



**X-ray & Neutron Scattering in Multiferroic and Ferroelectric Materials Research
Workshop III**

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National Physical Laboratory, Teddington, TW11 0LW, UK

Abstracts

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Invited Talks

Magnetically driven dielectric properties of Bi_{0.5}La_{0.5}FeO₃: competition between geometry optimisation and magnetism

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Rare earth doping has been demonstrated as an effective way of mitigating both the thermodynamic metastability and leakage current in the widely studied multiferroic perovskite BiFeO₃. We have investigated the structure-property relations in La- and Nd-doped BiFeO₃ using a combination of temperature dependent powder neutron diffraction and immittance spectroscopy. Specifically, structural variations were studied using a combination of both conventional “bond angle/bond length” and symmetry mode analysis. The latter is particularly useful as it allowed the effects of A-site displacements and octahedral tilts/distortions to be considered separately. The structural variations in these materials occur due to a changing balance between magnetic properties and other bonding contributions. This results in changes in the magnitude of the octahedral tilts and A-site displacements giving rise to phenomena such as negative thermal expansion and invariant lattice parameters i.e., the invar effect. I will specifically discuss the composition Bi_{0.5}La_{0.5}FeO₃ which adopts an orthorhombic GdFeO₃-type structure (space group: *Pnma*) with *G_z*-type antiferromagnetism. The temperature dependent dielectric permittivity is controlled by changes in the FeO₆ octahedral tilt magnitudes, accompanied by a structural distortion of the octahedra with corresponding A-site displacements along the *c*-axis; this behaviour is unusual due to an increasing in-phase tilt mode with increasing temperature. The anomalous orthorhombic distortion is driven by magnetostriction at the onset of antiferromagnetic ordering resulting in an Invar effect along the magnetic *c*-axis and anisotropic displacement of the A-site Bi³⁺ and La³⁺ along the *a*-axis.

"What first principles can do for you and what you can do for first principles"

Claude Ederer

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In this talk I will discuss two recent first principles (density functional theory) studies of multiferroic and ferroelectric materials: i) Can we find a good multiferroic material in the Aurivillius phases? Here, I will present our recent results for the Aurivillius phase material Bi₅FeTi₃O₁₅, compare our calculated properties with available experimental data, and discuss the challenges for designing Aurivillius phases with robust multiferroic properties. ii) Studies of the electrocaloric effect using first principles effective Hamiltonians. In both cases I will highlight in particular the possible interaction between theoretical and experimental studies and how the computational results can point towards new directions for future research.

Imaging ferroelectric control of magnetic domains using Photoemission Electron Microscopy

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Diamond Light Source

PhotoEmission Electron Microscopy (PEEM), combined with polarised soft X-ray spectroscopies such as X-ray Magnetic Circular Dichroism (XMCD) and X-ray Magnetic Linear Dichroism (XMLD), allows high-resolution imaging of ferromagnetic and ferroelectric domains. Here I will present some recent results from $\text{La}_{0.7}\text{Ca}_{0.3}\text{MnO}_3$ (LCMO) and Ni thin films grown on BaTiO_3 (BTO) substrates [1,2]. The LCMO/BTO system exhibits a giant, reversible magnetocaloric effect, not present for the bulk material, whereas the Ni/BTO system allows control of perpendicular magnetism through a strain mediated coupling.

[1] X. Moya *et al.*, *Nat. Mater.* **12**, 52 (2013).

[2] M. Ghidini *et al.*, submitted.

Ferroelectric / Multiferroic Measurements at *XMaS*

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New developments in the study of ferroelectric and multiferroic materials at the *XMaS* beamline in Grenoble will be presented. These include a ferroelectric measurement system which is fully integrated into the beamline diffraction control system, allowing real time data collection to be employed. We will highlight how both the electrical polarization and diffraction can be measured simultaneously.

