

Novel Style of Structure Determination for π -d System by Synchrotron X-ray Diffraction

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Molecular conductor (DBr-DCNQI)₂Cu undergoes a novel metal-insulator transition at 160K caused by π -d electron interaction, due to the simultaneous appearance of charge order in Cu ions [1] and the CDW in DCNQI molecules in the insulator phase. This phase transition is understood as a unique type of electronic instability caused by cooperation of the Peierls and Mott instabilities. However, the actual three-dimensional (3D) arrangement of these orderings has not been revealed.

In order to obtain the electron distribution in the unit cell by means of synchrotron x-ray measurements, the spatial relation between the charge ordering and the CDW was examined. The charge ordering in the Cu sites as Cu⁺ Cu⁺ Cu²⁺ along the stacking axis was observed by utilizing the anomalous scattering technique, consistent with previous studies. As for the CDW pattern on DCNQI columns, single crystal structure analysis was conducted.

As a result of these two x-ray experiments' combination, we successfully obtained the 3D pattern, which is different from the structure previously observed. We discuss the implementation to the mechanism.

[1] Hiraki K., Kobayashi Y., Nakamura T., Takahashi T., Aonuma S., Sawa H., Kato R., Kobayashi H., *J. Phys. Soc. Jpn.*, 1995, **62**, 1470.

Keywords: CDW, synchrotron x-ray radiation, structure analysis