PEROVSKITE STRUCTURE AND PHASE TRANSITION DUE TO TEMPERATURE

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Abstract

Phase transitions (symmetries) in ceramic and crystalline materials are widely explored in electrical-electronic devices. In this paper, we present the symmetries of the perovskite structure and the phase transitions due to temperature.

keywords: perovskite structure, crystalline structure, phase change, ceramics, barium titanate.

Introduction

1. Ceramic and crystalline materials are formed by stable physico-chemical structures called symmetries [1, 2].
2. The perovskite structure is organized into 5 symmetries: cubic, tetragonal, orthorhombic, rhombohedral, and monoclinic. Symmetry changes are due to temperature variation, induced polarization or impurities added in the unit cells [3–5].

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Methods

3. A systematic literature review was carried out in the area of materials science and engineering.

Results and Discussion

4. Ferroelectric materials are formed by structures of the perovskite type represented by ABO_3 , where A and B are cations, respectively with valences 1, 2, 3 and 4, 5, 6 and “O” is oxygen.
5. Perovskite structures are characterized by the cell parameters: a , b , c , α , β , and the polarization vector (P_s) of the electric dipole.
6. Unit cell with $\alpha = 90^\circ$, $\beta = 90^\circ$, $a = b = c$ has cubic symmetry, and is classified as paraelectric (non-ferroelectric, because $P_s = 0$):
7. Unit cell with $\alpha = 90^\circ$, $\beta = 90^\circ$, $a = b \neq c$ has tetragonal symmetry, Fig. 1, is classified as ferroelectric, because $P_s > 0$:

Figure 1: Tetragonal symmetry.

8. Unit cells with $\alpha \neq 90^\circ$ or $\beta \neq 90^\circ$ are distorted concerning cubic and tetragonal symmetry. If $\alpha = 90^\circ$ and $\beta \neq 90^\circ$, then the symmetry is orthorhombic. If $\alpha \neq 90^\circ$ and $\beta \neq 90^\circ$, then the symmetry is rhombohedral, see Fig. 2. These symmetries are ferroelectric, because $P_s > 0$:

Figure 2: symmetries: a) orthorhombic, b) rhombohedral.

9. Symmetry transitions are also called phase changes or phase transitions.
10. Phase transitions are investigated due to anomalies in the real dielectric permittivity (ϵ'), as shown in Fig. 3. In this figure, Fig. 3, refers to ferroelectric ceramic $BaTiO_3$. Phase transitions are in $+123^\circ C$ (cubic - tetragonal), $+5^\circ C$ (tetragonal - orthorhombic) and $-90^\circ C$ (orthorhombic-rhombohedral) [6, 7].

Figure 3: Anomalies in ϵ' of $BaTiO_3$ as a function of temperature.

Final Remarks

11. Material properties are optimized by manipulating the symmetries.

Open Invitation

*Review, add content, and **co-author** this paper [8].*

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