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Short Communication

Tailoring Phase Transition and Dielectric Response in $BaTiO_3$ Ceramics via Sb_2O_3 Doping

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Abstract

The practical applications of ferroelectric materials are highly dependent on their phase transition behaviors and dielectric properties. To broaden the application scope of $BaTiO_3$, direct Sb_2O_3 introduction was adopted as a strategy to modulate the phase transition in this work. Experimental results demonstrate that Sb_2O_3 doping induces a structural transformation of $BaTiO_3$ from tetragonal to pseudo-cubic symmetry, and facilitates the transformation of the original first-order phase transition to a diffuse type, while simultaneously shifting the Curie temperature toward room temperature. This modification pathway provides a promising avenue for optimizing the comprehensive performances of $BaTiO_3$ and expanding its application potential in pyroelectric, electrocaloric and energy storage fields.

Introduction

Ferroelectric ceramics are extensively utilized in advanced fields such as pyroelectric sensors, energy storage devices, and electrocaloric refrigeration systems. These applications are highly reliant on their phase transition behavior and dielectric properties. For instance, remarkable pyroelectric and electrocaloric effects are typically achieved near the Curie temperature (T_C), where the ferroelectric-to-paraelectric phase transition occurs [1]. Similarly, superior energy storage performance, characterized by low energy loss, requires excellent relaxor ferroelectric characteristics [2].

Barium titanate ($BaTiO_3$) is a classic lead-free ferroelectric material that undergoes a sharp first-order ferroelectric-to-paraelectric phase transition around $T_C \approx 125°C$ [3]. This inherent feature severely restricts its room-temperature pyroelectric, electrocaloric performances, and energy storage capability. To broaden its application scope, cation substitution is the most conventional and effective strategy for tailoring the phase transition and dielectric response. Typical routes include replacing Ba^{2+} with Ca^{2+}, Sr^{2+}, or rare-earth ions (RE^{3+}, where RE = La, Ce, Nd, Sm, Eu, Gd, Dy, Er) and substituting Ti^{4+} with Zr^{4+}, Sn^{4+}, or Hf^{4+} [4].

Different from the conventional cation substitution strategy, this work proposes directly introducing the metal oxide Sb_2O_3 into $BaTiO_3$ ceramics to tailor its phase transition and dielectric response. This novel modification approach is expected to optimize its pyroelectric, electrocaloric, and energy storage performances, thereby further expanding its application scope.

Experimental

$BaTiO_3$+xSb_2O_3 ceramics (x = 0, 0.01, 0.02, 0.03) were prepared by a conventional solid-state reaction method, using $BaCO_3$, TiO_2, Sb_2O_3. The homogenized mixed powders were calcinated at 1150°C for 3 h, followed by sintering at 1350°C for 2 h to obtain bulk ceramics. The phase structures were characterized by an X-ray diffractometer (XRD, Shimadzu LabX, Japan). A differential scanning calorimeter (DSC, TA Q2000, USA) was employed to collect heat flow data. Dielectric properties were measured by precision impedance analyzer (Wayne Kerr WK6500P, UK) coupled with a temperature-control and data-collect system (BALAB DMS-2000, China).

