DOMAIN STATES IN PEROVSKITE STRUCTURE OF $GdFeO_3$ TYPE

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The perovskite-type structure appears in a large number of oxide compounds with the stoichiometry ABO_3. Under ambient conditions many perovskite-type materials turn out to be distorted from the ideal structural arrangement. Various phases occur due to atomic displacements from the high symmetry cubic positions. Among such low symmetry (distorted) perovskites many phases exhibit ferroelastic behaviour with the cubic structure as the prototype modification (parent phase). One of the most prominent phases among the ABO_3 compounds is the orthorhombically distorted perovskite structure of the $GdFeO_3$ type (space group Pbnm, Z=4) [1,2]. The aim of this study is to determine the symmetry operations, which relate different domain states in compounds of the $GdFeO_3$ type, as well as to enhance the crystallographic understanding of the domain structure on an atomic scale.

Symmetry operations of linking the different domain states in $GdFeO_3$ type crystals have developed using the group-theoretical analysis of prototypic and ferroelastic space groups. The group-theoretical analysis of prototype Pm3m and ferroelastic Pbnm space groups have allowed to find symmetry operations of linking the different domain states in $GdFeO_3$ type crystals. Every of 6 possible orientation states can be separated on 4 translation ones in $GdFeO_3$ type crystals. The models of crystalline structure for all possible domain pairs have been proposed.

The ion locations on the domain boundary were estimated as the intermediate positions between the ion sittings in both states. It has been shown that the boundary crystalline structure always tends to be the prototype phase structure – an ideal perovskite structure, though certain perovskite deformation retains. In addition to shifts of all ions the turns of oxygen octahedra of the some type and appropriate displacements of A ions should take place at switching of orientation states. The turns of octahedrons and displacements of A ions are sufficient to cause forming the translation states (antiphase domains). Antiphase domains may have boundaries between themselves along 3 faces of the orthorhombic cell.

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References

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