New insight onto the metal to insulator transition in Ca2RuO4

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Presentation type: Oral **Presentation time:** 11:45-12:00

Heavy transition metal oxides are model systems for investigating emergent electronic phases generated by the strong coupling between electron correlations, spin–orbit interaction, and lattice distortions. This interplay can produce unconventional Mott physics, spin and orbital ordering, and unusual collective excitations, while offering several routes to tune the electronic ground state. Ca RuO (CRO) is a compelling example, as its electronic properties are intimately linked to its crystal structure. At T=357 K, CRO undergoes an insulator-to-metal transition [1] accompanied by a structural transformation from an orthorhombic insulating phase to a tetragonal metallic phase. This transition can also be induced by pressure or doping [2], electric gating or applied electric current [3].

Conventional x-ray diffraction measurements on bulk crystals provide valuable information on the average structural changes associated with the transition. However, this approach is intrinsically limited in systems where multiple structural phases may coexist, as averaged diffraction signals can obscure the microscopic picture. This limitation is particularly relevant for CRO, where current-driven experiments indicate metastable regimes and phase coexistence over a wide range of applied currents [3].

Here, we use scanning x-ray diffraction microscopy with sub-micron beams [4] to investigate the current- and temperature-induced structural evolution of thin CRO flakes. This scanning approach provides both local structural details and global sample-scale trends, while thin-flake measurements aim to access the intrinsic material response away from bulk complexity, where large volumes, strain fields, defects, and percolative pathways may mask the fundamental behaviour under external fields.

By mapping diffraction signals as a function of applied current or temperature, we attain the visualisation of distinct domains characterized by different c-axis lattice parameters and their distribution within the samples. We observe that the current-driven transition proceeds through a highly inhomogeneous mechanism, with structurally inequivalent regions nucleating, expanding, coexisting, and partially reversing upon current cycling. In contrast, temperature-induced switching shows a more uniform structural evolution, demonstrating unequivocally that that different physical mechanisms drive the transition. These results cast a new light on the phase transition of CRO.

References

[1] M. Braden et al. (1998). Crystal and magnetic structure of Ca2RuO4.... Phys. Rev. B,58(847)
[2] J. Zhanget al. (2019). Nano-Resolved Current-Induced Insulator-Metal Transition. Phys. Rev. X9(0110302); Bertinshaw, J. et al., (2019). Unique Crystal Structure of Ca2RuO4. Phys. Rev. Lett.123(137204)
[3] C. Cirillo et al. (2019). Emergence of a metallic metastable phase .... Phys. Rev. B100(235142)
[4] D. Carbone and O. Bikondoa, (2023). Focused and coherent X-ray beams ....Nuclear Inst. and Methods in Physics Research, B539 (127)