Results and Discussion

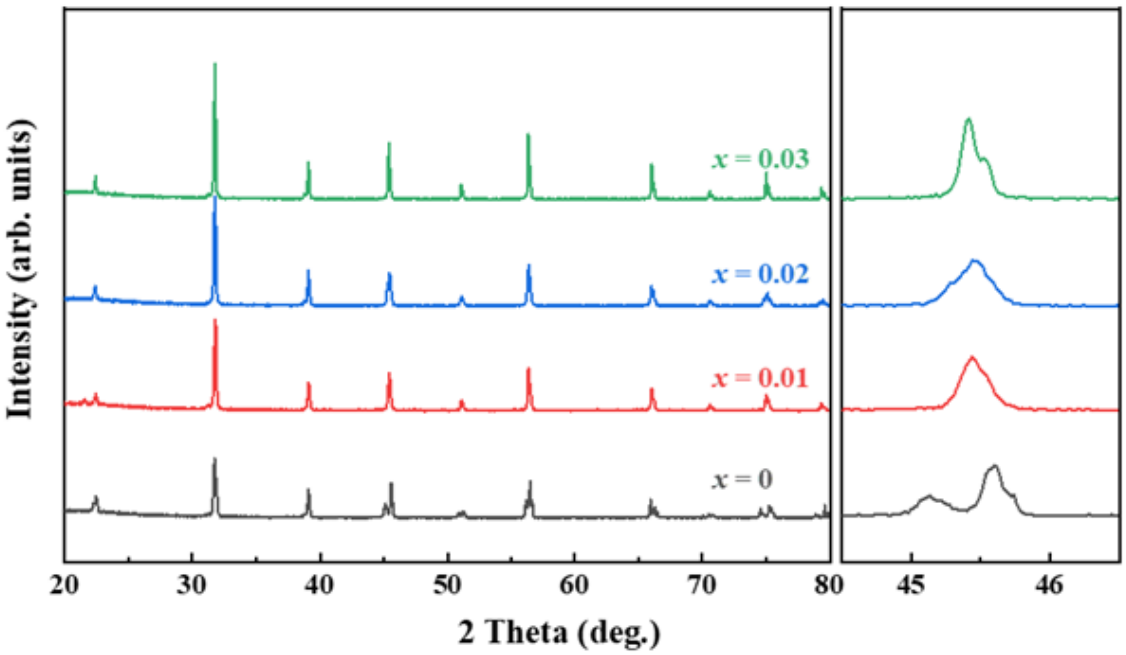

Figure 1: XRD patterns of $BaTiO_3$+xSb_2O_3 ceramics.

Figure 1 presents the XRD patterns of $BaTiO_3$+xSb_2O_3 ceramics. All samples exhibit a pure perovskite structure without detectable secondary phases, indicating that Sb_2O_3 has been fully incorporated into the $BaTiO_3$ lattice. Undoped $BaTiO_3$ displays a distinct (002)/(200) peak splitting at 2θ ≈ 45°, which is consistent with tetragonal (T) P4*mm* symmetry [5]. In contrast, a single diffraction peak is obtained near 2θ ≈ 45° for doped $BaTiO_3$, manifesting a pseudo-cubic structure. This result demonstrates that the introduction of Sb_2O_3 disturbs the long-range ordered lattice structure of $BaTiO_3$.

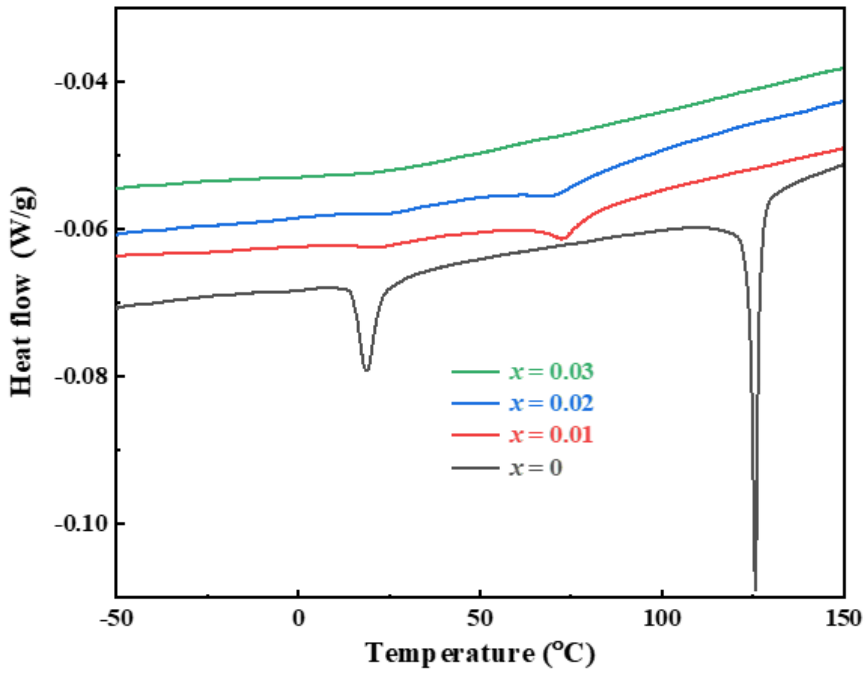

Figure 2: Heat flow curves of $BaTiO_3$+xSb_2O_3 ceramics.

