Incommensurate structures of $Pb(Zr,Sn)O_3$

M. Paściak[1], I. Jankowska-Sumara[2], M Podgórna[2], A. Majchrowski[3], M. Kopecký[1] and J. Kub[1]

[1]Institute of Physics of the Czech Academy of Sciences, Prague 8, Czech Republic;
[2]Institute of Physics, Pedagogical University, ul. Podchorążych 2, Kraków, Poland;
[3]Institute of Applied Physics, Military University of Technology, ul. Gen. Witolda Urbanowicza 2, 00-908 Warsaw, Poland

pasciak@fzu.cz

The prototype antiferroelectric material $PbZrO_3$ (PZO) features a peculiar transition from cubic (Z = 1, *Pm-3m*) to orthorhombic (Z = 8, *Pbam*) phase in which off-centre shifts of Pb^{2+} cations are accompanied with rotations of oxygen octahedra. These two displacive modes are present already in the cubic phase giving rise to strong structured diffuse scattering. Their coupling is considered to be at the core of the antipolar modulation of the PZO's ground-state structure.

Here we show that partial substitution of Zr^{4+} cations with Sn^{4+} adds another level of complexity to this system [1]. For 28 % of Sn two new intermediate phases appear before crystal reaches the known orthorhombic structure. The higher-temperature one is characterized by ordered system of octahedral tilts and signatures of incommensurate modulation. The latter properly develops at lower temperatures in the second intermediate phase. We track changes in the diffraction patterns in the wide temperature range, showing how diffuse scattering signal transforms to orders of magnitude stronger signal marking a critical growth of displacive modes correlation. These changes are discussed in the context of modes coupling.

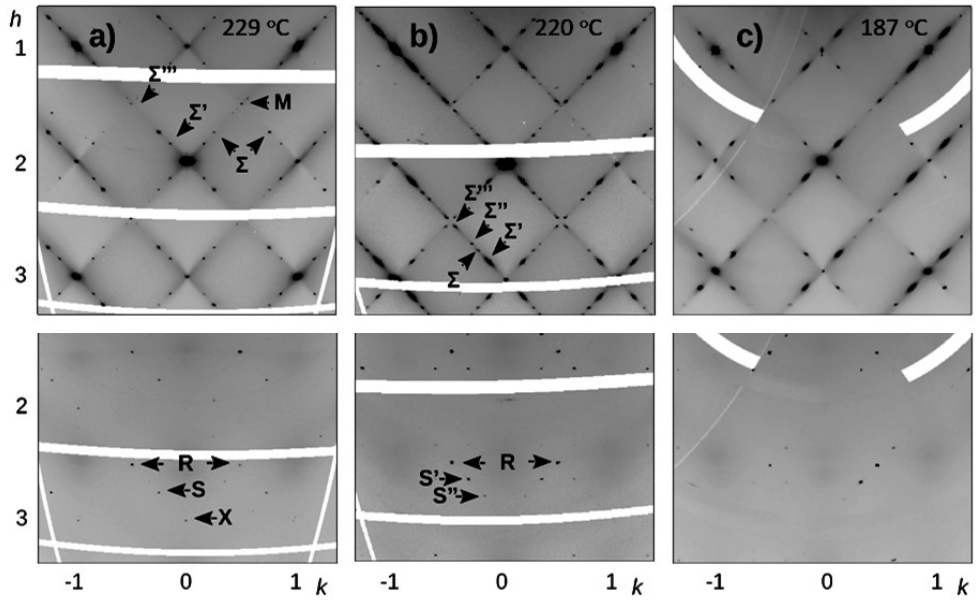

Figure 1. Diffraction in the incommensurately modulated phase of (a) $PbZr_{0.96}Sn_{0.04}O_3$, (b) $PbZr_{0.9}Sn_{0.1}O_3$, (c) $PbZr_{0.72}Sn_{0.28}O_3$. The upper and bottom rows show *hk*0 and 0.5 reciprocal planes, respectively. Reciprocal space points are those of the parent cubic structure.

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