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HIGH-DIELECTRIC-CONSTANT FERROELECTRIC THIN FILM AND BULK CERAMIC
CAPACITORS FOR POWER ELECTRONICS*

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High-Dielectric-Constant Ferroelectric Thin Film and Bulk Ceramic Capacitors for Power Electronics

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Abstract

Significant effort is presently focused on reducing the size and weight of power electronic modules. To achieve these goals in high-power capacitors, alternative materials and fabrication processes are needed. Thin film (<0.5 μm) and bulk capacitors that use perovskite-based ferroelectric dielectrics are promising alternative technologies.

Ferroelectrics possess high dielectric constants, thus offering substantial increases in volumetric capacitance. In thin film form, these materials display low loss and high breakdown strength. The unique properties of some of these materials, such as a nonlinear dielectric response or a high energy-storage capacity accompanying a phase change, can be exploited for power electronic capacitors.

Prototype capacitors of two such materials, $(\text{Ba,Sr})\text{TiO}_3$ and PbZrO_3 , have been fabricated in both thin film and bulk ceramic form. The influence of fabrication conditions on dielectric properties has been studied. Initial studies have demonstrated the viability of perovskite ferroelectrics for next-generation capacitor components.

Introduction

Significant achievements have been made in power electronic circuit designs and module components. Considerable attention is now concentrated on improving overall performance while reducing module size, weight, and cost. Although progress has been made in active components such as IGBT switches, substantial technological advances are needed in capacitors.

Aluminum oxide or tantalum oxide electrolytic capacitors are commonly used as DC bus capacitors due to their high energy densities. However, these capacitors are polar, exhibit high equivalent series resistance (ESR) that causes excessive thermal losses under high-frequency ripple currents, and their voltages must be substantially lowered to avoid catastrophic failure. Given these limitations and the excessive weight and size of these capacitors, alternative technologies are needed. Desired improvements include increased capacitance density, decreased electrical and thermal losses, improved packaging, and improved reliability and lifetimes.

Ferroelectric oxides, specifically $(\text{Ba}_{1-x}\text{Sr}_x)\text{TiO}_3$ (annotated as BST) and PbZrO_3 , exhibit high dielectric constants and breakdown fields with low dielectric loss. BST offers the advantage of relative ease of fabrication due to the absence of volatile lead, and lack of structural and ferroelectric phase

transitions under operating conditions. However, the antiferroelectric/ferroelectric (AFE/FE) transition in PbZrO_3 can be exploited to yield high volumetric capacitance densities.

Capacitor technologies can be compared in terms of their dielectric constants, breakdown fields, and energy storage volumetric densities (Table 1). Polymers and simple oxides are linear dielectrics and their energy densities can sufficiently be expressed by the dielectric constant (K) and breakdown field (E_b).^{1,2} Ferroelectrics, however, display a non-linear dielectric response. The dielectric constants and the energy density for BST thin films have been calculated on the basis of the Landau-Ginzburg-Devonshire formalism.³ The field given for BST films in Table 1 is that at which substantial leakage currents were observed in a 100 nm film.⁴ In AFE/FE PbZrO_3 , a linear polarization response is observed up to the phase-switch electric field (E_s) and then increases significantly as the dielectric switches from the antiferroelectric to the ferroelectric state (Fig. 1). High dielectric constants and energy densities are achieved at the switch field, well below the breakdown field. This non-linear dielectric response in the ferroelectrics can be exploited for non-linear snubber capacitors with reduced power losses.⁵

Material	K	E_b (E_s) (MV/cm)	Energy Density (J/cm ³)
Polymers	~2.5	~4	2
Electrolytic Alumina	9	8	26
AFE/FE PbZrO_3	12,000	0.12	3.2
BST film	500 (120)	1.0	11

Table 1. Dielectric constant (K), breakdown field (E_b) or switching field (E_s) for AFE/FE PZT, and energy density of dielectric materials. Dielectric constant at E_b for BST film is given in parentheses.

