A Reliability Model for Ni-BaTiO₃-Based (BME) Ceramic Capacitors

David (Donhang) Liu, Ph.D.
Sr. Staff Engineer II
ASRC Space and Defense
NASA Goddard Space Flight Center
Greenbelt, MD 20771

To be presented by David Liu at the International Microelectronics Assembly and Packaging Society (IMAPS) Chesapeake Chapter meeting, Johns Hopkins University Applied Physics Laboratory, Laurel, MD, July 23, 2014.
Outline

• General expression of reliability for ceramic capacitors with base-metal electrodes (BMEs)
  – Statistical model
  – Acceleration functions
    • Catastrophic: Power-law (Prokopowicz and Vaskas)
    • Slow degradation: Exponential

• Improved reliability model of BME ceramic capacitors
  – Impact of grain size
  – Impact of dielectric thickness
  – Impact of number of dielectric layers
  – Impact of chip size
  – General reliability model

• Application example(s)

• Summary
A General Expression of Reliability for MLCCs

\[ R(t) = \varphi(N, d, \bar{a}, S) \times AF(V, T) \times \gamma(t) \]

\( \gamma(t) \): Statistical distribution that describes the individual variation of properties (Weibull, log normal, normal)

\( AF(V, T) \): Function that describes the lifetime of a device in response to external stresses (independent of individual units)

\( \varphi(N, d, \bar{a}, S) \): Effects due to the characteristics of a capacitor device (structure, construction, etc.)

- Statistical distribution:
  - 2-parameter Weibull: \( \gamma(t) = e^{-\left(\frac{t}{\eta}\right)^\beta} \)
  - A function of time; always decreases with time
  - Probability of a failure occurring: \( \gamma(t) = [0, 1] \)
  - Durability of an MLCC that can function normally during wearout:
    - When \( \beta > 3 \) and \( t < \eta \), \( R(t) \sim 1 \), a reliable life span before \( \eta \)
    - When \( \beta > 3 \) and \( t > \eta \), \( R(t) \sim 0 \), parts failed rapidly after \( \eta \)
A two-stage dielectric wearout failure mode is better for describing the failure behavior in BME MLCCs with BaTiO$_3$ dielectrics (supported by recent failure analysis results)

- **Slow degradation**: leakage increases with time nearly linearly due to oxygen vacancy migration until the failure criterion (100 $\mu$A) is reached (parts failed prior to catastrophic failure)
- **Catastrophic failure**: leakage increases gradually, followed by time-accelerating catastrophic failures
Determination of Acceleration Functions (Cont’d)

• Previous studies have shown that for the two different failure modes, the acceleration functions appear to be different


  ➢ **Catastrophic** failures fit power-law (*P-V equation*):

\[
\frac{MTTF_1}{MTTF_2} = \left(\frac{V_2}{V_1}\right)^n \exp\left[\frac{E_a}{k} \left(\frac{1}{T_1} - \frac{1}{T_2}\right)\right]
\]

  ➢ **Slow degradation** failures fit exponential-law:

\[
\frac{MTTF_1}{MTTF_2} = \exp[-b(E_1 - E_2)] \exp\left[\frac{E_a}{k} \left(\frac{1}{T_1} - \frac{1}{T_2}\right)\right]
\]

where *MTTF* is the mean-time-tofailure and can be calculated from Weibull distribution

To be presented by David Liu at the International Microelectronics Assembly and Packaging Society (IMAPS) Chesapeake Chapter meeting, Johns Hopkins University Applied Physics Laboratory, Laurel, MD, July 23, 2014.
• Ceramic is a polycrystalline structure that contains a large number of closely packed single-crystal *grains*

• The microstructure of each grain is inhomogeneous; a core-shell structure is often reported due to the inhomogeneity between a grain boundary and the interior of a grain

  ➢ Core: ferroelectric BaTiO$_3$ single crystal

  ➢ Shell: non-ferroelectric, different composition and structure

To be presented by David Liu at the International Microelectronics Assembly and Packaging Society (IMAPS) Chesapeake Chapter meeting, Johns Hopkins University Applied Physics Laboratory, Laurel, MD, July 23, 2014.
II. Inhomogeneous Resistivity of BME Capacitors with BaTiO$_3$

Resistivity is significantly different between grain interior and grain boundary

- Core is relatively conductive; shell is highly resistive (bearing the insulating resistance (IR) for a BaTiO$_3$ grain)
- Applied voltage distribution is inhomogeneous
- Due to the formation of a highly **insulating** layer at the grain boundary, most of the voltage will be applied on the grain boundary region
**Improved Reliability Model of BME Capacitors**

**III. Impact of Grain Size**

- When applied voltage and dielectric thickness are identical for two capacitors, the one with the smaller grain size has a better dielectric strength.
- For this reason, powders with smaller particle sizes are always preferred for making BME capacitors.
- Voltage per grain is the key for characterizing the voltage robustness in BaTiO$_3$.

