A1

My Neutron Scattering Journey to Quantum Magnetic Materials in Japan

Hung-Cheng Wu[1,2*], Kazuhiro Nawa[2], Daisuke Okuyama[2],
Katsuki Kinjo[2], Taku J. Sato[2]

[1] *Department of Physics, National Sun Yat-sen University, Kaohsiung, 80424 Taiwan*

[2] *Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, Sendai 980-8577, Japan*

E-mail: tedwu@mail.nsysu.edu.tw

Abstract

Quantum magnetic materials [1-3] have attracted significant attention in both fundamental physics and applied science due to their peculiar physical properties. Understanding the microscopic magnetic structure in these materials remains a crucial challenge in current condensed matter physics and material science research. Among the available analytical techniques, neutron scattering stands out as the only method capable of directly probing magnetic properties, particularly magnetic structures. It allows for the precise determination of magnetic structure, providing key insights into the nature of quantum magnetic materials. Analyzing magnetic structures is a key step in understanding the physical properties of quantum magnetic materials, such as magnetic symmetry analysis, which enables the prediction of phenomena like the magnetoelectric or piezomagnetic [1] responses. This analysis helps us uncover fundamental physical characteristics and provides valuable guidance in designing novel materials and advancing the development of spintronics. During my 3.5-year stay in Japan, I performed various neutron scattering experiments at the Japan Research Reactor-3 (JRR-3) [2-4] and the Japan Proton Accelerator Research Complex (JPARC) [1] on selected quantum magnetic materials, with a particular focus on simple spin-1/2 systems involving Cu^{2+}, Ce^{3+}, and Yb^{3+} ions. Additionally, I served as an adjunct beamline scientist at the General-Purpose Triple-Axis Spectrometer located at JRR-3 [4] for over three years. In my talk, I will share my experiences and insights gained from neutron scattering research in Japan.

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A2

Crystal Structure Determination from Powder X-ray Diffraction Data on the Spin Transition Compounds

I-Jui Hsu *

Department of Molecular Science and Engineering, National Taipei University of Technology, Taipei 10608, Taiwan

*Email: ijuihsu@mail.ntut.edu.tw

Abstract

Structure determination is one of the most important techniques to discover new materials and new science in many scientific fields and even in industry. Traditionally, unknown crystal structure determination relies mainly on the single crystal x-ray diffraction data; however, if no good quality of single crystal can be obtained or if the crystal crashed during phase transition, the structure cannot be determined. Nowadays, with the benefit of high brilliance synchrotron light sources, unknown crystal structure determination from powder x-ray diffraction data (SDPD) can be performed in high resolution powder x-ray diffraction (PXRD) beamline at NSRRC. In this talk, a spin crossover complex of $\{[Fe(II)(2BTP)_2(bpy)](ClO_4)_2\}_n$ (**1**) (2BTP= 2-(2-benzyl-2H-tetrazol-5-yl) pyridine, bpy= 4,4'-bipyridine) was synthesized and its structure was determined from PXRD through standard procedure which the cell constants and space group are determined by indexing PXRD pattern and checking systematic absence, respectively. Then, the phase problem is solved either by direct method in reciprocal space or by global optimization with simulated annealing algorithm in real space. Finally, the structure is completed by Rietveld refinement.[1] The results indicate that Fe site consists of two bidentate 2BTP ligands at the equatorial position and a bpy ligand at axial position in a pseudo-octahedral $\{FeN_6\}$ core. The bpy is a bridging ligand further to connect two Fe(II) to form one-dimensional coordination polymer (1D-CP). The average bond distances of Fe-N at low spin (LS; t_{2g}^6) and high spin (HS; $t_{2g}^4e_g^2$) states are 2.04(1) Å and 2.20(1) Å, respectively. Incorporating ethanol molecules into **1** makes a $\{[Fe(II)(2BTP)_2(bpy)](ClO_4)_2{\cdot}C_2H_5OH\}_n$ (**2**) single crystal with 1D-CP structure. A replacement of bpy by 1,2-bis(4-pyridyl)ethane (bpea) produced $\{[Fe(II)(2BTP)_2(bpea)](ClO_4)_2\}_n$ (**3**) still keeping 1D-CP structure. The magnetic measurements showed that the spin transition temperatures $T_{1/2}$ of **1** and **3** are 350K and 320K, respectively, but **2** exhibits hysteresis loop 40K ($T_{1/2}\uparrow$=350K, $T_{1/2}\downarrow$=310K). How the molecular interactions affect the transition temperature will be discussed through the VT-PXRD, VT-XAS and differential scanning calorimetry (DSC) results.