Our current system will be augmented next year by the addition of an optical interferometer, enhancing the measurement of bulk and atomic displacements in piezoelectric materials. Thus, direct measurements of macroscopic strain, along with electrical polarization and diffraction will become possible. We will discuss some of the more technical details required to perform these measurements, such as sample mounting in complex sample environments. Ways of extending the use of these resources available at *XMaS* to the wider UK community through the use of a suite of offline instrumentation will be explored. Preliminary facilities will include a lab x-ray source compatible with the wide range of sample environments already developed on the beamline as well as stand-alone electrical measurements, such as PE loops and resistivity as a function of applied fields.

Direct view of spin dynamics in a large magnitude coherent electromagnon

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Multiferroics—materials with more than one type of ferroic ordering—have attracted strong interest for potential applications where electric fields control magnetic order. The ultimate speed of control via magnetoelectric coupling, however, remains largely unexplored. Here we report on an experiment in which we resonantly excite an electromagnon in multiferroic TbMnO_3 with an intense few-cycle terahertz (THz) pulse and observe the resulting coherent spin motion using time-resolved resonant soft x-ray diffraction. Our results show that it is possible to manipulate directly atomic-scale magnetic structures using the electric field of light on a sub-picosecond timescale.

Generating direct magnetoelectric behavior in EuTiO₃.

Philip Ryan,

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The phenomenon of magnetoelectric (ME) coupling, an interaction between magnetic and electric polarization, has the potential to allow control of the magnetic state of a material with an electric field (and vice-versa). This has enticing prospects for device engineering and could lead to multistate logic, new memory or advanced sensor technologies.

In this presentation I will review our ongoing project trying to untangle ME behavior in single phase systems and in the process demonstrate a ‘giant’ ME cross-field control capability in the rare earth perovskite, EuTiO₃ (1). In bulk form, this rare earth titanate material is both antiferromagnetic and paraelectric. However, both anti- and ferro-magnetic interactions are present between different nearest europium neighbors. By growing the titanate film upon a select substrate, we proposed that the induced structural distortion of the unit cell would result in a rebalancing of strengths between the competing magnetic interactions. The effect produced a precariously unstable magnetic environment. While still antiferromagnetic, any further distortion would collapse this magnetic order and allow for the emergence of ferromagnetism. By applying an electric field to the paraelectric material one could readily displace the central titanium atom by the tiniest fraction, unsettling the ground state leading to an altered magnetic structure. The moderate and easily achievable strain condition, the fact that ‘difficult to come by’ multiferroicity was not required, and the simplicity of the phenomenon itself, present a clear breakthrough in this field that may lead to new electronic functionality.

In addition, we have studied the pure single crystal form of the same system, EuTiO₃ (2). This material has one of the largest known Seebeck coefficients, and has an anomalously large magneto-dielectric response. We focused on understanding the potential structural instabilities in coupled electric and magnetic field environments, the response to which were thought to underlie several of the interesting macroscopic characteristics. This work led to the discovery of an unusual but naturally occurring superstructure comprised of two competing instabilities which do not typically coexist but in this system due to the precarious balance of degenerate states have found a way to cohabit. This finding generated a new understanding of how this material or similar systems could generate ‘giant’ ME phenomena circumventing the requirement of large permeability and permittivity to generate a strong linear ME effect.

1) P. J. Ryan, J. -W. Kim, T. Birol, P. Thompson, J. -H. Lee, X. Ke, P. S. Normile, E. Karapetrova, P. Schiffer, S. D. Brown, C. J. Fennie, D. G. Schlom, “Reversible Control of Magnetic Interactions by Electric Field in a Single Phase Material”, *Nat. Commun.*, 4, 1334, (2013)

2) Jong-Woo Kim, Paul Thompson, Simon Brown, Peter S. Normile, John A. Schlueter, Andrey Shkabko, Anke Weidenkaff, and Philip J. Ryan, “Emergent Superstructural Dynamic Order due to Competing Antiferroelectric and Antiferrodistortive Instabilities in Bulk EuTiO₃” *Phys. Rev. Lett.*, 110, 027201, (2013).

