

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.

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Keywords: liquid crystals, GISAXS, cubic phases

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

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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

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

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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 $10^{-1}-10^{-2} \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ 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 ($0.14 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$) 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.

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

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Functional nanostructured liquid-crystalline assemblies

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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.

Liquid crystals are ordered soft materials consisting of assembled molecules. They can be used as new functional materials for electron, ion, or molecular transportation, sensory, catalytic, optical, and bio-active materials [1,2]. Herein, we describe new approaches to functionalization of liquid crystals and show how the design of liquid-crystalline structures formed by supramolecular assembly and nano-segregation leads to the formation of a variety of new functional soft materials.

- 1) T. Kato, N. Mizoshita, K. Kishimoto *Angew. Chem. Int. Ed.* 2006, 45, 38.
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Keywords: liquid-crystal polymers, liquid-crystal structures, self-assembly supramolecular chemistry

MS.13.1

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Exploring the phase diagram of $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$: Spins, stripes, and superconductivity

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The layered structure of copper-oxide superconductors results in highly anisotropic properties. Single-crystal samples are essential for proper characterizations, especially with scattering techniques. While high-temperature superconductivity was first discovered by Bednorz and Mueller in $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$ (LBCO), this particular system has been one of the more challenging for the growth of crystals, at least for $x > 0.1$. The growth of LBCO crystals is complicated by the fact that the Ba concentration in the melt is much higher than that in the resulting crystal; nevertheless, persistent effort with the floating-zone technique has finally led to the successful growth of large crystals with x as large as 0.155. The availability of these crystals has enabled a broad range of characterizations, including elastic and inelastic neutron scattering, diffraction with soft and hard x-rays, infrared reflectivity, angle-resolved photoemission, scanning tunneling microscopy, magnetization, and transport measurements. We have been able to demonstrate the presence of charge and spin stripe ordering over a range of doping centered on $x=1/8$. Furthermore, although stripe order correlates with a strong suppression of bulk superconductivity, recent results provide evidence for two-dimensional superconductivity coexisting with stripe order at temperatures as high as 40 K. Another important cuprate system is $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+d}$. One of us (Gu) has recently succeeded in growing very large crystals (50 mm x 7 mm x 1-7 mm) of the 91-K superconductor. These have made possible direct studies of spin fluctuations and phonons by inelastic neutron scattering. Work at Brookhaven is supported by the Office of Science, U.S. Dept. of Energy, under Contract No. DE-AC02-98CH10886.

Keywords: crystal growth, copper oxide superconductors, charge density waves

MS.13.2

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High quality single crystals for neutron experiments

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To make headway on any problem in physics, high quality single crystals are required. In this talk, emphasis will be placed on the crystal growth of selected superconducting and magnetic materials (oxides, borides and borocarbides) using the Optical Image furnaces at the University of Warwick. The floating zone method of crystal growth used in these furnaces, produces crystals of superior quality, circumventing many of the problems associated with, for example, flux growth from the melt. Especially large volumes of crystal may be grown by this method, a prerequisite for most neutron scattering experiments. Some examples of experimental results from crystals grown at Warwick, selected from numerous in-house studies and our collaborative research projects with other UK and international groups will be discussed.

Keywords: floating zone technique, magnetic materials, neutron scattering techniques

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Tailor-made single crystal growth of high-Tc superconductors for characterization by spectroscopy

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Due to a tremendous scientific effort over the past 20 years, our understanding of high-temperature superconductivity in the lamellar copper oxides has greatly improved. In particular, significant progress in spectroscopic measurements, such as neutron and x-ray scattering, angle-resolved photoemission spectroscopy, scanning tunneling spectroscopies, have played a major role to probe the electronic properties and the nature of the elementary excitations in these class of materials. To make these experiments possible, availability of dedicated and well-characterized single crystal samples are always required, and indeed these samples have contributed in bringing a lot of interesting information. In my talk, I will discuss how the crystal growth efforts and spectroscopic studies are mutually benefitted from each other, mainly based on our case studies.

Keywords: high-Tc superconductivity, spectroscopy, floating zone method

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Layered and cubic cobaltites grown by floating zone, structural and magnetic properties study

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Cobaltites create a large family of compounds possessing a wide range of unique properties such as superconductivity in water