Incommensurate Crystallographic Shear Structure of $Ba_xBi_{2-2x}Ti_{4-x}O_{11-4x}$ (x=0.275)

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The 4d structure of the title compound consists of atoms with sawtooth-like modulation functions and step-like occupation functions (occupation domains, OD). Most of the structural parameters defining OD are concerned with γ (=0.36693), the **c*** component of the modulation wavevector. The 3d structure is closely related to the β-$Bi_2Ti_4O_{11}$ structure, where the linkage of TiO_6 coordination octahedra constructs the host framework providing the one-dimensional tunnel-like space for the accommodation of Bi ions. Domain boundaries are introduced by a kind of the crystallographic shear (CS) operation in the present structure. Namely, the layer unit consisting of $Bi_2Ti_2O_8^{2-}$ is removed from the β-$Bi_2Ti_4O_{11}$ structure, and remained blocks are displaced to fill the gap. The negative charge of the removed unit is compensated by the substitution of Ba^{2+} ions for Bi^{3+} ions in tunnels.

The unique character of this incommensurate structure is the aperiodic insertion of domain boundaries in contrast to usual (*i.e.* commensurate) CS structures. To the best of our knowledge, the present study is the first example of the quantitative analysis of the incommensurate CS structure.

Keywords: incommensurate structures, higher-dimensional structure analysis, crystallographic shear structures