Twistronics and Novel Functional Interfaces in Ferroelectrics

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Summary: This PhD project seeks to explore the manner in which twisting the lattices of two lithium niobate (LNO) ferroelectric crystals, across a bonded interface, affects the structural and functional characteristics of the interface. LNO is extremely insulating in bulk. However, we already know that interfaces at which the polarisation orientation reverses in single crystals of LNO can be strongly electrically conducting [1]. Now, in QUB, we have been the first to show that head-to-head polarisation reversal can be created at manually bonded interfaces between two single crystal wafers and these interfaces are conducting in the untwisted case. In conventional 2D materials, twisting can change conductors into profound super insulators, or equally robust 2D superconductors. We therefore seek to build on our success in making bonded "charged" interfaces, twist them and explore the consequences.

Background and Context: Remarkably, when brought into contact, two insulating dielectrics can sometimes generate an interface which is semiconducting, metallic or even superconducting [1-3]. This kind of "emergent" interfacial transport physics is usually most apparent when there is a discontinuity in the electrical polarisation associated with the abutting dielectrics [2]. It is therefore no surprise that materials in which polarisation naturally develops (such as ferroelectrics) are of very great interest in the generation and study of the physics of emergent interfacial conductivity [1]. Ferroelectric interfaces form spontaneously in the form of domain walls, or can be created through conventional growth of thin film stacks. In both these cases, there is strict crystallographic matching across the interface.

Currently, an exciting variation of emergent interfacial physics is being seen in hand-made multi-layered structures involving 2D sheet materials such as graphene. Researchers have noticed that the transport properties of the interfaces created in the multilayer stacks become even more exotic whenever there is a slight twist in the orientation of the layers, to produce Moire superperiodicities [4]. The electronics of such twisted stacks has been termed "twistronics" and is a white-hot area of research at the moment.

This Project: We will create twisted interfaces with polarisation discontinuities in ferroelectrics by thermomechanically bonding two wafers of lithium niobate together with different twist angles (initial work already done to insure viability – figure 1 below). We will then probe the nature of the interfaces created, in terms of polarisation microstructure, crystal orientations, local interfacial fields and emergent functionality. This would be one of the first studies of its kind and would combine the rich physics seen in two slightly separate branches of solid-state materials research: the first being the emergent interface physics associated with ferroelectric domain walls or interfaces with polar discontinuities and the second being 2D multilayer "twistronics". The project will be supported the recently awarded EPSRC £6M CAMIE Programme Grant, which has distinct workpackages on Moire physics at interfaces.

References:

[1] C. J. McCluskey *et al.* "Ultrahigh Carrier Mobilities in Ferroelectric Domain Wall Corbino Cones at Room Temperature" Adv. Mater. **34** 2204298 (2022)

[2] Z. Chen *et al.* "Two-Dimensional Superconductivity at the $LaAlO_3/KTaO_3$ (110) Heterointerface". Phys. Rev. Lett. **126** 026802 (2021)

[3] A. Ohtomo and H. Y. Hwang “A high mobility electron gas at the $LaAlO_3/SrTiO_3$ heterointerface”, Nature **427** 423 (2004)

[4] P. He *et al.* “Graphene moiré superlattices with giant quantum nonlinearity of chiral Bloch electrons” Nat. Nano. **17** 378 (2022)

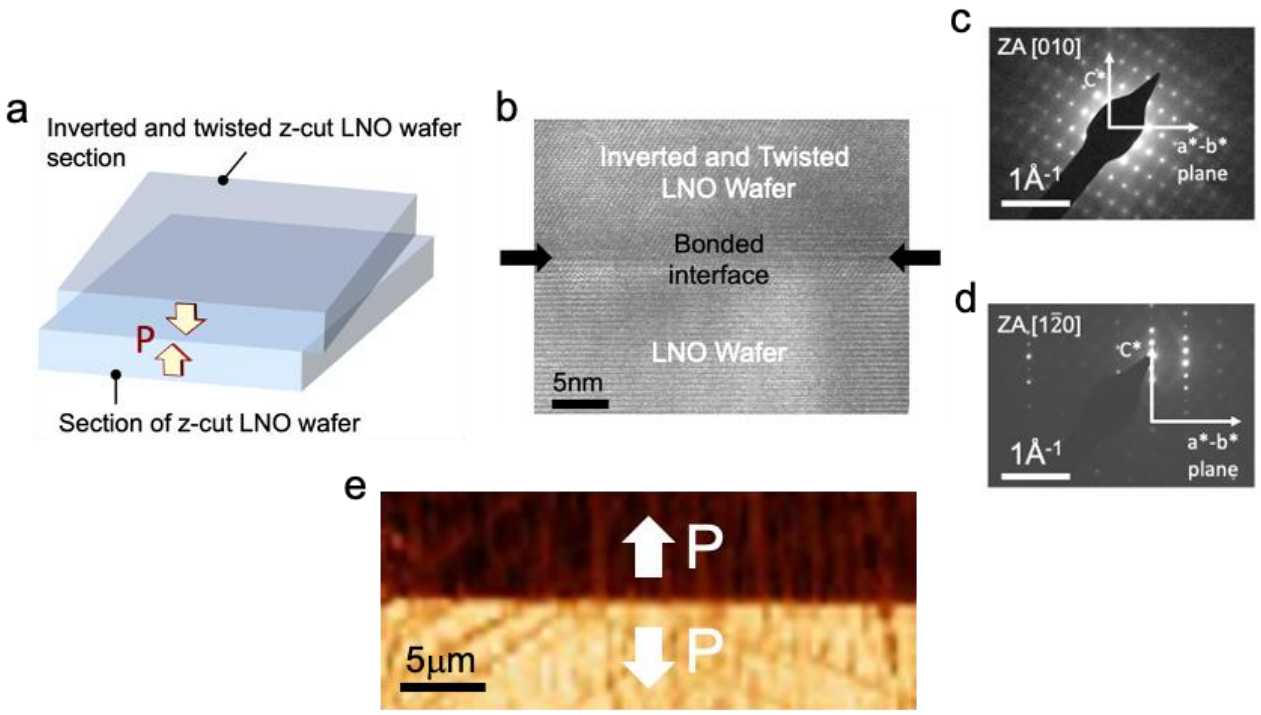

Figure 1: Fabrication of twisted charged interfaces in ferroelectrics. (a) Schematic of the manner in which twisted charged interfaces are created – sections of monodomain z-cut lithium niobate wafer are placed on top of one another in either head-to-head or tail-to-tail configurations and thermo-mechanically bonded at temperatures below the Curie temperature. (b) High-resolution transmission electron microscopy (HRTEM) confirms the successful generation of clean bonded interfaces. In this instance the viewing direction for the top wafer section is along the trigonal [010] (evident from the diffraction pattern in (c)) and the bottom one along $[1\bar{2}0]$ (evident from the diffraction pattern in (d)), confirming the deliberately exaggerated twist angle of 30° used. For twistronic effects on interfacial transport behaviour, much lower twist angles will be systematically probed. Piezoresponse force microscopy (PFM) across a bonded interface (e) confirms its charged nature (in this case a tail-to-tail interface has been created).