

Review

Research Progresson Crystal Structure, Defect Regulation, and Dielectric Property Modification of Barium Titanate Ferroelectric Ceramics

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Abstract: Because of its superior dielectric qualities, barium titanate (BaTiO₃), a common perovskite-type ferroelectric material, has found widespread use in electronics, telecommunications, and energy. However, its continued use has been constrained by problems such a high Curie temperature, a small temperature range, and a low dielectric constant at ambient temperature. This research explores the crystal structure of barium titanate, types of defects, and their mechanisms impacting dielectric performance by methodically evaluating pertinent contemporary local and foreign literature. Additionally, it offers a thorough examination of how nanocomposite technology and rare earth element doping optimize barium titanate's dielectric characteristics. According to research, barium titanate's crystal structure and dielectric characteristics may be efficiently controlled by rare earth element doping, and nanocomposite technology can improve the material's breakdown strength and dielectric constant by creating nano-scale heterostructures. Additionally, optimizing the sintering process parameters and other methods can also improve the performance of barium titanate to some extent. These modification strategies provide theoretical support and practical guidance for enhancing the overall



performance of barium titanate ceramics and expanding their applications in multilayer ceramic capacitors (MLCCs) and other electronic devices.

Keywords: Barium titanate; perovskite structure; defect; rare earth doping; nanocomposite; dielectric properties

1. Introduction

Ferroelectric materials have attracted a lot of research attention lately because of their important uses in the national defense, electronic communications, aerospace, and civilian sectors (Fu et al., 2008). Of them, barium titanate (BaTiO_3) is the first oxide of the perovskite type to be found to have ferroelectric characteristics. Less than a century of research by several scientists has demonstrated BaTiO_3 's high dielectric constant, enormous resistivity, high breakdown voltage, and exceptional insulating qualities since Wainer and Selomon found its good dielectric properties in 1942. It is one of the most extensively used materials in electronic ceramics because of these qualities, which allow it to be employed in the fabrication of capacitors, high-frequency electronic components, and electronic device encapsulation (Che and Chen, 2014).

Certain dielectric materials must have low dielectric loss, temperature stability, fine grain structure, high breakdown voltage, superior insulation, and aging resistance at the right permittivity values due to the trend toward electronic device downsizing (Shu et al., 2018). These characteristics make it possible to fabricate semiconductor-type parts like PTC thermistors and grain boundary capacitors as well as small, high-capacity micro capacitors (Colin et al., 2013). Consequently, a key area of study in the cutting-edge science of dielectric materials is the development of ceramics based on barium titanate that have exceptional all-around qualities. Rare earth ion doping in barium titanate ceramics provides substantial modification benefits, is a practical strategy for achieving higher overall performance in dielectric ceramic development, and is a potential future trend in dielectric ceramic materials. (Li et al., 2018)

2. Crystal Structure and Phase Transition Behavior of Barium

Titanate

2.1. Perovskite-Type Structural Features

Ferroelectric materials are mainly divided into four categories based on their crystal structures: hydrogen-bonded structures, fluorine-containing octahedra, oxygen-containing octahedra, and other ionic groups. The most researched of them are ferroelectric materials of the perovskite type that fall under the oxygen-containing octahedra category.

The molecular formula for perovskite materials is ABO_3 . Transition metal ions, including both variable-valency and high-valency metals (e.g., Zr, Y, Ti), usually occupy the B site, while alkaline earth metal ions, rare earth metal ions, and ions with larger radii are usually accommodated in the A site. (Guo, C. P.2013) Perovskite materials often assume an octahedral structure. Ternary compounds of the ABO_3 class, such as $CaTiO_3$, are examples of the so-called perovskite structure.

The most common perovskite ferroelectric material is barium titanate, in which the oxygen octahedral framework is formed by O^{2-} , the A site is occupied by Ba^{2+} , and the B site is occupied by Ti^{4+} . Barium titanate has a tetragonal phase (space group $P4mm$) at ambient temperature. The structural foundation for its ferroelectricity is the spontaneous polarization that results from Ti^{4+} 's deviation from the oxygen octahedron's center. Temperature affects barium titanate's crystal structure. Hexagonal, tetragonal, orthorhombic, and trigonal systems are the four crystal forms that it can take on in the solid state as it changes from high to low temperature (Liu, 2020). A series of phase transitions occurs in barium titanate as the temperature rises: tetragonal phase \rightarrow orthorhombic phase \rightarrow rhombohedral phase \rightarrow cubic phase. The nonpolar paraelectric phase is the cubic phase ($>120^\circ C$).

2.2. Phase Transforms and Property Correlations

Phase transition behavior features are closely linked to the functional performance of barium titanate material systems. Notably, controlling the Curie temperature has a significant impact on thermal stability parameters, dielectric characteristics, and the intensity of the piezoelectric action. This material is frequently utilized in temperature-sensitive electronic components because of its distinct change



in dielectric constant. The dielectric constant shows a maximum close to the Curie temperature when a structural transition takes place from the tetragonal crystal system to the cubic crystal system. The tetragonal phase exhibits considerable lattice distortion, leading to spontaneous polarization effects, whereas the cubic phase structure totally loses its ferroelectric capabilities because it is non-polar. Ferroelectricity originates from the cooperative changes in lattice distortion and oxygen octahedral tilt angles during the phase transition, according to analysis using transmission electron microscopy and X-ray diffraction. Examples demonstrate how these microstructural changes have a direct impact on the dielectric response spectrum properties and piezoelectric conversion efficiency of the material (Yang et al., 2023). Furthermore, the multi-field coupling properties of barium titanate materials are correlated with phase transition behavior. When an electric field or stress is applied, reversible switching enables the tetragonal ferroelectric domain structure to provide a notable piezoelectric effect. Examples demonstrate how domain wall pinning effects lead to a decrease in electromechanical conversion efficiency during the phase transition process.