Voltage Per Grain:  
\[
V_{\text{grain}} = \frac{V_{\text{applied}}}{d} = V_{\text{applied}} \times \left(\frac{\bar{r}}{d}\right)
\]

- $\bar{r}$ : average grain size (µm)  
- d : dielectric thickness (µm)

A key structural parameter that determines the dielectric strength and reliability!

To be presented by David Liu at the International Microelectronics Assembly and Packaging Society (IMAPS) Chesapeake Chapter meeting, Johns Hopkins University Applied Physics Laboratory, Laurel, MD, July 23, 2014.
III. Impact of Grain Size (Cont’d)

- Mean-time-to-failure (MTTF) data as a function of number of grains per dielectric layer has been measured at 150°C and 10 KV/mm
  - The more grains per dielectric layer, the longer the MTTF
  - When voltage per grain is normalized to a constant value, MTTF data are identical to a single grain

Prokopowicz and Vaskas equation:

$$MTTF = \frac{c}{V^{n}} \cdot e^{\frac{E_{a}}{kT}}$$

At a given temperature:

$$MTTF = \frac{c}{V_{\text{grain}}^{n}} = \frac{c}{V_{\text{applied}}^{n}} \times \left(\frac{d}{r}\right)^{n}$$

To be presented by David Liu at the International Microelectronics Assembly and Packaging Society (IMAPS) Chesapeake Chapter meeting, Johns Hopkins University Applied Physics Laboratory, Laurel, MD, July 23, 2014.
Improved Reliability Model of BME Capacitors
IV. Impact of Reliability Defects

• Reliability failures are caused by reliability defects
• Quality defects and reliability defects:
  - **Quality defects:** currently deficient products or components, particularly ones that are out of the standard specifications. Quality is generally expressed in percentages.
  - **Reliability defects:** failures that might occur in the future inside a product that has been working well so far. Reliability must therefore be regarded as a ratio expressed in terms of units of time.

• Reliability defects may behave in two ways:
  - They can be benign for the rest of the product life and not cause a failure
  - They can be catastrophic, depending on the feature size and the level of external stress

• Increasing the external stress level is equivalent to:
  - Increasing the applied voltage for a given dielectric thickness
  - Decreasing the dielectric thickness at a constant voltage
Improved Reliability Model of BME Capacitors
IV. Impact of Reliability Defects (Cont’d)

Dielectric layer reliability:

\[ R_i(t) \rightarrow 1, \text{when } d \gg r; \quad R_i(t) \rightarrow 0, \text{when } d \approx r. \]

For Weibull model:

\[ R(t) = e^{-\left(\frac{t}{\eta}\right)^\beta} \cdot \left[ 1 - \left(\frac{r}{d}\right)^\xi \right] \]

Since:

\[ r \approx c \times \bar{r}, \quad \bar{r} \text{ is the average grain size} \]

We have:

\[ P = \left[ 1 - \left(\frac{r}{d}\right)^\xi \right] = \left[ 1 - \left(\frac{\bar{r}}{d}\right)^\alpha \right], \quad (\alpha \geq 5) \]

\[ P \text{ is a geometric factor that determines the dielectric reliability with respect to the microstructure of an MLCC.} \]

To be presented by David Liu at the International Microelectronics Assembly and Packaging Society (IMAPS) Chesapeake Chapter meeting, Johns Hopkins University Applied Physics Laboratory, Laurel, MD, July 23, 2014.
Improved Reliability Model of BME Capacitors

IV. Impact of Reliability Defects (Cont’d)

With external stress: \[ \eta(V,T) = \frac{C}{V^n} \cdot e^{\frac{E_\alpha}{kT}} \]

