An Investigation of Polar Twinning in KTiOPO₄ and KTiOAsO₄. P.A. Thomas, T. Lyford. Department of Physics, University of Warwick, Coventry CV4 7AL, UK. P. Rejmankova-Pernot, F. Lorut, J. Baruchel European Synchrotron Radiation Facility, BP 220, F-38043 Grenoble Cedex, France. S.P. Collins CLRC, Daresbury Laboratory, Warrington, UK.

Keywords: twinning.

KTiOPO₄ (KTP) and KTiOAsO₄ (KTA) are well-known nonlinear optical materials which used for frequency-doubling and parametric oscillation applications. They are isostructural polar crystals described by orthorhombic space group Pna2₁. In principle, they are ferroelectric crystals, although they do not conform strictly to this definition at room temperature as the large ionic conductivity, brought about by mobile potassium ions and sub-stoichiometry on the potassium sites, does not allow a switching field to be sustained. However, they can be switched at low temperatures and this allows the writing of periodic gratings of inversion domains into the crystals for the purpose of creating so-called ‘quasi-phase-matched’ optical devices.

We have been investigating gratings of induced inversion domains using advanced x-ray techniques [1-4]. Two techniques have principally been used: (1) high-resolution diffraction at Station 16.3 of Daresbury Laboratory, which reveals structural information about arrays of domains through rocking curves with well-developed satellite reflections; (2) Bragg-Fresnel imaging [3,4] at ID19 of the ESRF. The detailed structural information accessible with these two techniques is presented, compared and contrasted. It is shown that it is possible to locate the pivot atom on a domain wall through the pseudomerohedric twinning of the KTiOPO₄ room temperature form the Cu⁺ ions are mobile within the framework [PSe₆] and their diffusion paths are evidenced by XRD by means of a combination of a non-harmonic Gram-Charlier expansion of the Debye-Waller factors and of a split model [3]. For the ambient temperature and low temperature forms of this compound the structure determination on single crystal was obscured by twinning. A method for searching crystallographic information from NMR has been established. This strategy is based on the concepts developed by Brown [2]. The sites symmetry observed by NMR can be related to compatible space groups [3]. XRD and NMR used together for structure search and resolution allowed us to find both polymorphs structures. By taking into account a merohedral twinning, the refinement of the Cu⁺-PSe₆ room temperature form structure leads to the residual factors R = 0.0297 (Rw = 0.0245) [1]. The pseudo-merohedral twinning of the Cu⁺-PSe₆ low temperature form has been described with six twin laws (R = 0.0466 / Rw = 0.0486) [1].