Figure 2 presents the heat flow curves of $BaTiO_3$+xSb_2O_3 ceramics measured in the temperature range of -50°C to 150°C during heating. For pure $BaTiO_3$, two sharp endothermal peaks are observed, among which, the low-temperature peak near 19°C corresponds to orthorhombic-tetragonal (O-T) first-order ferroelectric phase transition, while the high-temperature peak at 125°C, i.e T_C, arises from the tetragonal-cubic (T-C) first-order ferroelectric-to-paraelectric phase transition [6]. When Sb_2O_3 is doped at x=0.01, both endothermal peaks weaken significantly, and TC shifts to a lower temperature (75°C). With further increasing Sb_2O_3 doping content, the endothermal peaks gradually diminish. This indicates that Sb_2O_3 doping facilitates the transformation of the phase transition from a first-order to a diffuse type.

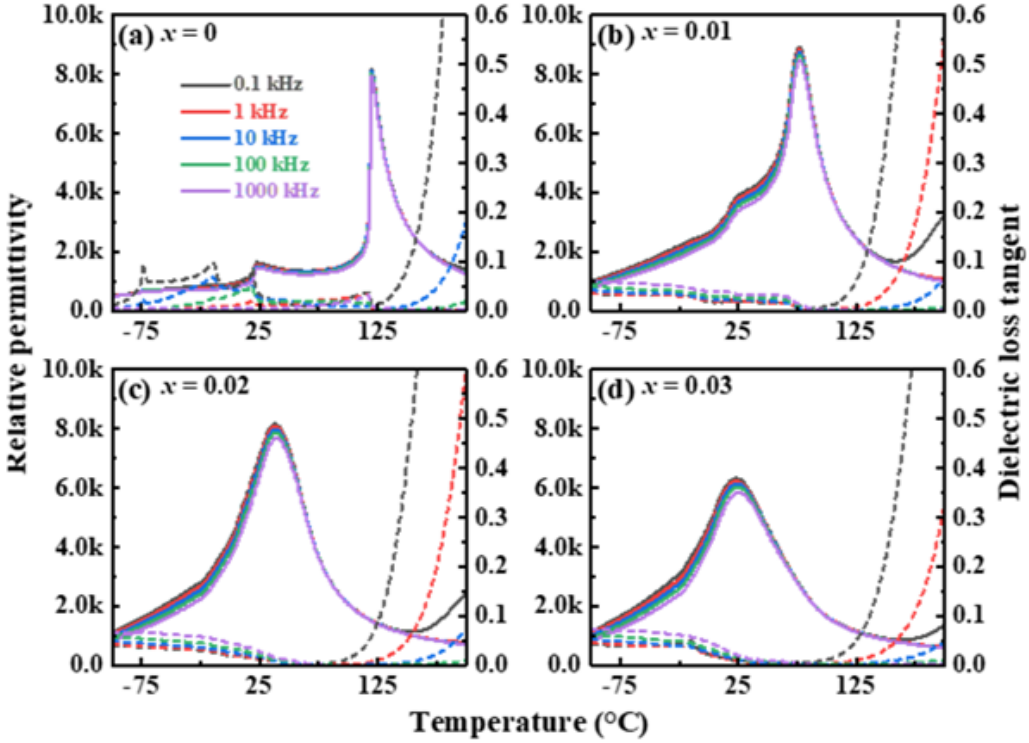

Figure 3: Temperature dependences of dielectric constants and losses of $BaTiO_3$+xSb_2O_3 ceramics.

Figure 3 illustrates the temperature dependences of dielectric constants (ε_r) and losses of $BaTiO_3$+xSb_2O_3 ceramics at frequencies ranging from 0.1 to 1000 kHz. Consistent with the heat flow results, pure $BaTiO_3$ exhibits first-order phase transitions around 19°C (O-T) and 125°C (T-C). Additionally, an extra dielectric peak is observed at -75°C, corresponding to the rhombohedral-orthorhombic (R-O) phase transition [6]. For the x=0.01 doped sample, the T_C shifts to 77°C, and the dielectric peaks corresponding to the R-O and O-T phase transitions become flattened. Notably, x=0.02 and x=0.03 samples only show a single dielectric peak corresponding to T_C at 38°C and 22°C, respectively, which is conducive to their room-temperature applications.