We have: \[ R_i(t) = R_w(t) \cdot \left[ 1 - \left( \frac{\bar{r}}{d} \right)^\alpha \right] = e^{-\left[ \frac{t}{C} \cdot V^n \cdot e^{\frac{E_\alpha}{kT}} \right]^\beta} \cdot \left[ 1 - \left( \frac{\bar{r}}{d} \right)^\alpha \right], \alpha \geq 5 \]

In general: \[ R_w(t \leq \eta) = e^{-\left[ \frac{t}{C} \cdot V^n \cdot e^{\frac{E_\alpha}{kT}} \right]^\beta} = 1 \]

So finally, single-layer dielectric reliability can be simplified as:

\[ R_i(t \leq \eta) \approx \left[ 1 - \left( \frac{\bar{r}}{d} \right)^\alpha \right] \]

\[ \alpha \text{ is an empirical constant that depends on the processing conditions and microstructure of a ceramic capacitor.} \]

\[ \alpha \approx 6 \ (V \leq 50) \text{ and } \alpha \approx 5 \ (V > 50) \text{ for BME MLCCs} \]

\[ \alpha \approx 5 \text{ for most PME MLCCs} \]
Improved Reliability Model of BME Capacitors

V. Impact of Number of Dielectric Layers

Total capacitance:

\[ C_t = C_1 + C_2 + C_3 \ldots + C_i \ldots + C_N = N \cdot C_i \]

Total reliability:

\[ R_t = R_1 \times R_2 \times R_3 \ldots \times R_i \ldots \times R_N = R_i^N \]

\( R_i(t) \): Single dielectric layer reliability, as discussed earlier

To be presented by David Liu at the International Microelectronics Assembly and Packaging Society (IMAPS) Chesapeake Chapter meeting, Johns Hopkins University Applied Physics Laboratory, Laurel, MD, July 23, 2014.
The reliability of an MLCC $R_t$ decreases with increasing $N$.

The value of $N$ can be as high as 1000!

$$\varphi(N, d, \bar{r}, S) = R_t(t < \eta) = R_i(t < \eta)^N = \left[1 - \left(\frac{\bar{r}}{d}\right)^{\alpha}\right]^N, \quad (\alpha \geq 5)$$

To be presented by David Liu at the International Microelectronics Assembly and Packaging Society (IMAPS) Chesapeake Chapter meeting, Johns Hopkins University Applied Physics Laboratory, Laurel, MD, July 23, 2014.
### Effective chip size 0805 is equal to 6.76 size 0402 MLCCs connected in parallel

### Reliability: $R_i(0805) = R_i(0402)^{6.76}$

### In general: $R_i(xy) = R_i(0402)^S$

### Where $S$ is the MLCC chip size scaling factor with respect to the chip size of an 0402 MLCC; $xy$ is the EIA chip size, $R_i$ is the reliability of a single dielectric layer
Improved Reliability Model of BME Capacitors
VI. Impact of Capacitor Chip Size (Cont’d)

- The reliability of MLCCs decreases with increasing chip size, but not significantly
- When the chip size scaling factor increases by a hundredfold, the reliability declines:
  - 45% when $R_i(0402) = 99\%$
  - 10% when $R_i(0402) = 99.9\%$
  - 1% when $R_i(0402) = 99.99\%$

- The reliability of a MLCC with chip size $xy$ and $N_{xy}$ layers of dielectric $R_t(xy)$ can be expressed as:
  \[ R_t(xy) = R_i(xy)^{N_{xy}} \]
  
  Since: \[ R_t(0402) = R_i(0402)^{N_{0402}} \]

One finally has: \[ R_t(xy) = \left[ R_i(0402)^{N_{xy}} \right]^S = \left[ R_t(0402)^{N_{xy}/N_{0402}} \right]^S \]
Improved Reliability Model of BME Capacitors

VI. Impact of Capacitor Chip Size (Cont’d)

• Reliability as a function of chip size:
  Since: \( N_{0402} \approx 70-80; \) and: \( N_{1825} \approx 280-300, S=100; \)

\[
R_t(1825) = \left[ R_t(0402) \frac{N_{xy}}{N_{0402}} \right]^S = R_t(0402)^{(3\sim4)\times100}
\]

• On the other hand, the dielectric thickness \( d \) also gradually increases with MLCC chip size, as shown in the plot below:

• Since the reliability of an MLCC follows a power-law increase with increasing dielectric thickness, one has:

\[
\frac{MTTF(1825)}{MTTF(0402)} = \left( \frac{d_{1825}}{d_{0402}} \right)^n = \left( \frac{7.8}{2.0} \right)^{3\sim5} \approx 56\sim902
\]

• The reliability decrease due to increasing chip size has been “compensated.”