Neutron scattering experiments on multiferroics at PSI: focus on thin films and skyrmion lattices

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I will present neutron scattering results obtained on two different magnetically-driven multiferroic systems. I will firstly discuss work done on multiferroic LuMnO_3 thin films grown on YAlO_3 substrates [1]. Unlike bulk LuMnO_3 which is a commensurate antiferromagnet, the films display drastically different properties and are simultaneously incommensurately antiferromagnetic *and* ferromagnetic at low temperature. Unraveling the details behind this rich behavior required input from numerous techniques, including pivotal polarized neutron reflectometry experiments from which we could spatially resolve the distribution of the ferromagnetism magnetization in the film. The key result is that ferromagnetism is most pronounced close to the film-substrate interface which is *strained* due to the lattice mismatch. This ties the origin of the ferromagnetism to the film strain, though open questions remain concerning how this is achieved at the microscopic level. We could further show the ferromagnetism and antiferromagnetism in the film to be directly coupled, and so demonstrate the promising functional properties of these films.

Secondly I will turn the attention to our study of the topologically protected magnetic spin vortices, or skyrmions, in the chiral-lattice compound Cu_2OSeO_3 . Until 2012, skyrmions had been observed only in conducting B20 compounds where it is known that they can be manipulated by conduction electrons. The discovery of a skyrmion lattice (SkL) phase in *insulating* Cu_2OSeO_3 caused great excitement since the material is a well-known magnetoelectric, and the important open question was to learn if the SkL could be manipulated by electric fields. Our small-angle neutron scattering experiments demonstrate successfully the manipulation of skyrmions by applied electric fields in Cu_2OSeO_3 [2]. For our chosen experimental geometry, we discover that the effect of applying an electric field is to controllably rotate the reciprocal SkL around the magnetic field axis in a manner dependent on both the size and sign of the electric field. These results provide the first evidence for a new manifestation of the electric field control of topologically-protected magnetism in magnetoelectrics, and further show the electric field to be a new experimental parameter for studying the basic physics of skyrmions inside chiral-cubic lattices.

[1] J.S. White *et al.*, Phys. Rev. Lett. **111**, 037201 (2013)

[2] J.S. White *et al.*, J. Phys.: Condens. Matter **24**, 432201 (2012)

Posters

Observation of the *piezomagnetolectric* effect in $0.7\text{BiFeO}_3 - 0.3\text{PbTiO}_3$ employing neutron diffraction.

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Magnetolectric (ME) materials offer a tremendous technological advantage by coupling electric and magnetic polarisations, manipulated by magnetic or electric fields respectively. This phenomena enables future technologies including advanced electronic memory, combining electronic speed and efficiency with magnetic robustness.

Low cost polycrystalline ME materials however are limited and excluded from most commercial applications, as they only exhibit this phenomena at cryogenic temperatures, require impractically large operating electric/magnetic fields, or exhibit low ME coefficients (1-100 mV/cm.Oe). Efforts to maximise ME device outputs have resulted in the engineering of thin film and composite structures, coupling room temperature piezoelectric and magnetostrictive particulates or laminates by interfacial strain to achieve usable ME coefficients in the order 10^3 mV/cm.Oe. Despite these systems, the technological potential of single compound ME coupling has continued to drive research in to multiferroic materials over the last two decades.

Here we show that through atomic strain engineering within the polycrystalline, room temperature multiferroic $0.7\text{BiFeO}_3 - 0.3\text{PbTiO}_3$ compound, we can exhibit a reversible, piezoelectric strain controlled ME effect. Employing a novel neutron diffraction experiment on the Polaris beamline at ISIS, we have demonstrated that this *piezomagnetolectric* effect manifests with applied electric field at the onset of piezoelectric strain, engineered in to the compound through crystallographic phase mixing. This produces a remarkable intrinsic ME coefficient = 1276 mV/cm.Oe in the single compound, comparable to commercial composite structures.

