Leakage Mechanisms

- Thin films, fully depleted
  - Leakage controlled by combined thermionic / field emission across the Schottky barrier at the film-electrode interfaces. Film quality effects barrier height, and mobilities of carriers.

- Thicker films of interest for higher voltage applications
  - Poorly understood
Much effort has gone into studying the **leakage** of perovskite-
type titanate thin films, including SrTiO$_3$, (Ba,Sr)TiO$_3$, and
Pb(Zr,Ti)O$_3$:

Proposed conduction mechanisms for BST thin films:

- Fowler-Nordheim tunneling (interface, bulk)
- Poole-Frenkel effect (bulk)
- Thermionic emission across Schottky barriers (interface)

The most favored mechanism:

Schottky-barrier limited current flow
### “Bulk” -Controlled vs. “Interface” -Controlled (Injection-Limited)

<table>
<thead>
<tr>
<th>“Bulk” -Controlled</th>
<th>“Interface” -Controlled</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ionic (high T, long time)</td>
<td>Schottky Emission</td>
</tr>
<tr>
<td>Tunneling (through film) (High E)</td>
<td>Field Emission</td>
</tr>
<tr>
<td>Bulk Doping (acceptors, donors, etc.)</td>
<td>Contact Photoexcitation</td>
</tr>
<tr>
<td>Photoexcitation (light effect)</td>
<td>Fowler-Nordheim Tunneling (can be bulk as well)</td>
</tr>
<tr>
<td>Trapping/Detrapping (Poole Frenkel)</td>
<td>Space-Charge-Limited (can be bulk as well)</td>
</tr>
<tr>
<td><strong>Hopping Conduction (Localization)</strong></td>
<td></td>
</tr>
</tbody>
</table>

### Thin Films                Thick(er) Films                Failure Mode

NC State
Lack of complete and careful analyses of leakage in BST thin films

- Experimental: Using a ramp or voltage step technique.
  - danger of relaxation currents contribution in the analyses
- Field and temperature dependencies:
  - Only field- or temperature-dependent data not sufficient for understanding the mechanism!
- Assumed values for the parameters in the model such as Richardson constant.
- Inhomogeneity of Schottky barrier, interfacial roughness, etc.
Leakage vs. A:B Site Ratio

\[ t = 30 \text{ nm}; \quad T = 125, 150, 175, \text{ and } 200^\circ\text{C}, \quad 0 < V < 3.5V \]
Leakage vs. A:B Site Ratio

\[ \ln \left( \frac{J}{T^2} \right) = \ln A^{**} + \frac{\alpha E^{1/2} - W_b}{k_B T} \]
Leakage vs. A:B Site Ratio

\[ J = A^{**}T^2 \exp\left( \frac{\alpha E^{1/2} - W_b}{k_B T} \right) \]

<table>
<thead>
<tr>
<th>Ti Content</th>
<th>( W_b ) (eV)</th>
<th>( \alpha )</th>
<th>( A ) (A/cm(^2)K(^2))</th>
</tr>
</thead>
<tbody>
<tr>
<td>51%</td>
<td>1.05</td>
<td>0.00085</td>
<td>4.0e-6</td>
</tr>
<tr>
<td>51.5</td>
<td>1.28</td>
<td>0.00066</td>
<td>4.2e-3</td>
</tr>
<tr>
<td>52</td>
<td>1.44</td>
<td>0.00080</td>
<td>1.2e-2</td>
</tr>
<tr>
<td>53</td>
<td>1.17</td>
<td>0.00069</td>
<td>9.1e-5</td>
</tr>
<tr>
<td>53.5</td>
<td>0.92</td>
<td>0.00084</td>
<td>3.3e-9</td>
</tr>
</tbody>
</table>
Depletion Widths

❖ **Issue:** What are the depletion lengths?
  ➢ 5 – 10 nm
  ➢ > film thickness (i.e. > 100 nm)

❖ **Why is this an issue?**
  ➢ Explanation of C-V behavior
  ➢ Affects development directions and ultimate performance predictions

❖ **Case for fully depleted film**
  ➢ Field dependence in a thickness series:
    J(E,T) is almost independent of thickness ➔ Field dropping across entire film thickness
  ➢ Frequency dependence of permittivity
    ✦ Depletion layer ➔ step frequency dependence
Consider 2 cases for a 200 nm film

\[ d_i = 10 \text{ nm} \]
\[ \tau = C_i \times R \]

