

[o.m1.p9] Satellite reflections from lateral hetero-structures of inversion domains in LiNbO₃, KTiOPO₄ and KTiOAsO₄. T. S. Lyford[†], P. A. Thomas[†], S. P. Collins[‡] & D. Laundry[‡]. [†] Crystallography Group, Physics Department, University of Warwick, Coventry, CV4 7AL, UK. [‡] Daresbury Laboratory, Warrington, WA4 4AD, UK. Keywords: ferro-electricity, NLO materials.

Periodically domain-inverted ferroelectric crystals, in which arrays of inversion domains are written by an electric field, have been of interest for optical applications for a number of years. Because the periodicity is of the order of microns, they have also proved interesting systems for study using advanced x-ray sources: they have provided a means of examining the Talbot effect, produced interesting phase-contrast image¹ and have given rise to the diffraction technique of combined “Bragg-Fresnel” imaging^{2,3}.

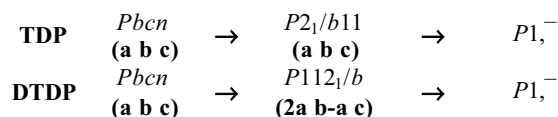
Whilst the principle emphasis has been on studies of periodic arrays of inversion domains using imaging techniques at 3rd-generation synchrotron sources such as ESRF, a theme of continuing and simultaneous interest is the application of high-resolution diffraction methods to the study of periodically domain-inverted crystals⁴⁻⁶. In this poster the results of recent experiments at SRS Station 16.3, Daresbury Laboratory, are presented. The rocking curves recorded from LiNbO₃ (LN), with a grating period of ~5µm, KTiOPO₄ with a grating period of 9 µm and KTiOAsO₄, with a grating period of 39 µm are shown. In all cases, remarkably clear satellite reflections corresponding to the period of the lateral grating are observed, with important differences in the details of the satellites between different samples and different reflections from the same sample. It is suggested that to reproduce the occurrence of satellites, it is only necessary to invoke the analogue of an optical diffraction grating of the appropriate period, with phase differences between adjacent “slits” corresponding to the difference in phase between the structure factors F_{hkl} and F_{-h-k-l}. The results so far are discussed in the context of this interpretation, together with the additional structural detail that can be derived from the diffraction data.

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[o.m1.p10] Isotope Effect in TiH₂PO₄. Structural Study of the Antiferroelectric Low Temperature Phases of TiH₂PO₄ and TiD₂PO₄. E. Álvarez, G. Madariaga, T. Brezewski. *Departamento de Física de la Materia Condensada Universidad del País Vasco, Apdo 644, 48080 Bilbao, Spain*
 Keywords: isotope effect, hydrogen-bonds, ferroelastic domains

TiH₂PO₄ (TDP) and its deuterated form TiD₂PO₄ (DTDP) belong to a large family of (anti)ferroelectric materials of the type of KDP. All of them show as common characteristic a remarkable isotope effect: when the H atoms that build their hydrogen-bond system are substituted by D atoms, the Curie temperature changes considerably. There is nowadays controversy regarding the origin of such an effect, whether it is due to a pure quantum effect because of the different tunneling power of the two isotopes through the hydrogen bonds, or there is an additional geometrical effect due to a decrease of the O-H bonding distances for the deuterated compound¹.

In the case of TDP this isotope effect notably implies a huge antiferroelectric-temperature shift of more than 100 degrees, but also a completely different sequence of phase transitions^{2,3}:



The aim of this work is to determine the triclinic phases of both isotopes.

The study has been carried out by X-Ray diffraction. A structural model for the low temperature phase of TDP has been achieved despite the difficulties due to strong pseudosymmetries and the presence of several ferroelastic domains owing to both the symmetry reduction after the phase transitions, and domain wall relaxation effects. The space group is *P1*⁻. The suspected analogy with the antiferroelectric phase of DTDP seems not to be accomplished. The positions of hydrogen atoms could not be well determined, so no conclusion can be stated about the influence of the H-bonds in the isotope effect.

DTDP shows additional problems related to the degree of deuteration of the samples. Nevertheless, 2nd harmonic generation measurements have strongly suggested the presence of an inversion center, and the analysis of the diffracted intensity distribution together with some refinement trials confirm *P1*⁻ as the space group for DTDP. Neutron diffraction experiments devoted to a more accurate location of H atoms are in progress.

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