Determination of Molecular Density Distribution by SEM in Mixed Crystals of Organic Metals

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As the lattices of organic conductors are flexible, it is an important technique to apply an external pressure and to study the lattice transformation of the crystal. In this case the distance between molecules changes, and the overlapping integral between molecules changes. When we want to make a temperature-pressure phase diagram, sometimes there is the case where we want to know a so called negative pressure area, in other words the phase states below the ambient pressure for the aiming crystal system. The representative strategy to cope this case is to make mixed crystals. We can use the similar molecules of the different sizes to make mixed crystals. In this case we should resolve the problem to decide the real density distribution of constituent molecules in the obtained samples. Sometimes, a possibility of inhomogeneous distribution of molecules is not avoidable, and it produces additional effects due to randomness. We have been studying the properties of mixed crystal using TMTSF and TMTTF molecules by ESR techniques [1] . In this report we show and discuss a simple and rather reliable technique to decide the relation between the real density and the aimed density of molecules by SEM (Scanning Electron Microscopy).

The SEM system (Keyence VE-9800SP) has a versatile EDX (Energy Dispersive X-ray spectroscopy) detector with a moving sample stage. Therefore, we can easily analyze the density of Se and S distribution along the conducting direction. Though we have applied this technique to the cation distribution at present, it is also effective for the determination of anion distribution. The EDX technique has been also applied to analyze the change of the crystal state from metallic to semiconducting for the κ–(BEDT-TTF)$_2$Ag(CN)$_2$ H_2O system.

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[1] K. Oshima *et al.*, J. Low Temp. Phys. 142 (3-4), 551-554 (2006).