

order on the 2-20 nm scale were discovered. Secondly, a complex cubic phase of some polycatenar LCs (rod-like molecules with more than one appended terminal chain) is investigated. Thirdly, packing of gold nanoparticles coated with nematogens is studied. Powder, single domain and fibre patterns are used, as appropriate, with GISAXS proving particularly useful. Electron density reconstruction is used routinely, but to help solve the phase problem a number of methods are used, including different variants of isomorphous replacement, model building and refinement, and supporting neutron scattering experiments. The main conclusion is that, with the ever increasing complexity of liquid crystal phases, the simple comparison of spacings and molecular dimensions as a method of structural characterization, often used in the past, is increasingly becoming a thing of the past.

1. G Ungar, XB Zeng, *Soft Matter*, 2005, 1, 95.
2. Prehm, M., Liu, F., Baumeister, U., Zeng, X.B., Ungar, G., Tschierske, C. *Angew. Chem. Int. Ed.*, 2007, 46, 7972
3. Xiangbing Zeng^a, Liliana Cseh^b, Georg H. Mehl^b and Goran Ungar, *J. Mat. Chem.*, in press
4. B Glettner, F Liu, XB Zeng, M Prehm, U Baumeister, G Ungar, C Tschierske, *Angew. Chem. Int. Ed.*, in press

Keywords: liquid crystals, GISAXS, cubic phases

MS.12.3

Acta Cryst. (2008). A64, C32

Molecular aggregation structure of exotic liquid crystals formed by thermotropic mesogen BABH(n)

Kazuya Saito¹, Kazumi Ozawa¹, Yasuhisa Yamamura¹, Syuma Yasuzuka¹, Hiroyuki Mori², Shoichi Kutsumizu²

¹University of Tsukuba, Department of Chemistry, Graduate School of Pure and Applied Sciences, 1-1-1 Tennodai, Tsukuba, Ibaraki, 305-8571, Japan, ²Gifu University, 1-1 Yanagido, Gifu 501-1193, Japan, E-mail : kazuya@chem.tsukuba.ac.jp

1,2-Bis(4'-n-alkoxybenzoyl)hydrazines [BABH(n), n: the number of C atoms in an alkoxy chain] exhibit micro phase separated liquid crystalline phases: smectic C (lamellar) and two bicontinuous types of cubic phases (Ia3d & Im3m). According to Babinet's principle, reflection intensities do not give any information concerning the electron density, and consequently, the location of molecules. To locate molecules in complex structures, the authors utilized the chain length (n) dependence. For the Ia3d phase, widely observed in lyotropics and block copolymers, it is deduced that Gyroid, a triply periodic minimal surface (TPMS), is formed by the terminal methyl groups while the molecular cores aggregate as rods. This structure remains in $3 < n < 23$, in contrast to simple continuum theories of micro phase separation, which predict the interchange of roles of two components at both sides of the lamellar phase region appearing around the equivolume composition. For the Im3m phase ($12 < n < 17$) that is observed only for low-molecular weight thermotropics, MEM analyses were systematically performed as the similar analysis to the Ia3d phase failed. The MEM formula was modified to use only their magnitude for reflections other than two main ones. The n dependence of the MEM results successfully solved the phase problem while making the theoretical consideration on the phase stability. The solution revealed that the molecular cores form a spreading jungle gym having three-fold junctions and spherical shells. The rods of the jungle gym are nearly on a TPMS (P surface). This structure of the Im3m phase clearly has similarities with both of the Ia3d phase and the lamellar phase: Spreading jungle gym with three-fold junctions and sheet-like aggregate (though closed on a sphere).

Keywords: liquid-crystal structures, maximum-entropy method, minimal surface

MS.12.4

Acta Cryst. (2008). A64, C32

Mesophase semiconductors: Design for 3D-mesophases with effective paths for electronic charge hopping

Yo Shimizu¹, Benoit Heinrich², Daniel Guillon², Motoo Shiro³, Hiroato Monobe¹, Kazuma Oikawa⁴

¹National Institute of Advanced Industrial Science and Technology, Kansai Center, Nanotechnology Research Institute, Synthetic Nano-Function Materials Group, Midorigaoka 1-8-31, Ikeda, Osaka, 563-8577, Japan, ²Institut de Physique et Chimie des Matériaux, Strasbourg, ³Rigaku Corp., ⁴Kanto Chemicals Corp., E-mail : yo-shimizu@aist.go.jp

Liquid Crystalline Semiconductors are now evolved into Mesophase Semiconductors because of the importance of the highly ordered structure of mesophase [1]. On the other hand, Organic Electronics is a most interesting category of researches on organic condensed matter in terms of polymer-based thin film electronic devices and more efficient design strategies for the molecules are required. Recent studies on calamitic liquid crystalline systems have insisted the better situation to obtain the faster mobility of charged carriers does not meet ordinary and typical liquid crystalline phases such as nematic and smectic A phases and the more highly ordered systems do have an advantage in the mobility improvement. We recently reported that a mesogenic 8TNAT8 (an alkylated dithienyl naphthalene) showing a highly ordered mesophase with a 3D lattice have a fast carrier mobility in the order of 10^{-1} - 10^{-2} cm² V⁻¹ s⁻¹ in the mesophase where the molecules align just like a smectic layered phase. The application of this compound to a field effect transistor (FET) exhibits the comparable mobility (0.14 cm² V⁻¹ s⁻¹) at room temperature (crystalline solid) [2]. In this work, the 3D-mesophase structure was studied by powder X-ray diffraction (XRD) with a dilatometry technique and by single crystal XRD of the room temperature crystal. It was found that the room temperature crystal and the mesophase one are so similar to each.

References

- [1] Y. Shimizu, K. Oikawa, K. Nakayama and D. Guillon, *J. Mater. Chem.*, 17, 4223 (2007).
- [2] K. Oikawa, H. Monobe, K. Nakayama, T. Kimoto, K. Tsuchiya, B. Heinrich, D. Guillon, Y. Shimizu and M. Yokoyama *Adv. Mater.*, 19, 1864 (2007).

Keywords: organic electronics, liquid crystalline semiconductor, charge hopping path

MS.12.5

Acta Cryst. (2008). A64, C32-33

Functional nanostructured liquid-crystalline assemblies

Takashi Kato

The University of Tokyo, Department of Chemistry and Biotechnology, Hongo, Bunkyo-ku, Tokyo, 113-8656, Japan, E-mail : kato@chiral.t.u-tokyo.ac.jp

Soft materials are molecular-based materials such as polymers, liquid crystals, and colloids. They are becoming important as functional materials because of their dynamic nature. Although soft materials are not as highly durable as hard materials such as metals and ceramics, they can respond to stimuli and environment. The introduction of molecular order into soft materials induces new dynamic functions.