced light intensity $\mathscr{I} = I/I_0$ (b) against the propagating depth normalized by the attenuation length of the trans-state azobenzene d_t for a film of thickness $20d_t$ with various tilt angles ϕ under diffuse light illumination. The vector $\vec{k}$ shows the light propagating direction and $\vec{n}$ is the director. $\alpha = 10\beta = 30$ is used here.

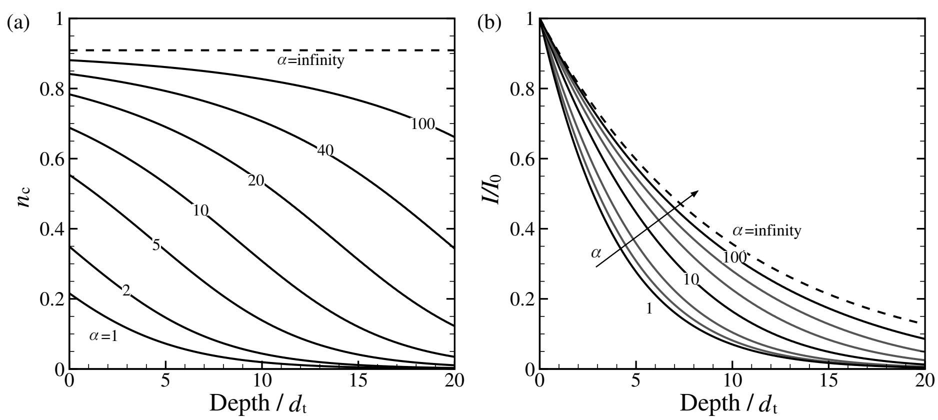

Fig. S2 Volume fraction of the cis-state azobenzene n_c (a) and the reduced light intensity $\mathscr{I} = I/I_0$ (b) against the normalized propagating depth for increasing α with a constant ratio $\alpha = 10\beta$. A tilted director with $\phi = 45°$ is chosen. A higher conversion level of cis ensues under a larger source intensity, at the cost of an increased amount of absorbed energy. The corresponding reduced light intensity increases, indicating that there is a larger portion of the input light getting transmitted and being ineffective.

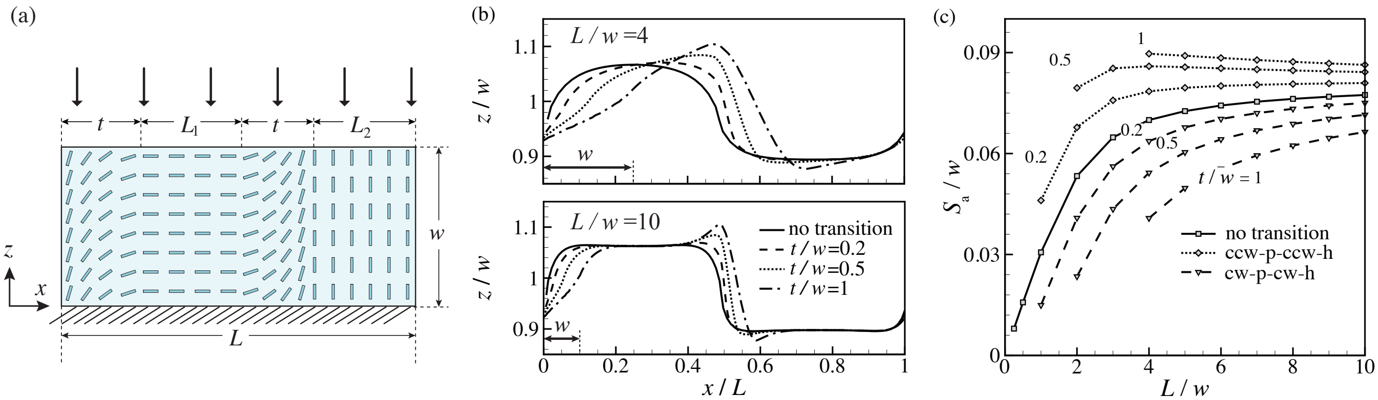

Fig. S3 (a) A schematic of the asymmetric transition region in a planar/homeotropic patterned film (denoted by cw-p-ccw-h; cw: clockwise rotation; ccw: counter-clockwise rotation). (b) The corresponding surface profiles for various ratios of t/w with $L/w = 4$, 10 and $L_1 = L_2$. (c) Variations of S_a/w as functions of L/w with various t/w for the symmetric clockwise transition (cw-p-cw-h) and the symmetric counterclockwise transition (ccw-p-ccw-h).

S2 Effect of transition regions

To illustrate the effect of transition regions inside patterned Azo-LC coatings, a planar/homeotropic film is chosen here, and two transition regions of size t are added, as schematically shown in Fig. S3. The characteristic length scales for this system are the length of the transition region t, the thickness of the coating w, the attenuation length of trans d_t and the length of the domains, i.e., L, L_1 and L_2. Simulations were conducted by fixing the thickness, $w/d_t = 10$, changing the length of the unit cell to obtain different L/w, and varying t to study the effect of t/w.

We study four idealized transition schemes here. The first one is denoted as the asymmetric transition scheme, in which the director rotates counterclockwise from the planar orientation to the homeotropic orientation in the right transition region, and the director rotates clockwise from the homeotropic to the planar state in the left transition regime (abbreviated as cw-p-ccw-h; p: planar; h: homeotropic; cw: clockwise; ccw: counterclockwise), as schematically shown in Fig. S3(a). The second asymmetric transition type is where the director rotates clockwise in the right transition region from the planar to the homeotropic and rotates counterclockwise in the left region (ccw-p-cw-h). Note that the second asymmetric scheme is a mirror image of the first one. The third and fourth possibilities are both symmetric transitions in which the director rotates either clockwise or counterclockwise in the two transition regions (cw-p-cw-h and ccw-p-ccw-h).

Figure S3(b) shows the predicted surface profiles of the asymmetric transition scheme (cw-p-ccw-h) with $L/w = 4$ and 10 and various values for t/w. The results without transition regions (i.e., $t = 0$) are also added for comparison. The transition region that features counterclockwise rotation is found to induce the formations of peaks close to the planar part and valleys close to the homeotropic region, which is due to the accumulation of the negative shear strains ε_{xz} inside the counterclockwise rotation region. In contrast, the out-of-plane deformations are suppressed by the clockwise rotation transition. Those distinct effects from the two rotation types (i.e., cw or ccw) are more dominant in the two symmetric transition schemes. The above results qualitatively match the measured surface profiles featuring a pair of peaks and valleys located at the domain boundary[1,2].

Figure S3(c) shows the normalized average height, S_a/w, of the symmetric clockwise transition (cw-p-cw-h) and the symmetric counterclockwise transition (ccw-p-ccw-h) as a function of L/w with various ratios t/w. The S_a/w increases for the counterclockwise rotation transition and decreases for the clockwise scheme, and these effects are more pronounced for larger transition region lengths. If the counterclockwise and clockwise rotation regions are more or less equally distributed at the patterning boundaries throughout the whole film, their influence is expected to cancel out, leading to a final roughness close to the prediction without the transition regions. Furthermore, for coatings with large in-plane dimensions, it is anticipated that the transition regions only affect the surface profiles in the vicinity of the patterning boundaries and have limited influence on the generated roughnesses, as indicated by the results with $L/w = 10$ in figures S3(b)-(c).

Note that more accurate studies on the effect of transition areas need insight on the exact director rotation of liquid crystal molecules, which might be beyond those in Fig. S3, such as Néel wall and Bloch wall[3,4] or complex director distributions around defects[5].

References

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