Molecular Crystals and Liquid Crystals Science and Technology. Section A. Molecular Crystals and Liquid Crystals

Publication details, including instructions for authors and subscription information:
http://www.tandfonline.com/loi/gmcl19

Materials for Liquid Crystal Displays with Reduced Power Consumption

Peer Kirsch [a], Matthias Bremer [a], Annette Kirsch [a], Atsutaka Manabe [a], Eike Poetsch [a], Volker Reiffenrath [a] & Kazuaki Tarumi [a]

[a] Merck KGaA, Liquid Crystals Division, 64271, Darmstadt, Germany

Version of record first published: 24 Sep 2006

To cite this article: Peer Kirsch, Matthias Bremer, Annette Kirsch, Atsutaka Manabe, Eike Poetsch, Volker Reiffenrath & Kazuaki Tarumi (2000): Materials for Liquid Crystal Displays with Reduced Power Consumption, Molecular Crystals and Liquid Crystals Science and Technology. Section A. Molecular Crystals and Liquid Crystals, 346:1, 193-199

To link to this article: http://dx.doi.org/10.1080/10587250008023878

Mol. Cryst. Liq. Cryst., 2000, Vol. 346, pp. 193-199
Reprints available directly from the publisher
Photocopying permitted by license only

Materials for Liquid Crystal Displays with Reduced Power Consumption

PEER KIRSCH, MATTHIAS BREMER, ANNETTE KIRSCH, ATSUTAKA MANABE, EIKE POETSCH, VOLKER REIFFENRATH and KAZUAKI TARUMI

Merck KGaA, Liquid Crystals Division, 64271 Darmstadt, Germany

A significant reduction of the power consumption of a liquid crystal display can be achieved either by application of a lower driving voltage or – even more effectively – by use of a holographically structured reflective scattering type of display without colour filters. The first option requires strongly polar materials with extremely high reliability, the second one new types of liquid crystals with a birefringence as high as possible in order to optimize the scattering effect. A molecular modeling based method for the prediction of reliability parameters is presented.

Keywords: liquid crystals; active matrix display; molecular modeling

1. INTRODUCTION

The reduction of the power consumption of active matrix liquid crystal displays (AM-LCD) is a predominant target on the way to an increased mobility of battery powered devices. The largest contribution to the overall energy consumption of a display comes from the backlight. Reflective displays could therefore reduce the power consumption by around 90%. A potential for the further decrease would be the use of a lower driving voltage.

2. MATERIALS WITH ULTRA-HIGH PURITY AND ULTRA-HIGH RELIABILITY

The reduction of the driving voltage of a AM-LCD implies the use of a liquid crystalline material with increased dielectric anisotropy ($\Delta\varepsilon$). This type of materials is known to be highly sensitive towards ionic impurities which decrease the voltage holding ratio, and finally lead to observable flicker or contrast inhomogenities of the display.[1] There are two possible reasons for the increased sensitivity of highly polar materials: First, the faciliated dissociation of ion-generating impurities in a medium with a high dielectric constant. Secondly, the solvation and mobilization of ions due to complexation by specific substructures of liquid liquid crystals.

It could be shown, that there is a strong reciprocal correlation of the voltage holding ratio of different types of liquid crystals with the calculated (semiemirical, AM1) heat of interaction with so-called „sparkles", models of hard-sphere ions with a positive or negative charge but no molecular orbitals.[2]

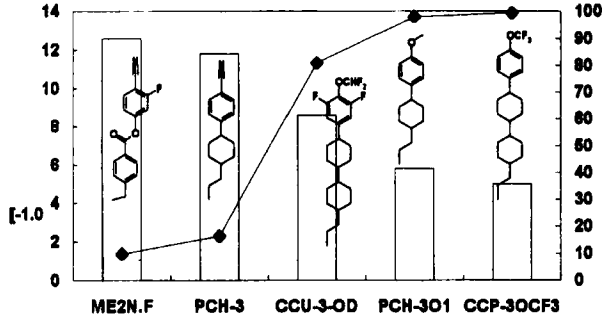

FIGURE 1 Correlation between voltage holding ratio (♦) and calculated heat of interaction (bars) with a „sparkle" (semiempirical, AM1) of some representative liquid crystals.

