ANISOTROPIC CRITICAL X-RAY DIFFUSE SCATTERING FROM KMnF3 AND NaNbO3 SINGLE CRYSTALS

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ANISOTROPIC CRITICAL X-RAY DIFFUSE SCATTERING FROM KMnF₃ AND NaNbO₃ SINGLE CRYSTALS

Abstract. — We have shown previously [1] that the cubic paraelectric phase of BaTiO₃ and KNbO₃ is disordered: the atoms are displaced from the high symmetry position of the ideal perovskite structure and the displacements are correlated along lines parallel to the cubic axes. The anisotropic fluctuation domains or « correlation chains » involve the correlated motion of about 20 unit cells and give rise to an intense diffuse X-Ray scattering localized in { 100 } reciprocal planes.

The case of KMnF₃ and NaNbO₃ is different since these crystals undergo, when the temperature is lowered, a structural transition from the cubic phase to a quite different tetragonal phase: due to the rotation of the fluorine or oxygen octahedra [2], [3] there is a doubling of the unit cell parameters. The X-Ray diffuse scattering patterns show that the cubic phase of these materials is highly disordered.

For KMnF₃, the scattering is restricted to the < 100 > reciprocal axes passing through the superlattice nods of the lower temperature phase [4]. This means that the atomic displacements related to the octahedra rotation are correlated in the { 100 } planes of the crystal, and involve a local doubling of the unit cell even in the cubic phase.

The case of NaNbO₃ is even more complex: the two kinds of scattering (planes and rods) are present on the X ray pictures. The two kinds of disorder are present simultaneously in the cubic phase: correlation chains related to the off-centering of atoms (and the ferroelectric effect), correlation planes associated to the octahedra rotations [5].

Fig. 1. — Variation of the intensity of the scattering restricted to reciprocal axes as a function of temperature : a) KMnF₃, b) NaNbO₃.

The two scattering have a quite different behaviour with temperature. In the first case, the intensity is nearly constant in the cubic phase [1], but in the second, the intensity variation is critical with a maximum at the transition temperature and a slow decrease in the cubic phase (Fig. 1).

References