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Comment on "Structure of Smectic Defect Cores: X-Ray Study of 8CB Liquid Crystal Ultrathin Films"

Michel *et al.* [1] claim that (1) the energy of a grain boundary in a smectic *A* (Sm*A*) is "more than 1 order of magnitude higher than the values usually proposed in the literature" and that (2) "the disclination and focal conic core energy per unit length are closer to (10–100)K than to K," where K is the Sm*A* splay constant. In this Comment we show that (1) the energy of the wall observed in Ref. [1], when calculated per unit area, is of the *same* order or even *smaller* than the literature values [2], and (2) the energy per unit length of a disclination core or a focal conic defect (FCD) core deduced from data [1] is closer to K than to (10–100)K, in accord with the de Gennes' model [3] but contrary to the claim [1].

(1) The Sm*A* elastic energy density, $f = \frac{1}{2}K(\mathrm{div}\mathbf{n})^2 + \frac{1}{2}B\varepsilon^2$, is comprised of the director $\mathbf{n}$ splay term and the layers dilation term [4]. The Young modulus B and K define the so-called penetration length, $\lambda = \sqrt{K/B}$, of the order of interlamellar spacing; for 8CB, $\lambda \approx 1$ nm [4]. The highest possible density of Sm*A* distortions is $\varepsilon \sim 1$ and $\mathrm{div}\mathbf{n} \sim 1/\lambda$. Therefore, the *maximum* energy per unit *area* of a Sm*A* wall is $\sigma \sim f_{1V}\lambda \sim K/\lambda$ [2], where $f_{1V} \sim B \sim K/\lambda^2$ is the maximum density per unit volume. Michel *et al.* [1] dealt with the wall of thickness 1 nm and "perimeter" $L_y = 350$ nm and concluded that its energy per unit length is $E_{1l} \approx (40\text{–}110)K$. The first dimension, 1 nm, is nothing else but λ, while the second is apparently the width of the wall dependent on thickness e of the film [1]. Taking E_{1l} as in [1], one finds $\sigma \approx E_{1l}/L_y \approx (40\text{–}110)K/350\ \mathrm{nm} \approx (0.1\text{–}0.3)K/\lambda$, which is of the *same* order or *less* than the literature value $\sigma \sim K/\lambda$ [2], when properly calculated as the energy per unit area of the wall. Note that for an extended sample, one of the dimensions of the wall might indeed become larger than λ, as determined by the sample size, surface tension, anchoring, and by the bulk parameters (the smectic twist grain boundary phases represent an example with essentially infinite grain boundaries).

(2) The FCDs are formed by special layers configurations, namely, Dupin cyclides, for which the 2D singular focal *surfaces* degenerate into *linear* defects, e.g., an ellipse and a hyperbola [4]. The reduced dimensionality greatly reduces the core energy, from $\sigma L^2 \sim f_{1V}\lambda L^2 \sim KL(L/\lambda)$, to $F \sim f_{1V}\lambda^2 L \sim KL$. The energy per unit length of the line is thus $E_{1l} \sim F/L \sim K$, the *same* as in literature [2–4], but definitely *much smaller* than (10–100)K claimed in Ref. [1]. Even a smaller $E_{1l} \approx (0.1\text{–}0.3)K$ is obtained if the data [1] are used to calculate f_{1V} as $f_{1V} \approx \sigma/\lambda \approx (0.1\text{–}0.3)K/\lambda^2$.

In Ref. [1], the core energy of a wall is compared to the line core energy. Even if the different dimensionality of the two were accounted for, such a comparison is still incomplete, as it does not take into account other major factors. Really, the two structures in Fig. 1 and Fig. 4 of Ref. [1] might differ not only in the "splitting" of a disclination into a rotating grain boundary (RGB), but also in the excess surface area at the Sm*A*-air interface (and thus in the surface tension energy), in surface orientation of $\mathbf{n}$ (and thus in the anchoring energy), and in the distortions outside the cores (and thus in additional elastic terms). All these contributions might be as high as the RGB energy and thus must be added to the analysis. For example, the anchoring energy of a Sm*A*-solid interface for large misalignment is $\sigma \sim K/\lambda$ [5]; the elastic energy per unit area of a wall in Fig. 1 of Ref. [1] is also of the same order, as calculated by the authors previously [6]: $\sigma \approx E_W/(2Re) \approx (K/\lambda) \times (\pi \sin\theta_0 - 2\theta_0) \approx K/\lambda$, where E_W, $2R$, and e are the total energy, length and width of the wall, respectively; $\theta_0 \approx 20^0$ is the misalignment angle for which $(\pi \sin\theta_0 - 2\theta_0) \approx 0.99$.

At last, we wish to draw the attention against the wrong conclusion that emerges from an unfitted reading of the Letter [1], namely, that the RGB model of a disclination core and the large total energy it carries are generic features of FCD disclination lines. The results [1] are characteristic of ultrathin films (100 layers or so), and crucially depend on a delicate balance between the distortion energy in the film and the surface tension of the free surface and the anchoring energy. It would be interesting to repeat the same (certainly beautiful and original) x-ray experiments on samples with different anchoring energy and for much thicker samples.

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