Our work reveals how piezoelectric strain can provide the link between the ferroelectric and antiferromagnetic orders on an atomic scale, and a mechanism in which it can be manipulated. We anticipate this work to encourage further investigations in to strain engineered nano-structures to realise low-cost ME devices designed from the atoms up, as well as contribute to the deeper understanding of the complex single phase ME coupling mechanisms involved.

Dysprosium Doped Bismuth Ferrite Ceramics

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The drive to find novel materials for applications such as data storage, spintronics, and microelectronics has led to resurgence in research into multiferroic materials. To date the most widely studied multiferroic is BiFeO_3 primarily due to its room temperature (anti)ferromagnetic ($T_N \sim 360$ °C) and ferroelectric ($T_C \sim 825$ °C) ordering. More recently researchers have looked to improve the ceramic properties of BiFeO_3 by incorporating cations onto either the A and/or B sites of the perovskite. Furthermore, doping BiFeO_3 with Dy_{3+} has been suggested to lead to an effective suppression of the magnetic spiral spin structure making them more attractive for application. Previous studies suggest that with increasing Dy content a transition from rhombohedral to orthorhombic symmetry occurs. However, there is some debate within the literature as to compositional limits and the nature of this orthorhombic phase (i.e. polar vs. non-polar). Furthermore, much of the previous work has centered on PXRD studies with little complimentary magnetic or electrical measurements performed.

Our research has centered on understanding the structure-property correlations in $\text{Bi}_{1-x}\text{Dy}_x\text{FeO}_3$ ($0 \leq x \leq 0.5$) materials. Our results indicate a compositional driven phase transition between $x = 0.06$ (polar) and $x = 0.30$ (non-polar). Furthermore, whilst $\text{Bi}_{0.94}\text{Dy}_{0.06}\text{FeO}_3$ exhibits a complex high temperature (paraelectric – ferroelectric) structural phase transition which is heavily correlated to the magnetic behavior, $\text{Bi}_{0.70}\text{Dy}_{0.30}\text{FeO}_3$ exhibits low temperature relaxor-like character. Interestingly, magnetic measurements suggest both phases exhibit similar magnetic states. In this paper we will present a full powder neutron diffraction study elucidating the structure-property correlations in these materials.

Ab Initio Random Structure technique (AIRSS) for phase predictions of perovskites.

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AIRSS is a powerful technique that allows prediction of new phases at high pressure and ambient conditions for various systems. In this work we applied AIRSS to predict sequence of phase transitions in BaTiO₃, PbTiO₃, PbZrO₃. The technique successfully describes R-O-T-C sequence for BaTiO₃; T-C sequence for PbTiO₃. We also found that PbZrO₃ exhibits a complex sequence of phase transitions. Finally, we applied AIRSS to characterise structure of Pb(Zr_{50%}Ti_{50%})O₃ (PZT). Using statistical approach we modelled structural variations of PZT that related to the mutual order of Zr and Ti cations and showed that the symmetry of statistically averaged phase is directly compared to experimental findings.

Optical properties of Pb(ZrTi)O₃.

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We use *ab initio* calculations to characterise optical properties of Pb(Zr_{50%}Ti_{50%})O₃ (PZT). We used statistical approach to describe structural variations of PZT related to mutual ordering of B-cations. We have found that the nature of the bottom of the conduction band strongly depends on the character of Zr- and Ti-cations ordering. The latter leads to variations of the edge of absorption band.