These calculations were reproduced and refined on the *ab initio* level (HF/6-31G*) with sodium cations, providing a semi-quantitative affinity scale of various liquid crystals with cations.

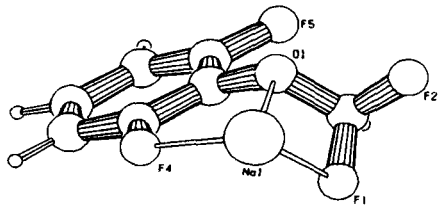

FIGURE 2 One of the possible complexes between a sodium cation and 2,6-difluoro(difluoromethoxy)benzene (*ab initio*, HF/6-31G*: ΔH_f^0 = –35.3 kcal·mol^{-1}). The relatively high heat of interaction can be explained by the chelation of the cation by three binding sites.

Experimental support was also obtained by fast atom bombardment mass spectrometry (FAB-MS) where clusters of liquid crystal molecules with protons or sodium cations are observed with intensities fitting the calculated affinity scale.

3. NEW MATERIALS WITH ULTRA-HIGH BIREFRINGENCE

Displays based on the reflective scattering mode (RSM) require no backlight. Holographic structuring of the polymer dispersed liquid crystal droplets makes also the strongly light-absorbing colour filters obsolete. Requirement on the liquid crystal side is an extremely high birefringence (Δn). The current limit for birefringence of commercially used liquid crystalline single compounds is around 0.32, wheras a reasonable minimum requirement for an effective RSM is 0.35. The optimum Δn value for a liquid crystal mixture would be larger than 0.5.

Even if there are some materials known with very high Δn, the main obstacles for the practical application of such highly birefringent liquid crystals are their UV instability, poor solubility and - possibly – insufficient compatibility with active matrix technology. In order to overcome these problems, a number of new materials was synthesized. The first of such high Δn liquid crystals are based on tolane (diphenylacetylene) substructures and the isothiocyanato group as a polar terminus. Optimization of the side chain lenghts and the fluorination pattern led to materials with highly promising properties.

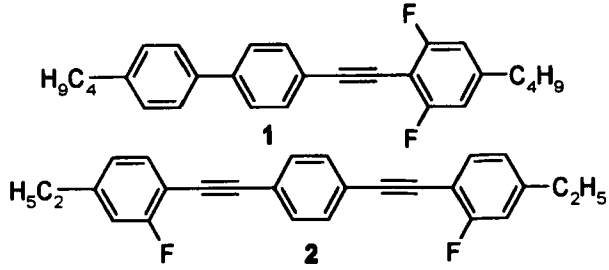

FIGURE 3 Tolane based liquid crystals with very high birefringence (Δn) but low dielectric anisotropy ($\Delta \varepsilon$).

Whilst material **1** still photochemically stable, materials with more than one acetylenic triple bond have an increased tendency towards photochemical degradation even after exposure to ambient room light.

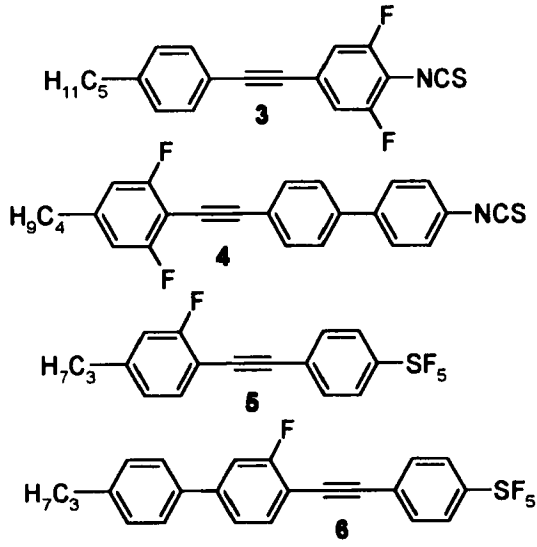

FIGURE 4 Polar liquid crystals with very high birefringence (Δn) based on tolane substructures.

