

DEISA project: On the molecular working of a twisted nematic cell

Period: 01.07.06 - 1.5.07

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Short report for dissemination:

One of the most successful stories in advanced materials is that of liquid crystal (LC) displays. The basic concept underlying the most classic among these devices, the twisted nematic (TN) display, is that a pixel is activated by a change of molecular organization in a few micron thick cell. According to this concept, an initial configuration of the local preferred direction (the director) is established between two orienting surfaces (rubbed glass or polyimide), rotated 90 degrees from one another, that confine the LC. An experimental fact is that polarized light is going through the pixel in this "rest" state and this is compatible with a microscopic helical configuration. If the chosen LC has a positive dielectric anisotropy and a suitable voltage is applied across the cell in correspondence of the pixel, then polarized light is not rotated and light does not go through the device, compatibly with a monodomain organization. When the field is switched off the original organization is re-established.

The classic textbook picture explaining the working of a TN-LCD, is that of uniformly twisted layers, but to the best of our knowledge there is little evidence that the molecular organization at rest is a uniform helix at molecular level. Moreover, the way the organization is established is not obvious, for instance as the organization at rest is re-established after an aligning cycle does the reorganization take place from the centre of the cell or from the surface? Uniformly or not? Is a uniform helix really formed? Or how helical is the structure?

Trying to work out the microscopic working of the TN display is a particularly challenging problem, as it imply considering a huge number of degrees of freedom, which are to follow for very long times from a microscopic point of view, as the average TN-LCD response vary in the range 8-15 milliseconds, while the typical time scales we are to date able to access through conventional computer simulations is of the order of nanoseconds.

Within the DEISA project, we have tackled this problem setting up a molecular resolution model of a TN cell containing  $O(10^6)$  model particles, simulated using the Monte Carlo (MC) method. To this purpose, we developed an MPI parallel MC code using a replicated data scheme, by modifying the canonical Markov chain of the Metropolis algorithm to allow for multiple simultaneous moves to be performed at the same time by different processors. This kind of moves are not possible in conventional MC algorithms due to the intrinsic non deterministic nature of MC, but in our case the

big sample size allow every processor to pick an energetically independent particle in suitably chosen cells in which the whole sample is subdivided.

We modeled the LC rod-like molecules contained in the LCD cell as Gay-Berne single ellipsoidal interaction sites, discarding all the intramolecular degrees of freedom.

Our TN cell is arranged as to model a 0.1 micron x 0.1 micron x 0.05 micron display cell. Although a fully realistic model would have to consider an order of magnitude bigger sample, this is currently unfeasible with the available resources. The initial configuration (see fig.1 a), is characterized by the LC molecules uniformly aligned perpendicular to the display surfaces to give the dark pixel state, while the display boundaries are modeled with layers of fixed particles oriented along the incoming and outgoing polarizers directions (rotated 90 degrees from one another). The system is then allowed to relax through MC simulation to the "rest" equilibrium state, which is reached only after 150000 hours of computing time (see fig.1 b.).

Following the time evolution of this equilibration process we can notice that the mechanism of clearing of the pixel proceeds by the local induction of order by the two confining surfaces which induce an almost parallel alignment to their orientation on the LC molecules filling the display. This is a very slow process, characterized by the progressive alignment of the molecular layers, starting from those closer to the two surfaces. The resulting distribution of local directors at this point is far from being that of a perfect linear helix. On the contrary, the molecular layers align almost parallel to the closest display surface, and are not affected by the farthest surface. Some sort of helicoidal ordering starts to form only when the two fronts of perpendicular oriented particles, come into contact in the middle of the sample. However, the temperature dependent fluctuations of molecular orientations in the middle of the sample make the conventional picture of an uniformly helicoidal configuration too simplistic, and evidences how this requirement is not necessary to achieve a good optical behavior.

Having reached an equilibrated configuration corresponding to a light pixel, we switched on an electric field in the central region of the display. Our aim was to investigate on the mechanics underlying the disruption of helicoidal order to give a black pixel. The interesting result is that the dark region of the pixel starts to grow from the centre of the square area affected by the field, expanding in concentric spherical shells, instead of uniformly all over that area (see fig. 2).

The calculations were carried out at the CSC in Finland, employing 128 processors and at CINECA in Italy, using 64 processors, for a global amount of 200000 CPU hours.