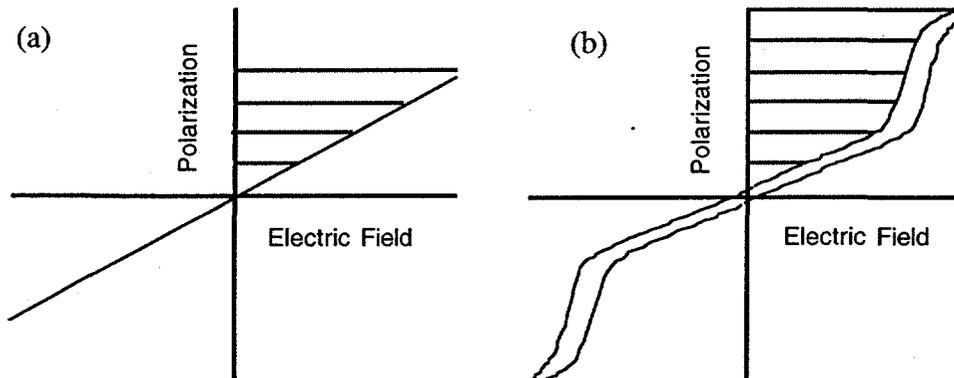


Fig. 1. Schematic polarization-electric field plots for (a) linear dielectric and (b) AFE/FE. Total electric energy stored in a dielectric material is represented by the hatched areas.

Capacitor architecture also plays a significant role in device performance. Ceramic capacitors are typically tape-cast structures consisting of 10 to 100 μm thick ceramic dielectric layers sandwiched between interdigitated noble-metal electrodes. Vapor-deposited thin film dielectric layers ($<0.5 \mu\text{m}$) exhibit better materials uniformity, higher density, and smoother electrode-dielectric interfaces, all of which lead to higher breakdown strengths. Indeed, vapor-deposited BST thin film capacitors have shown⁶ breakdown fields as high as 3 MV/cm, and dissipation factors of $\approx 0.2\%$ over several frequency decades.⁷ Additionally, mechanical clamping of the dielectric film by the substrate improves the temperature stability.³ Thin film capacitor technologies will also result in smaller device footprints and the possibility of integrating capacitors directly onto silicon-based switching circuits.

Initial results on BST thin films and AFE/FE PbZrO_3 capacitors are discussed in the following sections.

BST Thin Film Capacitors

BST thin film capacitors have been fabricated by two vapor deposition techniques extensively used in the semiconductor industry, i.e. metalorganic chemical vapor deposition (MOCVD) and sputtering. Both of these techniques offer compositional and morphological uniformity with high device yields. Prototype capacitors were fabricated by depositing BST films on 1200 \AA Pt/3000 \AA SiO_2 coated Si (100) substrates (Fig. 2). The Pt layer had a (111) out-of-plane orientation and served as the bottom electrode. The BST films were characterized by X-ray diffraction (XRD), Rutherford backscattering spectroscopy (RBS), scanning electron microscopy (SEM), atomic force microscopy (AFM), and X-ray fluorescence spectroscopy (XRF). Pt top electrodes (1000 \AA) were deposited by electron beam evaporation, and electrical transport measurements (Keithley 237 source-measurement unit) and dielectric measurements (HP4192 impedance analyzer at 10 kHz and 0.2V AC oscillation) were made on the capacitors.

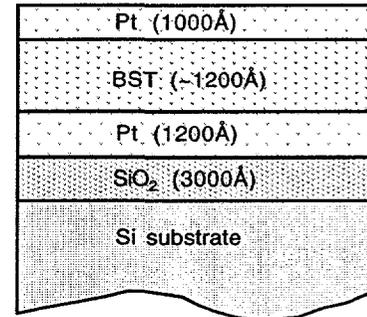


Fig. 2. Schematic diagram of the thin film capacitor structure.

BST thin films by MOCVD

Chemical vapor deposition (CVD) uses heterogeneous gas/solid reactions to synthesize a thin film. Gaseous precursors are introduced into the reactor and a solid film is formed by chemical reactions on or near the heated substrate. In MOCVD, these precursors are evaporants of metalorganic species that pyrolyze at moderate substrate temperatures. Excellent thickness and compositional uniformity over large areas have been demonstrated by MOCVD. Because the reactants diffuse to the growth surface, the process is not line-of-sight and therefore conformal coverage of complex topographies can be obtained. Indeed, CVD has been used to deposit conformal dielectric films on etched Si substrates with a 85x increase in surface area while maintaining a small footprint.⁸