Discharge Measurement of High Temperature Capacitors

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There has been rapid progress in recent years in the development of high temperature power electronics driven by a wide range of applications such as low carbon vehicles and energy management from renewable sources. These systems need passive components that can operate under the same high temperature conditions. Capacitors are a key component in systems such as DC-DC converters and power controllers, and represent a significant portion of the cost and weight of a power conversion system. Capacitors present a particular difficulty in this respect because conventional ceramic and electrolytic devices have poor temperature stability and/or low maximum operating temperatures and often need to be cooled. This poster presents a new measurement system to measure discharge current in capacitors up to 200 °C. Results are presented on the energy and power density and temperature stability for a new class of high operating temperature dielectric material (HITECA).

Synthesis and study of the magnetoelectric ($\text{Ga}_{2-x}\text{Fe}_x\text{O}_3$)-class of materials

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An interesting sub-class of the multiferroic materials are the multiferroic magnetoelectrics, in which a coupling between the two ferroic order parameters (magnetic and electric) exists, of which the ($\text{Ga}_{2-x}\text{Fe}_x\text{O}_3$)-class of materials is a good example. These compounds are now well-known for their high transition temperature as well as for the potential interaction between their ferrimagnetic and piezoelectric properties. In addition, their crystallographic and magnetic structure are quite complicated, due to the existence of internal site disorder.

In order to study the physical properties of these compounds, single crystals of $\text{Ga}_{2-x}\text{Fe}_x\text{O}_3$ ($x=0.90, 1.00$ and 1.10) have been synthesized by the floating zone method in an infrared image furnace, using different growth conditions. $\text{Ga}_{2-x}\text{Fe}_x\text{O}_3$ samples crystallize in the $\text{Pc}2_1n$ space group as determined from Rietveld refinement of the X-ray and neutron diffraction patterns (powder and single crystals). The cell parameters and the Néel temperature (T_N) of the $\text{Ga}_{2-x}\text{Fe}_x\text{O}_3$ single crystals varies linearly with the iron content (x). The occupation factors were calculated by refinement and the results showed a disordered structure (25% of the iron is found on the native gallium sites). The magnetic excitations spectra measured for the $\text{Ga}_{2-x}\text{Fe}_x\text{O}_3$ single crystals by inelastic neutron scattering revealed a coexistence of a ferrimagnetic ordering and a diffuse scattering signal below the Néel temperature. The diffuse signal suggests the existence of a spin glass like component due to the internal site disorder. Dielectric investigations showed no temperature dependent anomaly of the dielectric constant for the GaFeO_3 single crystal, suggesting a lack of a magnetoelectric coupling in this system.

The evidence for glassy behavior in the $\text{Ga}_{2-x}\text{Fe}_x\text{O}_3$ system highlights the importance of site disorder in determining the ground state magnetic properties [1].

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Electric energy storage properties of BiFeO_3 -based thin films

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In the quest for alternative technologies to store and convert energy, ferroelectrics have drawn considerable interest as these are characterized by high power density and fast charge/discharge time. Ferroelectrics are currently widely used to provide a cost-effective, temperature and vibration stable solutions for general electronic applications. We report investigations carried out in a new composition $0.4\text{BiFeO}_3\text{-}0.6\text{SrTiO}_3$, where a high energy density 18.6 J/cm^3 at 972 kV/cm was measured at room temperature and an impressive thermal stability (temperature coefficient of capacitance below 11%) of the dielectric response at least up to $200 \text{ }^\circ\text{C}$ was observed.

High Pressure Neutron Diffraction Experiment On Triangular Lattice Antiferromagnet Using Hybrid Anvil Cell

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Since the introduction of sapphire anvils pressure cells to neutron diffraction, measurements above 3 GPa and at low temperature have been possible.[1] Osakabe has been developing a *hybrid-anvil-type* pressure cell with combination of two different anvils, WC and SiC for JRR3 in Tokai.(Fig. 1)[2] This cell is able to apply pressure up to 10 GPa, and combination with low temperature and magnetic fields are possible.

