Electrical conduction mechanism in high-dielectric-constant (Ba0.5,Sr0.5)TiO3 thin films
Shao-Te Chang and Joseph Ya-min Lee

Citation: Appl. Phys. Lett. 80, 655 (2002); doi: 10.1063/1.1436527
View online: http://dx.doi.org/10.1063/1.1436527
View Table of Contents: http://apl.aip.org/resource/1/APPLAB/v80/i4
Published by the American Institute of Physics.

Related Articles
Reduced leakage current, enhanced ferroelectric and dielectric properties in (Ce,Fe)-codoped Na0.5Bi0.5TiO3 film
Modified Johnson model for ferroelectric lead lanthanum zirconate titanate at very high fields and below Curie temperature
Engineering titanium and aluminum oxide composites using atomic layer deposition
J. Appl. Phys. 110, 123514 (2011)
High dielectric tunability of (100) oriented PbxB1xTiO3 thin film coordinately controlled by dipole activation and phase anisotropy
J. Appl. Phys. 110, 124107 (2011)
Kelvin probe force gradient microscopy of charge dissipation in nano thin dielectric layers
J. Appl. Phys. 110, 084304 (2011)

Additional information on Appl. Phys. Lett.
Journal Homepage: http://apl.aip.org/
Journal Information: http://apl.aip.org/about/about_the_journal
Top downloads: http://apl.aip.org/features/most_downloaded
Information for Authors: http://apl.aip.org/authors

Submit Now
Explore AIP’s new open-access journal
- Article-level metrics now available
- Join the conversation! Rate & comment on articles

ADVERTISEMENT
Electrical conduction mechanism in high-dielectric-constant (Ba$_{0.5}$,Sr$_{0.5}$)TiO$_3$ thin films

Shao-Te Chang and Joseph Ya-min Lee

Department of Electrical Engineering, Tsing-Hua University, Hsinchu, Taiwan, Republic of China

(Received 18 July 2001; accepted for publication 15 November 2001)

The electrical conduction mechanism of (Ba$_{0.5}$,Sr$_{0.5}$)TiO$_3$ (BST) as a function of the temperature was studied. Au/BST/Pt metal–insulator–metal capacitors were fabricated. The temperature range was from 300 to 423 K. The conduction current depended on the voltage polarity. At high electrical field (>800 kV/cm) and with the Pt electrode biased negatively, the Pt/BST interface forms a Schottky barrier with a barrier height of 0.58 eV from 300 to 373 K. The Au/BST interface forms an ohmic contact. The conduction current when the Au electrode is biased negatively shows space-charge-limited-current behavior. An energy band diagram is proposed to explain the experimental results.

The paraelectric barium strontium titanate (Ba$_{0.5}$,Sr$_{0.5}$)TiO$_3$ (BST) is a promising candidate for application of dynamic random access memories (DRAMs) in very large scale integrated (VLSI) circuits due to its large dielectric constant with no aging and fatigue effects. However, before BST films can be fully utilized, its electrical properties such as its conduction mechanism$^{1–10}$ and resistance to degradation$^{5,9}$ need to be better understood. Considerable effort has been made to reduce the leakage current level and to identify the conduction mechanism in BST thin film capacitors. The leakage mechanisms proposed include Schottky emission,$^{1–4,6,7}$ Poole–Frenkel emission,$^{2,3,7}$ space-charge-limited current,$^5$ ionic space-charge-limited current,$^8$ and modified Schottky emission.$^{10}$ Schottky emission is most widely used to describe the conduction mechanism at the Pt/BST interface. But the extracted values of the barrier height in the literature vary widely from 0.46 to 1.7 eV.$^{1,3,4,7,11}$ In this letter, the temperature dependence of the conduction current of BST capacitors is studied to identify the conduction mechanism. The electrical characteristics at both the Pt/BST and the Au/BST interfaces are discussed.

N-type (100) orientation silicon wafers with a resistivity of 8–10 Ω cm are used as the starting substrates. A thermal silicon dioxide layer with a thickness of 500 nm is grown first. A double layer of titanium (150 nm) and platinum (100 nm) is then deposited. The titanium is used to improve adhesion and the platinum is used as the bottom electrode. The BST thin films are deposited by rf magnetron sputtering at a substrate temperature of 550 °C. The composition of the sputtering target is (Ba$_{0.5}$Sr$_{0.5}$)TiO$_3$. The sputtering gas is a mixture of Ar and O$_2$. The flow rates of Ar and O$_2$ are 13.5 and 5 sccm, respectively. The total pressure during deposition is 10 mTorr. The film thickness is measured by ellipsometry and the BST film thickness is about 190 nm. The 300-nm-thick top Au electrode is evaporated and patterned using a lift-off process. The top gold electrodes are squares of 150 μm × 150 μm.

The crystalline phase of the BST thin films was identified by x-ray diffraction (Shimatzu XD-5). The current–voltage (I–V) characteristics were measured by a Keithley 236 electrometer. The sample temperature was varied by using a hot plate. The capacitance–voltage (C–V) characteristics were measured by a HP4294 precision LCR meter. All experimental data reported in this letter are average values of at least five specimens.

