X-ray diffraction in molecular conductor $TPP[Fe(Pc)(CN)_2]_2$

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Molecular conductor $TPP[Fe(Pc)(CN)_2]_2$ (TPP : tetraphenylphosphonium, Pc : phthalocyanine) shows giant negative magnetoresistance [1,2]. The $Fe(Pc)(CN)_2$ molecule forms a one-dimensional chain along the *c* axis, whose stacking provides a 3/4-filled band of the HOMO in Pc. There is a local moment in the next HOMOs of the Fe 3d orbitals. Since the $Fe(Pc)(CN)_2$ has these molecular orbitals contributing to both the electron conduction and the local moments, one can expect the strong intramolecular π-d interactions. The resistivity increases at the lower temperatures. The negative magnetoresistance is observed below 50K. In order to investigate the origin of the gigantic magnetoresistance, it is necessary to clarify the nature of the insulating ground state. We measured the X-ray Diffraction by use of the Low temperature vacuum camera in BL02B1(SPring-8) and a highly sensitive monochromatic Laue camera Okayama University. We find the diffuse streak in the position of $(1/2)c^*$ at the low temperatures. The intensity of this diffuse streak is six orders of magnitude smaller than that of the Bragg peak. The intensity of the diffuse streak increases below 80K, in lowering the temperature, in accord with the enhancement of the resistivity. Even at the lowest temperature (6K), the diffuse streak spreads along the a^*b^*plane, suggesting very weak interchain correlation. Taking into account the 3/4-filled HOMO band, this diffuse streak can be ascribed to the $4k_F$ charge disproportionation, and suggests the carrier localization due to the electron correlation.

[1] N.Hanasaki et al., J.Phys.Soc.Jpn., **75**, 033703 (2006).
[2] H.Tajima et al., Phys.Rev.B, **78**, 064424 (2008).