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A3

Comprehensive structural insights from dual-space synchrotron high-resolution powder diffraction and pair distribution function analysis

Yu-Chun Chuang *, Bo-Hao Chen, Chung-Kai Chang, Yen-Chung Lai, Xu-Feng Luo, Po-Ya Chang

Materials Science Group, Scientific Research Division, Hsinchu, Taiwan

*Email: chuang.yc@nsrrc.org.tw

Abstract

Advancements in crystallography have been greatly enhanced by the dedicated high-resolution X-ray powder diffraction beamline TPS 19A and the general-resolution 2D X-ray diffraction beamline TPS 20A. These state-of-the-art facilities are tailored to support a broad range of crystallographic applications, including structure determination, precise structure refinement, cell parameter analysis, estimation of crystalline size, characterization of crystal morphology, and the investigation of stacking faults.

The integration of dual-space resolution techniques, which combine X-ray diffraction (XRD) and pair distribution function (PDF) analysis, represents a significant leap forward in structural characterization. XRD excels in elucidating the long-range crystalline order, while PDF analysis provides critical insights into both short-range and long-range structural arrangements in disordered or amorphous materials. This complementary approach bridges the gap between real-space and reciprocal-space data, offering unparalleled structural insights.

At the TPS 19A beamline, high-energy X-rays (~30 keV) and the cutting-edge MYTHEN 18K large-angle one-dimensional detector facilitate total scattering measurements with a maximum Q value,Q_{max}, of 27.5 $Å^{-1}$. This setup ensures the simultaneous acquisition of high-Q and high-delta-Q resolution data, enabling comprehensive structural analysis in dual spaces.

By leveraging these advancements, our approach emphasizes the integration of XRD and PDF analysis as a powerful framework for unraveling the structural complexities of materials. Whether crystalline, amorphous, or exhibiting mixed-order characteristics, this method provides a holistic perspective on material architecture. The development of such dual-space techniques paves the way for transformative applications across various scientific fields, demonstrating the versatility and depth of modern synchrotron-based crystallography.

A4

Quantifying Structure Dynamics and Distortions Symmetry-Adapted Analysis and HRPD

Wei-Tin Chen[1,2,3] *

[1] *Center for Condensed Matter Sciences (CCMS), National Taiwan University, Taipei, Taiwan*
[2] *Center of Atomic Initiative for New Materials (AI-Mat), National Taiwan University, Taipei, Taiwan*
[3] *Taiwan Consortium of Emergent Crystalline Materials (TCECM), National Science and Technology Council, Taipei, Taiwan*

*Email: weitinchen@ntu.edu.tw

Abstract

The exploration of novel emergent materials and quantum matters with intriguing physical phenomena and functionalities is essential in modern condensed matter sciences. In order to unraveling the mechanisms of the exotic physical phenomena, it is fundamental to examine the crystal structures and their evolution to obtain critical insights into the intertwined relationship between lattice, charge, orbital, spin degrees of freedom and the material properties. Diffraction is a crucial and indispensable tool for structure analysis of solid state materials. With utilising x-ray and neutron diffraction techniques and extracted structural information, one can derive detailed insights of materials such as charge distribution, orbital ordering, or spin arrangement.

Benefit from ultrahigh angular resolution provided by High Resolution Powder Diffraction (HRPXRD) beamline 19A at Taiwan Photon Source (TPS), subtle structural distortion and weak superlattice reflections in temperature-induced phase transition can be detected. Built on group theory principles, symmetry analysis tools such as ISODISTORT [1] and AMPLIMODES [2] are developed recently. The observed structural changes are connected with their underlying symmetry breaking, using a systematic approach to explore structural instabilities in crystalline materials by analyzing symmetry-adapted modes. The symmetry modes such as rotation, tilting, displacive distortion can be deconvoluted and quantified, and the evolution of these amplitudes can be determined and correlate to the exotic physical phenomena.