3. Types of Defects in Barium Titanate and Their Effects

3.1. Wire Defects and Their Impact on Performance

Dislocations are the main type of linear defects in barium titanate, usually brought on by pressures during crystal formation or processing. Dislocations reduce the material's piezoelectric response by impeding domain wall mobility. Increased leakage currents could result from localized electric fields created by lattice distortions around dislocations. For example, local conductivity can be increased by an order of magnitude when edge dislocations build up on {100} crystal surfaces. Additionally, under cyclic electric fields, the dislocation network weakens the material's mechanical strength and increases the likelihood of fatigue cracks.

3.2. Twin crystal

Grain borders and phase boundaries are examples of surface defects, which are flaws with larger dimensions in two directions and smaller dimensions in one. Here,



twins are the main topic of discussion. When two identical crystals coexist in a mirror-symmetrical configuration, twins are created. There is just one symmetry plane, one symmetry center, and a secondary rotation axis in their symmetry relationship.

Ferroelectric domains are commonly referred to as a type of twin structure in the study of ferroelectric materials. In the 1940s, for example, P.W. Forsberg Jr. studied domain structures in great detail and proposed that twins form domains: two converging twin planes produce wedge-shaped layered domains. Conventional twins are usually immobile lattice defects, although ferroelectric domains can move under electric fields.

Due to lattice mismatch at the twin plane, twinning modifies the local stress field in addition to influencing crystal formation and creating unique morphologies. Because twinning may encourage development at particular sites, this can result in an increased number of lattice faults in the final crystal.

4. Strategies for Barium Titanate Modification

4.1. Rare earth doped modification

Due to their distinct electrical structure and chemical characteristics, rare earth elements offer substantial advantages when it comes to altering barium titanate (BaTiO_3). Barium titanate's crystal structure and dielectric characteristics can be effectively controlled by doping it with rare earth elements. For example, lanthanum (La) doping improves the stability of barium titanate's dielectric constant and dielectric loss while

This is because oxygen vacancies are created to preserve charge balance when lanthanum ions take the place of some barium ions. The degree of lattice distortion is changed by oxygen vacancies, which has an impact on the dielectric characteristics of the material (Li et al., 2018). Additionally, yttrium (Y) doping improves barium titanate's dielectric characteristics; in high-frequency applications, yttrium-doped barium titanate shows reduced dielectric loss. This is mainly because yttrium ion doping optimizes the dielectric response properties of barium titanate by changing the lattice parameters and oxygen octahedron tilting (Fu et al., 2008).

4.2. Modification by Nanocomposite Technology



By mixing nano-scale second-phase materials with barium titanate composites, nano-composite technology is an efficient way to improve characteristics. For example, adding nano-titanium dioxide (TiO₂) to barium titanate produces a nanoscale heterostructure in the matrix. In barium titanate, this structure successfully inhibits grain development, producing more consistent and finer grain sizes. As a result, the material shows improved breakdown strength and dielectric constant (Che and Chen. 2014).

Additionally, the presence of nano-titanium dioxide can absorb and scatter electromagnetic waves to a certain extent, thereby reducing the dielectric loss of the material (Jun and Jun, 2019). Furthermore, nanocomposite technology can also regulate the properties of barium titanate through interfacial effects. Charge transfer and polarization phenomena occurring at the interfaces between different materials can significantly influence the dielectric properties of barium titanate (Jun and Jun, 2019).

4.3. Other modification methods

There are many more ways to modify barium titanate in addition to the two primary approaches listed above. Sintering temperature, holding time, and atmosphere are just a few of the variables that can be controlled throughout the sintering process. This maximizes the qualities of barium titanate by controlling defect generation and grain growth. Reducing the sintering temperature or holding time can result in a more equal distribution of grain sizes. Examples demonstrate how suppressing excessive grain formation improves density and dielectric characteristics (Jiao et al., 2016).

The employment of specialist techniques like sol-gel technology and chemical co-precipitation is very important in the creation of barium titanate materials. It is feasible to produce materials with particular qualities by achieving precise control over structure and composition at the tiny scale. Examples demonstrate how the use of these sophisticated procedures has created new opportunities for performance characteristic optimization (Gong et al., 2014).

5. Conclusion



The dielectric characteristics of barium titanate can be efficiently optimized by methods like rare earth doping and nanocomposite techniques, which offer theoretical justification and useful advice for its use in electronic devices like multilayer ceramic capacitors (MLCCs). However, major problems including excessive dielectric loss and inadequate temperature stability still prevent barium titanate-based ceramics from being further promoted in high-performance electronic systems. To increase the variety of applications for high-performance barium titanate, efforts should be undertaken in the future to develop additional doping and composite systems as well as to further improve the preparation procedures.

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