Structural study of ferroelectric charge ordered state in α'-ET_2IBr_2

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α'-ET_2IBr_2 is one of typical organic conductors with quasi-two-dimensional anisotropic triangular lattice. This material is semi-conductive in all temperature region, but it exhibits three sequential phase transitions as follows; the first one is from the room temperature phase (Phase-I) to the higher resistive phase (Phase-II) considered as *charge ordered state* at 204 K, the second one is from Phase-II to Phase-III with larger *SHG signal* at 160 K, and the third one is from Phase-III to the *nonmagnetic* Phase-IV at 25 K. In other word, the resistivity increases at 204 K, SHG signal increases at 160 K, and magnetic susceptibility decrease to zero at 25 K. Nevertheless, the space group symmetry at room temperature is P-1 that consists of inversion symmetry only. [1]

In this study, low temperature X-ray diffraction experiments was conducted to reveal the nature of each phase at BL-8A/KEK-PF and our laboratory. Anomalies in temperature dependence of lattice parameters were found at 204 K, 160 K and 30 K. Especially, the significant hysteresis was found at 30 K. In addition, formation of super lattice of *a* x *b* x 2*c* was found in Phase-II as shown in the lower panel of Fig. 1. The direction *c* is inter-conducting layer direction. As shown in Fig. 1, these superlattice reflections were weakened by irradiation damage. Crystal structure analyses were carried out at 220 K (Phase-I), 175 K (Phase-II), 120 K (Phase-III) and 15 K (Phase-IV). On the basis of the result of crystal structure analyses, it was indicated that 1) No static charge order exists in Phase-I, 2) In Phase-III, charge aligns to make ferroelectric polarization (charge ordered phase), 3) In Phase-II, charges may align ferroelectric in the intra-layer direction and antiferroelectric in the inter-layer direction, and 4) Phase-IV seems to be spin-Peierls phase.

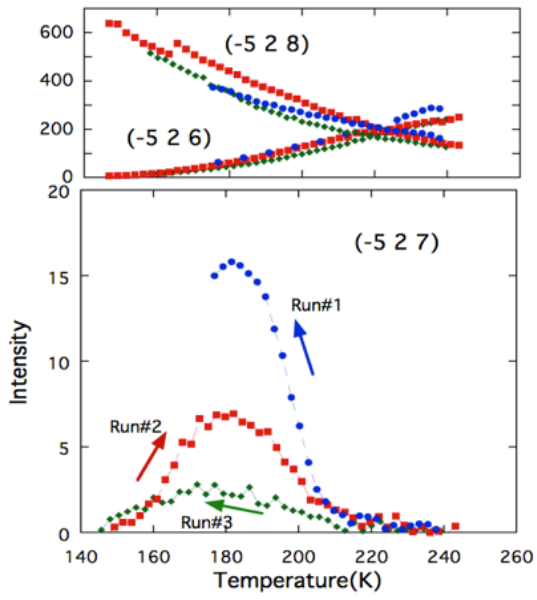

Fig. 1. Temperature dependence of intensity on Phase-Ⅱ. Upper is the fundamental Bragg and the lower is superlattice reflection.

[1] Y. Yue et al., JPSJ, 78(2009), 004