The crystal structure of a new mixed anion compound with SCN anion

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In recent years, mixed-anion compounds, which are inorganic solid materials containing multiple types of anions within a single compound, have attracted attention. [1] In mixed-anion compounds, unique structures and properties, unattainable in single-anion systems, can emerge due to differences in the size and electronegativity of the anions.[1] While the exploration of mixed-anion compounds has mainly focused on combinations of single anions such as O^{2-} and N^{3-}, incorporating molecular anions into these systems would significantly increase their degree of freedom. Moreover, molecular anions exhibit fundamentally different characteristics compared to single anions, such as molecular shape, stretching, and rotation, making their influence on structures and properties particularly intriguing.

Recently, we found new compounds composed of fluoride (F^-) and thiocyanate (SCN^-) anion in single compounds. By using lab XRD, we found that this new phases can be indexed by rhombohedral lattice with the lattice parameters of a = 4.3 Å, c = 34.5 Å. The long c axis suggest that it has layered structure. The analysis of synchrotron XRD allows us to determine the position of heavy elements in the lattice. Moreover, we found that they exhibit relatively high fluoride ion conductivity at moderate temperature. However, it is difficult to determine the position of light element such as fluorine and carbon by means of XRD. Therefore, we propose detailed structural analysis using neutron powder diffraction data collected using HERMES at JRR-3.

Figure 1 shows the fit of Rietveld refinement using NPD patterns of new fluoride thiocyanate. The refinement assuming layered structure provide good fit with the reliability factors of GOF = 2.38, R_p = 7.23% and R_{wp} = 9.53%. We found that the refinement of neutron powder diffraction data allows us to determine the position of fluoride anions. However, it was difficult to determine the position and orientation of thiocyanate. We speculate the thiocyanate orient randomly or move dynamically in the lattice. Therefore, another experiments such as Raman measurement is necessary to discuss its crystal structure.

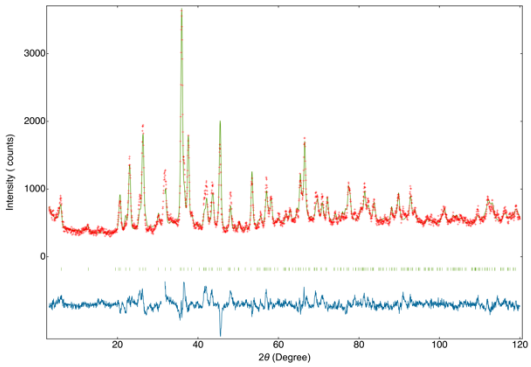

Fig. 1. Rietveld refinement using neutron diffraction data collected at HERMES.

1. H. Kageyama, K. Hayashi, K. Maeda, J. P. Attfield, Z. Hiroi, J. M. Rondinelli and K. R. Poeppelmeier, Expanding frontiers in materials chemistry and physics with multiple anions, *Nat. Commun.*, 2018, **9**, 772.