In order to obtain higher statistic magnetic diffraction data and make use of the wide angle coverage on time of flight neutron instruments, which allows multiple Bragg peaks to be collected simultaneously, we are developing the cell on WISH in ISIS.

Recently, we have succeeded in measuring several magnetic reflections of multiferroic CuFeO₂ under pressure. The incommensurate and commensurate phase transition, occurring at 11 K at ambient pressure, is clearly shifted to 9 K under 1.4 GPa.(Fig.2) Statistics of these data on WISH were much better than in the previous experiment.[3]

In this presentation, we would like to introduce utilization of the hybrid-anvil-cell for neutron diffraction measurements under high pressure, low temperature and magnetic field conditions.

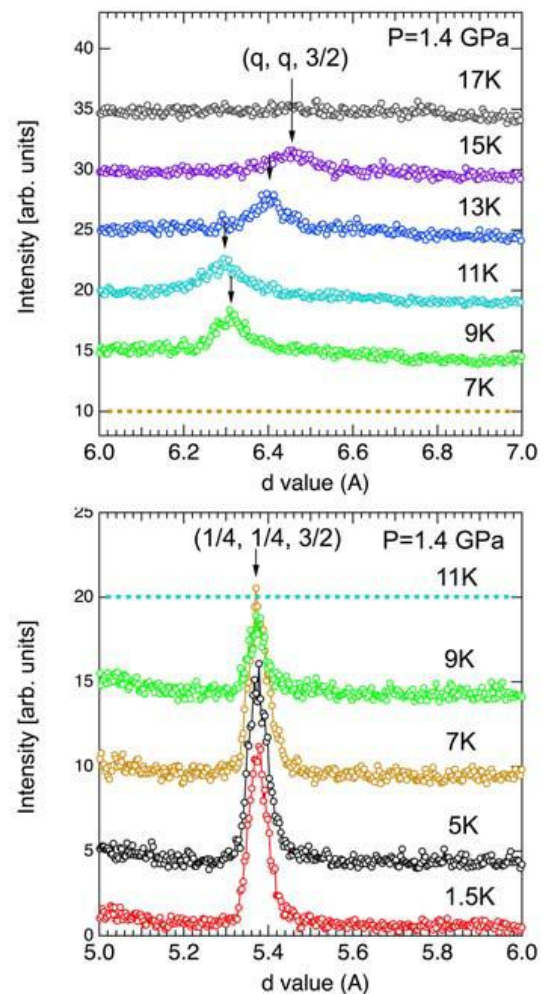
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Fig. 1 Photograph hybrid-anvil-type high pressure cell.[2]

Fig. 2 Temperature dependence of the magnetic diffraction profiles of CuFeO₂ in 1.4 GPa, measured with WISH.



RXD experiment on Ba₂CuGe₂O₇

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Materials which, at a certain temperature, show a spontaneous polarization are called ferroics. If such a material, at a given temperature, shows more than one order is probed to be multiferroic (MF). MFs compound have been studied since the sixties and in the last decade they returned to be matter of studies due to the magnetoelectric (ME) effect shown by a subset of the MFs called improper-MFs. Fundamental research is still in progress, as ME materials show electronic mechanisms which still wait to be explained [1]. Besides, the properties of these multifunctional compounds raise our imagination to new application, such as in memories technologies and low consumption devices. The key factor of these compounds is the cross-interaction between electric and magnetic phenomena, as for example the possibility of controlling the magnetic hysteresis cycle via an external electric field. Besides to the perovskite related transition metal oxides, which lead the field, new compounds revealed ME properties. Among these, the Ba₂CuGe₂O₇ non-centrosymmetric, non-polar, tetragonal crystal (space group: P-4₂m) [2] (Fig. 1a), has been matter of our studies. Any attempt of understanding the ME phenomena should start from the comprehension of the microscopic electronic structure, and resonant X-rays diffraction (RXD) is suitable for this purpose. On resonance we can focus the attention on a particular electronic shell. The atomic scattering factor shows its tensorial nature allowing the appearance of forbidden reflection in non-symmorphic space groups (as in our case) [3]. Therefore the technique has a high sensitivity to the symmetry of the shell investigated and can easily show any local distortion. In suitable conditions, focusing our attention on the outer electronic shell, we can determinate the magnetic properties of the compound [4]. It is therefore possible to study the interplay between the magnetic structure and the ferroelectric properties. For these reason, we performed a RXD experiment at Diamond Light Source (I16 beamline) and we present results obtained by fixed-Q energy scans (Fig. 1b) on forbidden reflections.