• Aspect ratio (\( d / \text{chip size} \)) is the KEY! The same design rule applies to CMOS gate capacitors.

To be presented by David Liu at the International Microelectronics Assembly and Packaging Society (IMAPS) Chesapeake Chapter meeting, Johns Hopkins University Applied Physics Laboratory, Laurel, MD, July 23, 2014.
A General Reliability Model of BME Capacitors

\[ R(t) = \varphi(N, d, \bar{r}, S) \times AF(V, T) \times \gamma(t) \]

\[ = \left[ 1 - \left( \frac{\bar{r}}{d} \right)^{\alpha} \right]^N \times \left\{ p \times e^{-\frac{t}{V_{\text{applied}}^n \times \left( \frac{d}{\bar{r}} \right)^n \cdot e\left( \frac{E_{a1}}{kT} \right)}} \right\}^{\beta_1} + (1 - p) \times e^{-\left[ K_0 t \right] \cdot e\left( \frac{E_k}{kT} \right)} \]

Where:

- \( d \): dielectric thickness
- \( \bar{r} \): average grain size
- \( N \): number of dielectric layers
- \( \alpha \): empirical constant
- \( p, \beta_1, \text{and } E_{a1} \): percentage, Weibull slope constant, and activation energy for failure mode 1: catastrophic failure

- \( E \): applied electric field
- \( K_0 e^{-\frac{E_k}{kT}} \): degradation rate constant of \( V_0 \)
- \( n \): power law constant
- \( C, c, \text{and } b \): constants

To be presented by David Liu at the International Microelectronics Assembly and Packaging Society (IMAPS) Chesapeake Chapter meeting, Johns Hopkins University Applied Physics Laboratory, Laurel, MD, July 23, 2014.
Application Example(s): $R(t=0)$

- When $t=0$, one has
  \[ R(t = 0) = \left[ 1 - \left( \frac{r}{d} \right)^{\alpha} \right]^N \]

- The initial reliability is only determined by the construction/processing parameters

- This also indicates that high-reliability MLCCs must be built for that; one cannot improve capacitor reliability by “up-screening”

- It has been noticed that if $R(t=0)$ is met
  \[ R(t = 0) = \left[ 1 - \left( \frac{r}{d} \right)^{\alpha} \right]^N = 1.00000 \]

most of commercial BME capacitors would pass Group B life testing per MIL-PRF-55681
Application Example(s): \( R (t=0) \) (Cont’d)

Testing Results

- Some commercial BMEs passed the life test; the life testing is still in progress!
- All of Automotive Grade BME MLCCs meet this requirement
- The formula described can be used as a simple rule of thumb when designing the BME MLCCs for high reliability applications
- It can also be used as an empirical criterion of construction analysis to reject a BME capacitor for high-reliability use prior to tedious life testing

\[
R(t = 0) = \left[1 - \left(\frac{t}{d}\right)^{\alpha}\right]^N = 1.00000
\]