❖ Case 1:

\[ \tau < 10^{-4} \text{ Hz} \]
\[ R_b \sim 10^{11} \Omega \]
\[ n \sim 10^{11} \text{ m}^{-3} \]

➤ Not high enough carrier density to cause band bending

❖ Case 2:

\[ \tau > 10^9 \text{ Hz} \]
\[ \sigma_b = \frac{d - 2d_i}{AR_b} \sim 30 \text{ (}\Omega \text{m})^{-1} \]

➤ This is strongly semiconducting.
Failure Modes: Resistance Degradation

- Change in resistivity of a sample caused by migration of charged point defects, leading to increased leakage and eventually breakdown


Resistance Degradation and Lifetime: Thickness Dependence

Observed thickness dependence manifests itself as a decrease in the activation energy with respect to temperature.

Waser: bulk SrTiO$_3$, $n \sim 2.5$ @ 2 kV/cm, 270°C

The measured resistance degradation lifetime at this temperature and in this field increases as the Ti content is increased to 52.0 at%Ti, and then decreases with higher at%Ti.
Resistance Degradation and Lifetime: Temperature Dependence

Temperature dependence clearly follows an Arrhenius-type behavior:

\[ t_d = t_0 \exp\left(\frac{Q_T(V)}{kT}\right) \]
Resistance Degradation and Lifetime: Voltage/Field Dependence

It is difficult to distinguish the different functional forms of voltage/field dependence, given the electric field range investigated:

\[ t_d = t_0 \exp \left( -\frac{qV}{Q_v(T)} \right) \]  

most conservative

\[ t_d = t_0 V^{-n} \]

\[ t_d = t_0 \exp \left( \frac{Q_v(T)}{qV} \right) \]  

least conservative
Resistance Degradation and Lifetime: Estimation of Lifetimes

51.0 at\%Ti BST Films

(Previously extrapolated to 1.6 V)

Extrapolated Lifetime, $t_d$ (s)

$1000/T$ (1/K)

85°C

10 years

(Previously extrapolated to 85°C)

Extrapolated Lifetime, $t_d$ (s)

1.6 V

10 years

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Resistance Degradation and Lifetime:
Modification Of Leakage Behavior

Oxygen vacancies are mobile defects under the given experimental conditions: electromigration toward cathode.

“Modification of Schotky barrier heights/band structure”
(different than bulk resistance degradation mechanism)

Also: Spatial modification of carrier concentrations due to the spatial variation in the oxygen vacancy concentration between the two electrode: change in conductivity of the bulk film.

The accumulation of oxygen vacancies in front of the cathode creates an internal built-in potential at the interface. This space charge modifies the band structure and thus interfacial energy barriers: The difference in barrier heights then appears as an internal bias in the film.
Resistance Degradation and Lifetime: Modification Of Leakage Behavior

The differences in barrier heights:

- $4\times t_s$: 0.13 eV
- $5\times t_s$: 0.21 eV
- $7\times t_s$: 0.22 eV

**Diagram 1:**
- 53.0 at% Ti
- Thickness: 40 nm
- T = 25°C
- **(-) Polarity**
  - 4xt$_s$ (- deg.)
  - 5xt$_s$ (- deg.)

**Diagram 2:**
- 53.0 at% Ti
- Thickness: 40 nm
- T = 25°C
- **(+) Polarity**
  - 7xt$_s$ (+ deg.)
  - Fresh
Resistance Degradation and Lifetime: Modification Of Leakage Behavior

The peak shift in C-V: 0.12 V
Resistance Degradation and Lifetime: Modification Of Leakage Behavior

The peak shift in C-V: 0.20 V

- 5 -4 -3 -2 -1 0 1 2 3 4 5
- 5 -4 -3 -2 -1 0 1 2 3 4 5

53.0 at% Ti
5t: 40 nm
T = 25°C

Peak Shift: 0.20 V

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Resistance Degradation and Lifetime: Modification Of Leakage Behavior

The peak shift in C-V: 0.20 V

53.0 at% Ti

- Bias (V)

C/A (F/μm²)

Peak Shift: 0.20 V

5.0 at% Ti

- Bias (V)

C/A (F/μm²)

Peak Shift: 0.20 V

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Resistance Degradation and Lifetime: Modification Of Leakage Behavior

Recovery anneal studies:
Negative polarity currents were completely recovered.
Positive polarity currents decreased further.

![Graph showing current density vs. V^{1/2} for different conditions.]

- 53.3 at% Ti
- Thickness: 40 nm
- T = 25°C

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C-V behavior indicates that resistance degradation is recoverable.