The leakage current in a dielectric consists of electronic conduction current and polarization current. The polarization current can be expressed as dP/dt, where P is the electric polarization and t is the time. The polarization current is expected to gradually saturate as the applied voltage increases. The BST leakage current in this work was measured with 0, 3, and 5 s delay times between each voltage step. Because the BST samples are paraelectric, the polarization current is relatively small. The leakage current at high electric field is dominated by the electronic conduction current. It was also observed that the BST films became stressed during leakage current measurements with delay times longer than 3 s and that the BST breakdown voltage degraded. Because an analysis of the conduction mechanism employs I–V data mainly at electric fields higher than 800 kV/cm, the leakage current data taken with zero delay time are used to minimize the degradation effect of the BST films.$^3$ The bias voltage is defined as positive when positive voltage is applied to the top Au electrode. Figure 1 shows the current and voltage characteristics under positive and negative biases in the temperature range from 300 to 423 K. The I–V characteristics depend on the bias polarity. As a result, the conduction mechanism should be electrode limited for at least one of the metal–insulator junctions.

The Schottky emission can be expressed as

$$J = A \frac{S}{2} T^{2} \exp \left( - \frac{q(\varphi_B - \sqrt{qE/4\pi\varepsilon_0\varepsilon_r})^2}{kT} \right) \right),$$

where $A$, $q$, $\varphi_B$, $\varepsilon_0$, and $\varepsilon_r$ are the effective Richardson constant, potential barrier height, permittivity of free space, and dynamic dielectric constant, respectively. If the conduction current is governed by Schottky emission, the log($J/T^2$) vs $E^{1/2}$ plot should be a straight line and the slope will give the dynamic dielectric constant. The dynamic dielectric con-
constant is about 4 according to the square of the refractive index $n^2$. Figure 2 shows the Schottky emission plot with the dynamic dielectric constants calculated. Although ideally the barrier height can be calculated from the intercept in Fig. 1, the error will be large due to the uncertainty in $A^\ast$. The barrier height is thus calculated using a plot of $\log(J/T^2)$ vs $1/T$. The barrier height is extracted from the slope and the uncertainty in $A^\ast$ will not be a factor. When the temperature is higher than 373 K, the conduction current is insensitive to the temperature and the calculated dynamic dielectric constant deviates from the ideal value of 4. The $\log(J/T^2)$ vs $10^3/T$ plot using the same set of data is reasonably linear between 300 and 373 K, but become somewhat saturated above 373 K at high field. The slope in the $\log(J/T^2)$ vs $10^3/T$ plot gives the effective barrier height $q(\varphi_B - \sqrt{qE}}/4\pi\varepsilon_0\varepsilon_r)$]. The barrier height $q\varphi_B$ of 0.58 eV at the BST/Pt interface is obtained by extrapolating the electric field to zero. Only the data at an electric field higher than 0.8 MV/cm are used in the calculation.

Figure 3 shows a log-log plot of the current density ($J$) versus the applied voltage ($V$) with the Au electrode biased at negative voltage. The slopes are all close to 1 in the low voltage range for all temperatures from 300 to 423 K. The Au/BST contact is thus ohmic at low electric field. At higher bias voltages above 1.8 V, the $\log(J)$ vs $\log(V)$ plot shows a slope of 2–3 which agrees well with space-charge-limited current (SCLC) theory. The conduction current from SCLC with traps can be expressed as

$$J = \frac{9}{8} \varepsilon_r\varepsilon_0\mu\frac{V^2}{d},$$

where $V$ is the applied voltage, $d$ is the film thickness, $\varepsilon_0$ is the permittivity of free space, $\varepsilon_r$ is the dielectric constant of the insulator, $\mu$ is the mobility, and $\theta$ is the ratio of free-to-trapped electrons. Assuming a discrete shallow trap level in the insulator, the trapped electron density ($N_t$) can be calculated from the trap-filled limit voltage ($V_{TFL}$) using

$$N_t = \frac{9}{8q}\varepsilon_r\varepsilon_0\frac{V_{TFL}}{d^2},$$

where $q$ is the electronic charge. Experimentally, $V_{TFL}$ and $\theta$ obtained from Fig. 3 are 4.6 V and $10^{-3}$, respectively. The calculated value of $N_t$ at 300 K is $1.2 \times 10^{18}/\text{cm}^3$. The trap level $E_t$ can be calculated using

$$\theta = \frac{N_c\exp[(E_t - E_c)/kT]}{gN_t},$$

where $N_c$ is the density of states at the Fermi level. The energy level $E_t$ can be calculated from the trap-filled limit voltage $V_{TFL}$ using

$$\theta = \frac{N_c\exp[(E_t - E_c)/kT]}{gN_t},$$

where $g$ is the density of states at the Fermi level.
where $N_c$ is the effective density of states in the conduction band, and $g$ is the degeneracy factor ($\sim 2$). $N_c$ is assumed to be $10^{21}/\text{cm}^3$. Thus $E_c - E_t = 0.335$ eV. Based on the above results, an energy band diagram of the Au/BST/Pt capacitor structure is proposed in Fig. 4.

In summary, the temperature dependence of the $I-V$ characteristics of (Ba$_{0.5}$Sr$_{0.5}$)TiO$_3$ thin film capacitors was studied. Au/BST/Pt MIM capacitors were fabricated. The potential barrier height of 0.58 eV at the Pt/BST interface was calculated from log($J/T^2$) vs $1/T$ plots. The Au/BST contact was ohmic. The conduction mechanism with the Au biased at negative voltage was space-charge-limited current. The trap density ($N_t$) in BST was calculated to be $1.2 \times 10^{18}/\text{cm}^3$ and the trap level ($E_t$) is 0.335 eV below the conduction band edge. An energy band diagram of the Au/BST/Pt structure was proposed based on the experimental results.

This work was supported by the National Science Council, Taiwan, Republic of China, under Contract No. NSC89-2215-E-007-044.