For instance, colossal magnetoresistance (CMR) was demonstrated in the archetypal manganite perovskites. To further examine the CMR effect, we have designed the (Na/Ca/La)Mn_7O_{12} quadruple perovskite solid solution with high pressure high temperature techniques. [3] Detailed crystallography works were performed with high resolution synchrotron x-ray and neutron diffraction, and the symmetry-adapted structural analysis was conducted with ISODISTORT and TOPAS program [4]. Examples of quantifying structure dynamics and distortions utilising the symmetry-motivated approach will be presented.

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B1

Exploring the electronic ordering of quantum materials using resonant x-ray scattering

Chao-Hung Du *

Department of Physics, Tamkang University, Tamsui 25137, Taiwan

*Email: chd@gms.tku.edu.tw

Abstract

Quantum materials have attracted lots of attention in condensed matter physics because of their exotic physical properties, such as topological insulators/superconductors, geometrical spin/charge frustrations, or Dirac and Weyl semimetals. It has been demonstrated that the different coupling strengths of electronic ordering with spins, orbital, and lattice are responsible for the occurrence of such exotic physical properties. Among the probes for studying these electronic ordered structures, x-ray scattering has the merits of high-spatial resolution, element selectivity, and distinguishable polarization over others. Using resonant x-ray scattering, including both hard and soft x-rays on the newly completed facilities on TPS 09A and 41A, we are able to study the modulations caused by the charge and spin ordering in some quantum materials, such as YBaCuFeO5, $TmMn_6Sn_6$ and Ir_2In_8Se, and demonstrate that the multiple magnetic sublattices can be studied in detail.

B2

High-resolution X-ray scattering for probing the static and dynamic structure of matter

Shih-Chang Weng *

National Synchrotron Radiation Research Center, Hsinchu city, Taiwan

*Email: weng.sc@nsrrc.org.tw

Abstract

High-resolution X-ray scattering is a versatile and non-destructive technique for probing the static and dynamic structures of materials at the atomic scale. Leveraging third-generation synchrotron radiation with advanced insertion devices, TPS 09A provides an exceptionally intense, collimated, and tunable X-ray source, far surpassing the capabilities of conventional X-ray systems.

This presentation highlights recent research conducted at TPS 09A, including studies on the grazing-incidence X-ray diffraction (GIXRD) of ultra-thin and monolayer films; X-ray scattering investigations of phase transitions and critical phenomena; resonant X-ray scattering with polarization analysis; and time-resolved X-ray diffraction (TR-XRD) employing laser-pump and X-ray-probe techniques. These advancements underscore the transformative potential of high-resolution X-ray scattering in material science and physics.

B3

Novel optical phenomena of GIXBD and its applications

Mau-Tsu Tang[1,*], Yun-Liang Soo[2], Bi-Hsuan Lin,[1] Tzu-Hung Chunag[1], Shih-Chang Weng[1], Yi-Wei Tsai[1] , Yang Song[1] and Shih-Lun Chen[1]

1 National Synchrotron Radiation Research Center, Hsinchu, 30076, Taiwan
2 Department of Physics, National Tsing Hua University, Hsinchu, 30013, Taiwan

*Email: mautsu@nsrrc.org.tw

Abstract

The Temporally Coherent X-ray Scattering Beamline at 09A Taiwan Photon Source (TPS) is equipped with world-leading ultrahigh energy resolution experimental setups, which have significantly advanced X-ray optics studies in severe energetic demanding environments [1]. At TPS 09A, we have recently observed a novel diffraction phenomenon, Grazing-Incidence X-ray Back Diffraction (GIXBD), where the incident angle nears the critical angle and the miscut angle approaches 90°. Inherited from the diffraction geometry of grazing-incidence, GIXBD excites the dynamical X-ray eigenmodes near the crystal surface, resulting in distinct diffraction patterns different from normal counter ones [2,3]. Specifically, as the miscut angle approaches 90°, significant optical dispersion is boosted to a level similar to that in the visible light region. We have successfully obtained an unprecedented angular dispersion rate (ADR) of 44.4 ± 9.3 μrad/meV, five times higher than ever reported before, from GIXBD on a highly miscut angle of 89.926° of the Si (12 4 0) crystal surface [4]. Our previous publication has already predicted the experimental results by both fully dynamical calculations as well as the kinematical Snell's law [5]. The results suggest the potential for fabricating sub-100 μeV X-ray optical devices using modern lithography techniques. The atomic surface depth of the excited X-ray modes indicates a promising experimental system for studying the direct interaction of surface X-ray waves with low-dimensional materials.

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