Charge density study of $(DBr\text{-}DCNQI)_2Cu$ by Synchrotron X-ray Diffraction

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The quasi-one-dimensional (Q1D) molecular conductors have attracted wide interest owing to their unique electronic structures and intriguing physical properties. A molecular conductor $(DCNQI)_2Cu$ system, where DCNQI is the *N*, *N'*-dicyanoquinonediimine, shows the novel metal-insulator (M-I) transition at low temperature[1,2]. The M-I transition is accompanied by the charge density wave (CDW) formation at the 1D DCNQI columns and the spatial charge ordering (CO) at the Cu sites. The CDW and CO have been revealed by various kinds of experimental studies, such as ESR, XPS and x-ray diffraction[2]. However, three dimensional (3D) structures of both CDW and CO, which provide crucial information for understanding the M-I transition, in $(DCNQI)_2Cu$ system have never been determined. High resolution synchrotron radiation (SR) single crystal x-ray diffraction study is one of the promising technique to reveal the 3D structures of CDW and CO. Actually, Wigner crystallization of CO arrangement in $(DI\text{-}DCNQI)_2Ag$ has been determined by the SR x-ray diffraction[3]. In this study, we have performed accurate structural analysis of $(DBr\text{-}DCNQI)_2Cu$ using the third generation synchrotron x-ray source, SPring-8.

The single crystal x-ray diffraction data were carried out using Weissenberg camera with an imaging plate as a detector installed at SPring-8, BL02B1 beam line. The wavelength of the incident x-ray is 0.35 Å. The temperature of the sample was controlled by He gas flow device. The crystal structure refinement was performed using SHELX97 software. The *R*-factor was less than 3.0 %. The high quality diffraction data with good *R*-factor and wide *d*-spacing range enables us to directly observe 3D CO and CDW structure by an experimental charge density study. The charge density studies by the Maximum Entropy Method, the Multipole Refinement, and the Bader topological analysis, are now in progress.

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