To further quantify the phase transition diffuseness, the modified Curie–Weiss law was employed [7]. Figure 4 displays the plots and linear fittings of $\ln(1/\varepsilon_r\text{-}1/\varepsilon_m)$ and $\ln(T\text{-}T_m)$ at 1000 kHz, where ε_m is the maximum dielectric constant and T_m is the temperature corresponding to ε_m. All sample data can be well fitted linearly, and the slope of the fitting line is defined as the diffusion factor (γ). With the increase of Sb_2O_3 doping content from x = 0 to x = 0.03, the diffusive factor increases from γ = 1.05 to γ = 1.99. A γ value close to 1 indicates a normal ferroelectric, while a γ value approaching 2 is characteristic of a relaxor ferroelectric. This result further confirms that Sb_2O_3 doping converts the phase transition of $BaTiO_3$ from a first-order to a diffuse type.

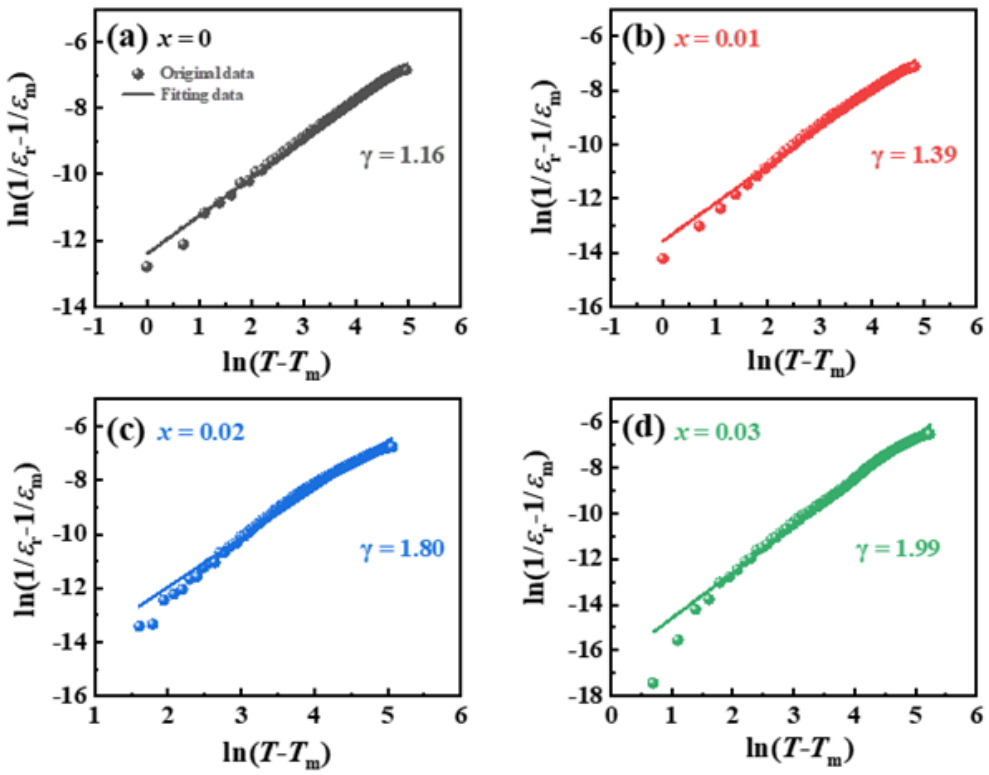

Figure 4: The plots and linear fittings of $\ln(1/\varepsilon_r\text{-}1/\varepsilon_m)$ vs. $\ln(T\text{-}T_m)$ at 1000 kHz.

Conclusion

This work achieves $BaTiO_3$ modification via direct Sb_2O_3 introduction. The results show that Sb_2O_3 can be fully dissolved into the $BaTiO_3$ lattice to form a pure perovskite phase, triggering a structural transformation from tetragonal to pseudo-cubic symmetry. Meanwhile, it converts original first-order phase transition of $BaTiO_3$ to a diffuse type, endowing the material with relaxor ferroelectric properties, and shifts the Curie temperature toward room temperature. This novel modification strategy provides effective support for optimizing the performances of $BaTiO_3$ and expanding its application prospects.

Acknowledgement

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