A primary consideration in MOCVD growth is a stable and robust precursor delivery system. Strict control of reactant gas chemistry is needed because the dielectric response of BST is strongly dependent on film composition. BST films were deposited with a commercial liquid precursor delivery tool (ATMI LDS-300B) that allows fine compositional control with a high degree of process reproducibility.⁹ Liquid solutions of the metalorganics are metered to a flash evaporator and the vapor stream is then directed into the reactor. The cold-wall quartz vertical reactor was designed at Argonne National

Laboratory and incorporates several features to prevent condensation and/or premature decomposition of the reactant gas stream. The gases exit the inlet through a showerhead mesh screen that distributes the vapor stream over a 15 cm deposition area.

BST films were deposited at 650°C at 4 Torr total pressure. Film composition was controlled by adjusting the LDS parameters to obtain Ba:Sr ratios of 70:30 and Ti compositions of 45-55 at.% as determined by RBS and XRF. XRD revealed the films to be polycrystalline without the need for a postdeposition anneal and typically exhibited a (111) out-of-plane orientation. Excellent film uniformity was obtained over a 100 mm diameter wafer as indicated by a uniform thickness fringe and confirmed by RBS. Growth rates were typically on the order of $\approx 5\text{-}10 \text{ \AA}/\text{min}$, but rates as high as $50 \text{ \AA}/\text{min}$ have been achieved over the course of reactor design cycles. Dielectric constants of 580 were measured at zero bias and 178 at an electric field of 0.4 MV/cm. This corresponds to a capacitance density of $4.3 \mu\text{F}/\text{cm}^2$ and $1.3 \mu\text{F}/\text{cm}^2$ respectively. Dissipation factors as low as 4% and breakdown fields of 0.5 MV/cm have been measured. A parametric study of the role of process variables on capacitor performance is currently underway.

Sputter deposited BST thin film capacitors

BST thin films were deposited in a commercial magnetron sputtering system (Edwards Auto 306). Films were deposited at 95 W Rf power in a 4:1 Ar-O₂ sputtering gas mixture. The substrates were positioned opposite a 7.6 cm Ba_{0.5}Sr_{0.5}TiO₃ target (Johnson-Matthey) in an rotating heated substrate holder that improved the film composition and thickness uniformity. The target-substrate distance was adjusted to obtain 7% thickness uniformity over a 7.6 cm diameter area with growth rates of $\approx 10 \text{ \AA}/\text{min}$.

Sputtered BST films were polycrystalline, with a mixed (100) and (110) out-of-plane grain orientation. The films exhibited a dense crack-free microstructure with an RMS surface roughness of 2 nm. Film composition, both Ba/Sr and (Ba+Sr)/Ti ratio, depended strongly on the sputtering pressure and had a significant influence on the electrical properties. Deposition at 10 mTorr resulted in a Ti-rich film and a low zero-bias dielectric constant of 293 (Fig. 3). Near-stoichiometric films deposited at 15 mTorr exhibited a zero-bias dielectric constant of 880. These films also exhibited dissipation factors of 2% and breakdown strengths of 0.9 MV/cm. Leakage current densities were on the order of $3 \times 10^{-8} \text{ A}/\text{cm}^2$ for a 2 V excitation.

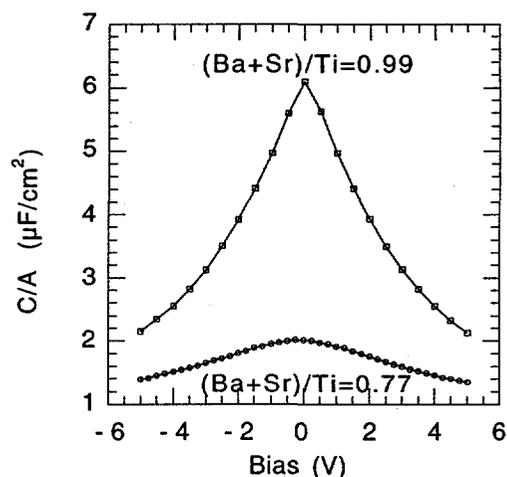


Fig. 3. Capacitance-voltage curves of two Pt/sputtered BST/Pt capacitors with two different (Ba+Sr)/Ti compositions.