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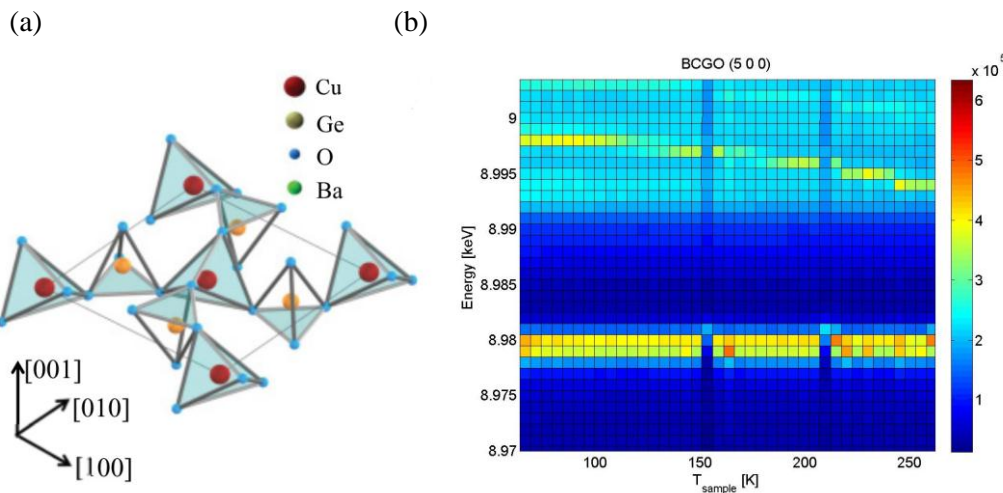


Fig.1
(a) Three-dimensional view of the crystal structure of Ba₂CuGe₂O₇

(b) Map of emission intensity as function of temperature and energy of the incident beam. $y = 0^\circ$ with respect to (010). At 8.98 keV is clearly visible the Cu pre-edge diffracted intensity.

National Physical Laboratory Strategy for Large Scale Facilities

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NPL is designing and building, in collaboration with x-ray and neutron large scale facilities around the world, new metrology systems to enable scientists from academia and industry to investigate and understand the coupling phenomena in ferroelectric and magnetoelectric materials. These include beamline devices and measurements kits, often associated with the development of advanced synchronisation and data reduction/analysis to enable complex experiments. Of particular interest are the cases where different techniques are combined in a single in-situ experiment to perform real-time measurements and monitor at the same time multiple correlated parameters. New physics can therefore be investigated and both static and dynamic properties of functional materials can be tracked as function of various external stimuli (H, T, E, ...).

National Physical Laboratory and ISIS Neutron Facility strategic collaboration

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ISIS neutron Facility and the National Physical Laboratory are joining together to form a strategic collaboration which will bring benefits to the UK. From this joint effort, both ISIS and NPL will be able, through scientific and technical collaboration, to produce scientific excellence by both sharing instrumentation and expertise in many science areas. In this partnership, whenever necessary, NPL and ISIS will work together in technical development of unique capabilities, effectively expanding the existing sample environment options benefitting both academic and industrial users. This collaboration will widen the use of ISIS by industry and grant NPL beamtime access to perform both frontier and applied research on world class neutron instruments, effectively bringing economic benefit to the United Kingdom.