The compatibility with active matrix technology could be improved by introducing the highly polar[3,4] pentafluorosulfuranyl function as a terminal group.[5]

No.	(Meso)phases	$T_{NI,extr}$	$\Delta\varepsilon$	Δn
1	C 32 N 159.5 I	197.4	3.6	0.319
2	C 128 N 193.7	236.1	1.4	0.437
3	C 46 I	22.0	18.3	0.381
4	C 102 S_A 208 N 259.8 I	228.1	15.8	0.460
5	C 78 I	-32.0	21.6	0.224
6	C 129 S_A 155 N 158.1 I	138.0	20.6	0.308

TABLE 1 Physical properties of tolane based materials with very high birefringence. Phase transitions and „virtual" clearing points ($T_{NI,extr}$) are cited in °C. $T_{NI,extr}$, $\Delta\varepsilon$ and Δn were extrapolated from a 10% w/w solution in the Merck mixture ZLI-4792 (T_{NI} = 92.8°C, $\Delta\varepsilon$ = 5.27, Δn = 0.0964) and corrected empirically for differences in the order parameter. The electrooptical parameters were measured at 20°C, the birefringence at a wavelength of 589 nm, and the dielectric anisotropy with an 1 kHz AC voltage.

The results of the „sparkle" calculations indicated, that the pentafluorosulfuranyl group does not coordinate very well to cations and does therefore not reduce the voltage holding ratio in spite of its strong dipole moment. This prediction was experimentally confirmed.

4. REDUCTION OF POWER CONSUMPTION BY VERY LOW THRESHOLD VOLTAGE – MATERIALS WITH ULTRA-HIGH VOLTAGE HOLDING RATIO

The computational models for reliability prediction, such as the „sparkle" affinity scale, were intended to be a guidance for the design of new structures for liquid crystals with improved voltage holding ratio. One of the results of such predictions is the introduction of the pentafluorosulfuranyl group which has a low affinity to ionic contaminants. Another type of materials promising improved reliability are alicyclic compounds containing no heteroatoms except fluorine.

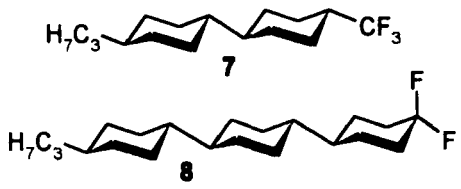

FIGURE 5 Fluorinated alicyclic liquid crystals with very high voltage holding ratio.

No.	Mesophases	$T_{NI,extr}$	$\Delta\varepsilon$	Δn
7	C 18 S_B 40 I	-43.0	6.8	0.054
8	C 42 S_B 161 I	88.9	3.1	0.062

TABLE 2 Physical properties of the fluorinated alicyclic liquid crystals with very high voltage holding ratio **7** and **8**. Phase transitions and „virtual" clearing points ($T_{NI,extr}$) are cited in °C. $T_{NI,extr}$, $\Delta\varepsilon$ and Δn were extrapolated from a 10% w/w solution in the Merck mixture ZLI-4792.

Nevertheless, in spite of their excellent reliability, materials such as **7** or **8** have strong tendency to form S_B mesophases. Therefore, the mesophase range of this type of materials is a parameter with potential for further improvement.

5. SUMMARY

Supported by molecular modeling as a powerful design tool, a number of new liquid crystalline materials, either with very high birefringence or with strongly improved voltage holding ratio was synthesized.

Acknowledgments
We thank A. Ruhl and R. Tavakoli for experimental assistance, and Dr. J. Krause, J. Haas and H. Heldmann for the physical evaluation of the new substances. This work was performed under the management of the *Association of Super-Advanced Electronics Industries* (ASET) in the R & D program of the Japanese *Ministry of International Trade and Industry* (MITI) supported by the *New Energy and Industrial Development Organization* (NEDO).

References

[1] A. Sasaki, T. Uchida, S. Miyagami, *Japan Display '86,* **1986,** 62.
[2] M. Bremer, S. Naemura, K. Tarumi, *Jpn. J. Appl. Phys.* **1998,** *37,* L88-L90.
[3] M. Bremer, K. Tarumi, *Adv. Mater.* **1993,** *5,* 842–848.
[4] M. Klasen, M. Bremer, A. Götz, A. Manabe, S. Naemura, K. Tarumi, *Jpn. J. Appl. Phys.* **1998,** *37,* L945-L948.
[5] P. Kirsch, M. Bremer, M. Heckmeier, K. Tarumi, *Angew. Chem.* **1999,** *111,* 2174–2178; *Angew. Chem. Int. Ed. Engl.* **1999,** *38,* 1989–1992 .