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 利用課題名 (日本語) : 蛍光 X 線ホログラフィー法によりの  $\text{Pb}(\text{Zr,Ti})\text{O}_3$  の局所構造の研究  
 Program Title (English) : Study of the local structure in  $\text{Pb}(\text{Zr,Ti})\text{O}_3$  (PZT) by x-ray fluorescence holography  
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 キーワード : 強誘電体, 局所構造, 蛍光 X 線ホログラフィー法

### 1. 概要 (Summary)

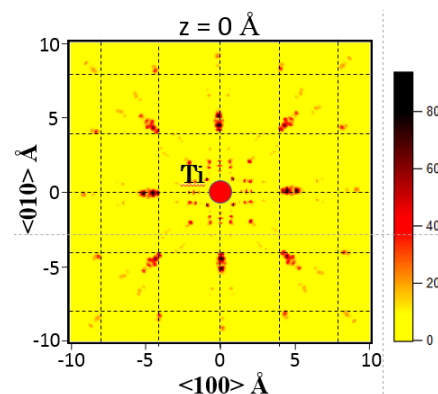
Lead zirconate-titanate  $\text{Pb}(\text{Zr,Ti})\text{O}_3$  (PZT) is the most widely used ferroelectric piezoelectric system in multilayer actuators, sonar and ultrasonic transducers, and ultrasonic motors owing to its excellent electro-mechanical properties [1]. Neither PZ nor PT are particularly good piezoelectrics, but mixing these materials gives rise to excellent piezoelectric response. Understanding of the microscopic origin leading to very high dielectric and piezo-electric responses and the local structure of PZT is essential for designing of new and improved materials. However, accurate local structure of PZT is not clear yet due to the difficulties in studying nano-scale inhomogeneity and growing sufficient large size of PZT single crystals. In this work, we investigated the local structure around Ti atoms in  $\text{Pb}(\text{Zi}_{0.7}\text{Ti}_{0.3})\text{O}_3$  single crystal [2] using x-ray fluorescence holography (XFH) technique.

### 2. 実験 (Experimental)

XFH experiment was carried out at BL22XU of SPring-8 synchrotron facility. The incident X-ray energies were 18.5 KeV - 22 keV with 0.25 keV steps. Ti K $\alpha$  (4.5 keV) x-ray fluorescence was collected using photodiode detector with a graphite-crystal analyzer. Using multi-energy holograms, 3D real space local structures around Ti were successfully obtained.

### 3. 結果と考察 (Results and Discussion)

Right figure shows reconstructed atomic image of center Zr/Ti plane, which paralleled to the (001) plane at  $z=0 \text{ \AA}$ . The crosses of dotted lines indicates ideal positions of Zr/Ti atoms and center red spot indicates the position of emitter Ti. Neighboring Zr/Ti atoms are clearly visible and the positions of obtained atomic images agreed with theoretical positions. However, Zr/Ti atomic images split along radiation direction, indicating existence of local distortion. For bettering understanding, local structure around Zr and Pb will be investigated in the future beamtime.



### 4. その他・特記事項 (Others)

[1] J. F. Scott, Science 315, 954 (2007).  
 XFH is a novel model-free technique for determining the 3D atomic arrangement around a specific element at atomic resolution.