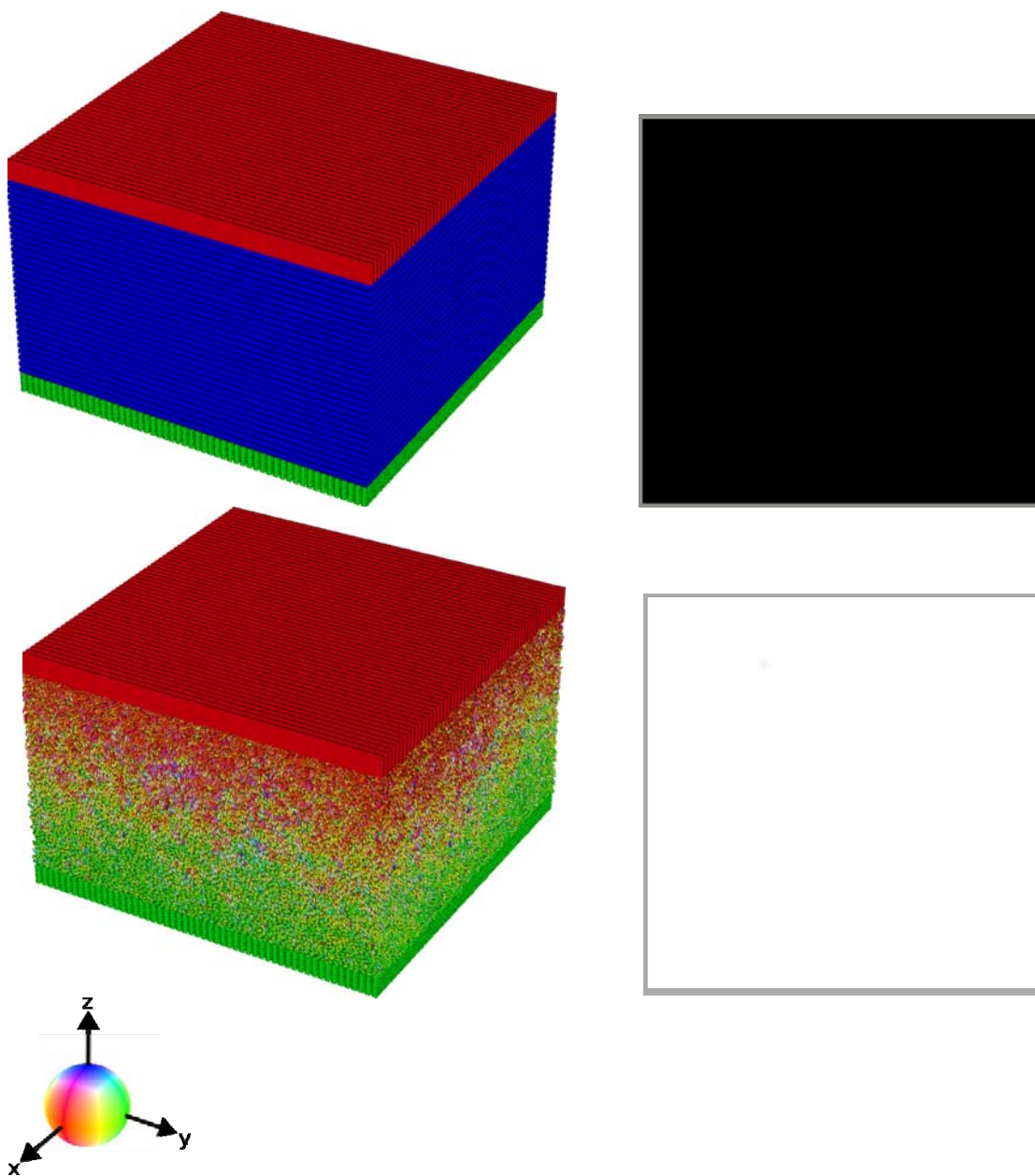


Fig 1. Snapshots of the molecular configurations (left) and corresponding computed pixel images (right) for: a) the initial dark state (top) and b) the final states (bottom), after 150000 hours of Monte Carlo simulation. Molecules are color coded according to their orientations as in the palette shown below.

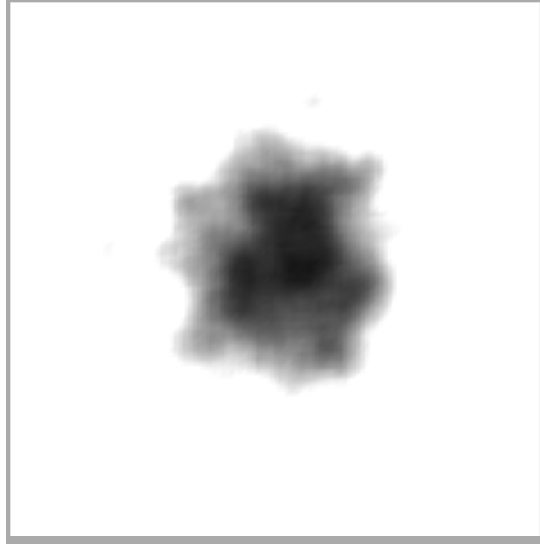


Fig. 2. Pixel image computed after 50000 cycles of MC simulation with an electric field switched on in the middle of the display.