Study of nanoscale local structural fluctuations in ferroelectrics using convergent-beam electron diffraction

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It is well known that $BaTiO_3$ undergoes successive phase transformations from the cubic paraelectric phase to three ferroelectric phases: tetragonal, orthorhombic and rhombohedral ones. Coexistence of the displacive and order-disorder characters in the phase transformations of $BaTiO_3$ was pointed out from many experiments and theories. However, local structures related to the order-disorder character were discovered neither in crystal structure analyses using neutron and X-ray diffraction nor by TEM observations. In the present study, the convergent-beam electron diffraction (CBED) method [1] was applied to examine nanometer-scale local structures of $BaTiO_3$.

Rhombohedral nanostructures were observed in the orthorhombic and tetragonal phases of $BaTiO_3$ using CBED [2]. It was found that the symmetry of the orthorhombic phase is formed as the average of two rhombohedral variants with different polarizations, and that of the tetragonal phase is formed as the average of four rhombohedral variants. These results indicate an order-disorder character in their phase transformations.

Similar rhombohedral nanostructures were also found in the ferroelectric orthorhombic phase of $KNbO_3$ [3], while it was confirmed that the ferroelectric tetragonal phase of $PbTiO_3$ does not have such rhombohedral nanostructures [4].

We also proposed a combined use of STEM and CBED methods (STEM-CBED method) to observe the nanostructures of polarizations [5]. Using the method, two-dimensional distributions of the rhombohedral nanostructures, or nanoscale fluctuations of the polarization clusters, were successfully visualized in the tetragonal phase of $BaTiO_3$. We are also planning to apply this method to the orthorhombic and cubic phases.

References

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