Investigation of microscopic origin of piezoelectric effect in $Bi_{12}SiO_{20}$

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The aim of this work was to investigate the atomistic origin of piezoelectric effect in $Bi_{12}SiO_{20}$ - one of a few non-polar materials with high piezoelectric response (20 times higher than that of the α-quartz). The point symmetry group (23) of $Bi_{12}SiO_{20}$ excludes the formation of ferroelectric / ferroelastic domains, i.e. the piezoelectric effect must have intrinsic nature (related to the crystal structure). The high intrinsic piezoelectric response in Bi-based structures is particularly interesting, as the piezoelectric effect of the same magnitude has recently been found in another (BiB_3O_6) Bi-based material [3]. In this work, we confirm the absolute structure of $Bi_{12}SiO_{20}$ and relate it to the anisotropy of the piezoelectric effect.

A single $Bi_{12}SiO_{20}$ crystal was grown by Czochralski technique, cut perpendicular to the [111] direction (~ 0.75 mm thick) and coated by thin gold contacts to apply external high voltage (up to +/- 1500 V). We implemented the stroboscopic technique (described elsewhere [2, 4, 5]) to detect small field induced changes of selected Bragg rocking curves at the D3@DORIS beamline.

We used the measured shifts of the Bragg positions under electric field to calculate the piezoelectric constant of $Bi_{12}SiO_{20}$ (d_{14} ~ -40 pC/N in agreement with Abrahams et al. [1]) and establish the direction of the positive / negative piezoelectric effect. Then we collected the set of absolute intensities to establish the absolute sense of the structure. The experiment was repeated at three different wavelengths (0.4, 0.7 and 0.93 Å) corresponding to the different magnitudes of anomalous scattering factors f''(Bi) (4.1, 10.9 and 4.9 correspondingly). We used analytical absorption correction for a plane-shaped sample to reduce the measured intensities to the structure factors. Two inversion related structures (shown on the Figure 1) were tested by calculating the R-factors - sum of the squared differences between calculated and observed structure factors.

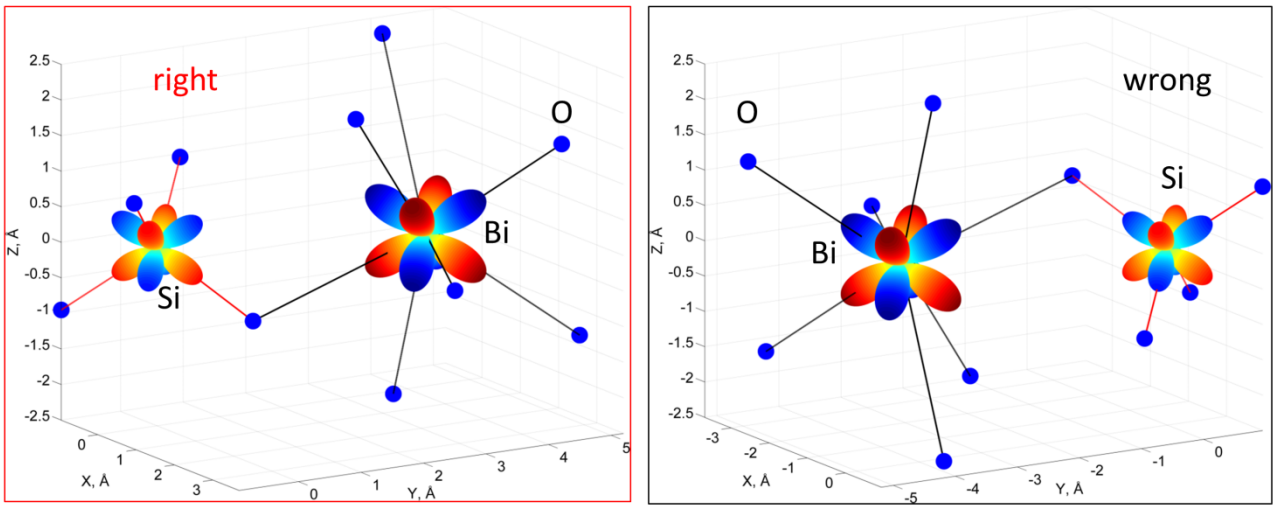

Figure 1: The fragment of two inversion related variants of absolute structure of $Bi_{12}SiO_{20}$ (SiO_4 structural tetrahedra on the left and BiO_7 structural polyhedra on the right) as determined relative to the representation surface of longitudinal piezoelectric effect. The coloured surfaces present the magnitude of the longitudinal piezoelectric deformation ($d'_{33} = d_{ijk}l_i l_j l_k$, where d is the tensor of piezoelectric constants and $\boldsymbol{l}$ is a unit vector). The red / blue parts of the surfaces correspond to the positive / negative piezoelectric effect.

Table 1. Summary of the collected data and the refinement results

Data Set	λ, Å	#Reflections	f''(Bi)	R (%), Structure 1	R (%), Structure 2
1	0.93	142	4.1	5.07	5.36
2	0.70	69	10.4	7.64	9.19
3	0.40	179	4.9	8.27	8.63

The Table 1 summarizes the results of the experiment and testing of the inversion-related structures. The number of collected Bragg reflections, the magnitude of anomalous scattering factor of Bi atom is presented for each data set. The last two columns show the R-factors corresponding to the tested structure. The better agreement between experimental and simulated structure factor is achieved for the structure 1 (the left on the Figure 1). Thus we confirmed that Si --> O directions in the SiO_4 tetrahedra of $Bi_{12}SiO_{20}$ correspond to the directions of the positive piezoelectric effect: the tensile mechanical stress along the direction of Si-O bonds brings a positive charge on the ‘’O’’ side and negative charge on the ‘’Si’’ side.

References

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