第 29回フロンティア材料研究所講演会

講師：Professor K. R. Poeppelmeier
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1月25日（水） 15時30分～17時 R3棟1階会議室にて
演題：**Low Temperature Synthesis of the Centrosymmetric and Noncentrosymmetric polymorphs of $KNaNbOF_5$ and the Dynamic Origins of Noncentrosymmetry**

This talk will present the hydrothermal synthesis of oxide-fluoride compounds as a strategy to target noncentrosymmetric (NCS) materials. NCS structures are required for a variety of useful materials properties including for example second-harmonic generation and piezoelectricity. Therefore, the design of NCS materials is an ongoing theme in crystal engineering. Analysis of dynamic phase transition processes can be used to identify factors that cause some compounds to adopt crystal structures that are noncentrosymmetric (NCS). We have examined a two-step, temperature driven reconstructive phase transition in the compound $KNaNbOF_5$ using empirical dynamic simulations, in-situ diffraction studies, and theoretical calculations.

We used cryogenic temperature (~15K) and variable-pressure (1-10 GPa) diamond anvil cell single crystal diffraction experiments on the NCS, $Pna2_1$ phase of $KNaNbOF_5$ to develop a set of empirical pairwise interatomic interaction functions of the complex five element system. Our investigation lead to the discovery of a dynamically disordered high temperature crystal structure and the mechanistic origin of the NCS phase stabilization upon cooling. The reconstructive transition going from the *P4/nmm* phase to the high temperature *Cmcm* phase is believed to result from a loss of O/F site ordering caused by rigid-type rotations of octahedral $[NbOF_5]^{2-}$ anionic units. The high temperature phase was found to exist in a dynamically disordered state involving two locally stable phases in the potential energy landscape with *Pbcm* and *Pnma* space group symmetries.

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