

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.
- 2) T. Kato *Science* 2002, 295, 2414.

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

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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

intercalated $\text{Na}_{1-x}\text{CoO}_{2-x}$, spin-state transitions of the Co^{3+} ion in LaCoO_3 , a metal-insulator (MI) accompanied by structural transition in $\text{LnBaCo}_2\text{O}_{5.5}$ (where Ln is a rare earth). We present our recent results on crystal growth of cobaltites: $\text{La}_{1-x}\text{Sr}_x\text{CoO}_3$ and $\text{LnBaCo}_2\text{O}_{5+x}$ using Optical Travelling Solvent Floating Zone method. The crystals were studied by different techniques and some of results will be discussed. A very small Sr doping level (0.2%) drastically changes magnetic properties of $\text{La}_{1-x}\text{Sr}_x\text{CoO}_3$ as found using inelastic neutron scattering and magnetisation measurements. This can be explained assuming that the slight hole doping in LaCoO_3 matrix creates magnetic polarons, which leads to a spin-state transition of Co^{3+} . On the background of the spin-state and orbital-ordering transitions of the Co^{3+} ion in $\text{LnBaCo}_2\text{O}_{5+x}$, the system shows a metal-insulator transition accompanied by structural one at temperatures above room temperature, three different magnetic phases below room temperature and a structural transition at temperature above MI transition. All these properties can be tuned by a kind of the rare earth ion and oxygen stoichiometry. Structural, magnetic and transport studies of layered cobaltites $\text{LnBaCo}_2\text{O}_{5.5}$ (Ln=Tb, Nd) especially near metal-insulator transition will be presented.

Keywords: crystal growth, crystal structure and properties, transition metal-rare earth oxides

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Micro-crystallographic structure of $\text{Sr}_2\text{RuO}_4/\text{Sr}_3\text{Ru}_2\text{O}_7$ eutectic crystals grown by floating zone method

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Directional solidification at high temperature gradients by Infrared Image Furnace of $\text{Sr}_2\text{RuO}_4/\text{Sr}_3\text{Ru}_2\text{O}_7$ eutectic crystals has shown that mainly two distinct eutectic morphologies occur, a regular lamellar structure and a wavy lamellar structure. High resolution X-ray analysis has shown that the two phases are stacked in a multilayer structure along their c-axis. The analysis of X-ray diffraction patterns by the Rietveld method has been used to determine the percentage of each phase in crystals grown starting from a different composition of the polycrystalline rod. The morphology of crystals with different fraction of Sr_2RuO_4 and $\text{Sr}_3\text{Ru}_2\text{O}_7$ phase has been investigated by optical and electron microscopy. Electron back scatter diffraction (EBSD) technique was used to characterize the crystallographic match at the interface between Sr_2RuO_4 and $\text{Sr}_3\text{Ru}_2\text{O}_7$ phases. In particular the crystallographic match has been investigated for interfaces along plane parallel and perpendicular to the growth direction. Moreover, the misorientations for sharp and wavy lamellar structure have been thoroughly investigated with EBSD technique.

Keywords: eutectic crystallization, float zone growth, back-reflection electron Kikuchi pattern

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Chirality realized only in the crystalline state: Inorganic and organic compounds

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Some compounds exhibit chirality only in the solid state through chiral supramolecular arrangement of achiral compounds or through trapping a chiral conformation of a flexible achiral compound. The chirality must be measured in the solid state, however, the macroscopic anisotropies of crystals, Linear Birefringence (LB) and Linear Dichroism (LD) cause parasitic artifact signals in CD (Circular Dichroism). Thus, we have designed and built a Universal Chiroptical Spectrophotometer (UCS-1¹, UCS-2²) and devised a set of procedures for obtaining artifact-free CD and CB (circular birefringence) based on the Mueller matrix method. We have studied inorganic crystals, $\alpha\text{-Ni}(\text{H}_2\text{O})_6 \cdot \text{SO}_4$ and $\text{Ni}(\text{H}_2\text{O})_6 \cdot \text{SeO}_4$, which exhibit natural optical rotatory power only in the crystalline state. Using UCS-1, we could show that true CD and CB signals satisfy the Kramers-Kronig relationship.³ Further we have discovered a remarkable sign inversion of single crystal CD in one of the Ni *d-d* transitions at near liquid nitrogen temperatures, although the crystal structure hardly changes.⁴ With UCS, we have also observed birefringence of a chiral cubic crystal of class T, NaClO_3 and NaBrO_3 , along the [100] directions for the first time and proved that the anisotropy is of an intrinsic nature. Only the non-birefringent axis is along the [111] directions.⁵ Photocyclization of dynamically achiral organic compounds also produces enantioselective reaction products if carried out in chiral crystal environment.⁶

- 1) R. Kuroda, T. Harada, Y. Shindo, *Rev. Sci. Instrum.* **72**, 3802-3810 (2001)
- 2) T. Harada, H. Hyakawa and R. Kuroda, *Rev. Sci. Instrum.* **79**, 0731033802(2008).
- 3) T. Harada, Y. Shindo and R. Kuroda, *Chem. Phys. Lett.*, **360**, 217-222 (2002).
- 4) T. Harada, T. Sato and R. Kuroda, *Chem. Phys. Lett.*, **456**, 268-271 (2008)
- 5) T. Harada, T. Sato and R. Kuroda, *Chem. Phys. Lett.*, **413**, 445-449 (2005).
- 6) R. Sekiya, T. Sato, T. Harada and R. Kuroda, to be submitted.

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Structure-property relationship in the crystals of chiral amino acids and their racemic counterparts

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Understanding structure-property relations in crystalline amino