AFE/FE Capacitors

Bulk PbZrO₃-based AFE/FE single layer capacitors were made by hot pressing pellets at temperatures $>1200^\circ\text{C}$ to achieve a high density. Polarization of a AFE/FE phase-switch material is shown in Fig. 4a. The stored energy of this capacitor is $\approx 3.2 \text{ J}/\text{cm}^3$, although energy densities as high as $12 \text{ J}/\text{cm}^3$ have been reported for PbZrO₃-based ceramic materials.¹⁰ The hysteresis loop area above the AFE/FE transition defines the energy lost in the dielectric. Large hysteresis losses will result in excessive heating of the capacitor at high inverter switching frequencies. However, the hysteretic losses, can be reduced by appropriate chemical formulations such as La, Sn, and other rare-earth

substitutions.^{11,12} The slope of the polarization versus electric field plot is proportional to the dielectric constant (Fig 4b). The dielectric constant is relatively modest at low fields and increases to >12,000 at the AFE/FE switch field of 0.12 MV/cm. This is a substantial improvement over common ceramic dielectric formulations that exhibit dielectric constants <1000 at electric field levels >0.10 MV/cm.²

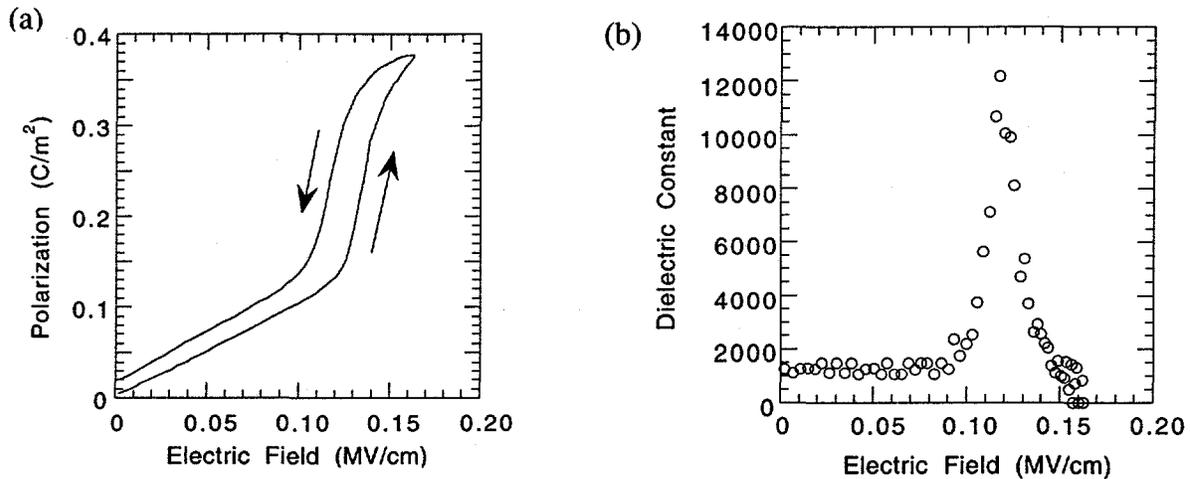


Fig. 4. PbZrO₃-based AFE/FE capacitor (a) AFE/FE polarization curve. Arrows indicate increasing or decreasing electric field. (b) Dielectric constant of PbZrO₃-based material derived from the slope of the polarization curve.

The required dielectric thickness of a capacitor made from an AFE/FE material is determined by the switch field and the application voltage. For example, 350 VDC bus capacitors for automotive applications would require a dielectric thickness of 290 μm . Layers of this thickness can be fabricated by tape casting, a common ceramic manufacturing technique. Future development of these materials will be directed toward minimizing hysteresis losses and controlling the temperature dependence of the AFE/FE switch behavior.

Conclusions

Initial results on high-dielectric-constant ferroelectric films and multilayers have shown these technologies to be viable solutions for advanced capacitors. A complete study of process parameter effects on performance is being investigated to develop a fundamental physical understanding of these materials and to arrive at robust processing schemes. In addition, integration of base metal electrodes to reduce capacitor cost is being explored. These efforts will lead to improved capacitor technologies for power electronic systems.

Acknowledgment

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