<table>
<thead>
<tr>
<th>CAP ID</th>
<th>Grain Size (μm)</th>
<th>Dielectric Thickness (μm)</th>
<th>No. of Dielectric layers N</th>
<th>Calculated ( R_t )</th>
<th>1000 hours</th>
<th>4000 hours</th>
</tr>
</thead>
<tbody>
<tr>
<td>A08X22525</td>
<td>0.305</td>
<td>3.89</td>
<td>211</td>
<td>0.99995</td>
<td>Fail</td>
<td>Pass</td>
</tr>
<tr>
<td>B08X33425</td>
<td>0.420</td>
<td>5.80</td>
<td>74</td>
<td>0.99999</td>
<td>Pass</td>
<td>Pass</td>
</tr>
<tr>
<td>A08X15425</td>
<td>0.460</td>
<td>9.80</td>
<td>43</td>
<td>1.00000</td>
<td>Pass</td>
<td>Pass</td>
</tr>
<tr>
<td>C06X10525</td>
<td>0.440</td>
<td>3.20</td>
<td>150</td>
<td>0.99999</td>
<td>Fail</td>
<td>Pass</td>
</tr>
<tr>
<td>A06X10425</td>
<td>0.470</td>
<td>7.89</td>
<td>62</td>
<td>1.00000</td>
<td>Pass</td>
<td>Pass</td>
</tr>
<tr>
<td>A12X47425</td>
<td>0.492</td>
<td>10.40</td>
<td>58</td>
<td>1.00000</td>
<td>Pass</td>
<td>Fail</td>
</tr>
<tr>
<td>C04X47325</td>
<td>0.386</td>
<td>4.40</td>
<td>60</td>
<td>0.99997</td>
<td>Fail</td>
<td>Pass</td>
</tr>
<tr>
<td>B12X47525</td>
<td>0.376</td>
<td>4.34</td>
<td>260</td>
<td>0.99989</td>
<td>Fail</td>
<td>Pass</td>
</tr>
<tr>
<td>P08X10425</td>
<td>0.790</td>
<td>20.20</td>
<td>23</td>
<td>1.00000</td>
<td>Pass</td>
<td>Pass</td>
</tr>
<tr>
<td>B06X10516</td>
<td>0.273</td>
<td>2.29</td>
<td>179</td>
<td>0.99948</td>
<td>Fail</td>
<td>Pass</td>
</tr>
<tr>
<td>A08X47416</td>
<td>0.319</td>
<td>3.75</td>
<td>208</td>
<td>0.99992</td>
<td>Fail</td>
<td>Pass</td>
</tr>
<tr>
<td>B12X68416</td>
<td>0.375</td>
<td>6.21</td>
<td>64</td>
<td>1.00000</td>
<td>Pass</td>
<td>Pass</td>
</tr>
<tr>
<td>C08X22516</td>
<td>0.224</td>
<td>3.81</td>
<td>212</td>
<td>0.99999</td>
<td>Pass</td>
<td>Fail</td>
</tr>
<tr>
<td>B08X22516</td>
<td>0.340</td>
<td>3.23</td>
<td>230</td>
<td>0.99969</td>
<td>Fail</td>
<td>Pass</td>
</tr>
<tr>
<td>B08X56416</td>
<td>0.373</td>
<td>4.21</td>
<td>80</td>
<td>0.99996</td>
<td>Pass</td>
<td>Fail</td>
</tr>
<tr>
<td>C08X47516</td>
<td>0.230</td>
<td>2.49</td>
<td>260</td>
<td>0.99984</td>
<td>Pass</td>
<td>Fail</td>
</tr>
<tr>
<td>B12X10516</td>
<td>0.475</td>
<td>7.82</td>
<td>99</td>
<td>1.00000</td>
<td>Pass</td>
<td>Pass</td>
</tr>
<tr>
<td>B04X10416</td>
<td>0.342</td>
<td>3.05</td>
<td>67</td>
<td>0.99987</td>
<td>Fail</td>
<td>Pass</td>
</tr>
<tr>
<td>B12X10606</td>
<td>0.365</td>
<td>3.11</td>
<td>348</td>
<td>0.99908</td>
<td>Fail</td>
<td>Pass</td>
</tr>
<tr>
<td>B04X10406</td>
<td>0.323</td>
<td>2.50</td>
<td>70</td>
<td>0.99967</td>
<td>Fail</td>
<td>Pass</td>
</tr>
<tr>
<td>B08X22506</td>
<td>0.419</td>
<td>3.42</td>
<td>230</td>
<td>0.99922</td>
<td>Fail</td>
<td>Pass</td>
</tr>
<tr>
<td>A08X10406</td>
<td>0.490</td>
<td>12.50</td>
<td>34</td>
<td>1.00000</td>
<td>Pass</td>
<td>Pass</td>
</tr>
<tr>
<td>B08X22046</td>
<td>0.373</td>
<td>4.01</td>
<td>67</td>
<td>0.99996</td>
<td>Pass</td>
<td>Fail</td>
</tr>
<tr>
<td>P06X10405</td>
<td>0.770</td>
<td>12.60</td>
<td>24</td>
<td>1.00000</td>
<td>Pass</td>
<td>Pass</td>
</tr>
</tbody>
</table>

To be presented by David Liu at the International Microelectronics Assembly and Packaging Society (IMAPS) Chesapeake Chapter meeting, Johns Hopkins University Applied Physics Laboratory, Laurel, MD, July 23, 2014.
**Application Example(s):** $R\ (t=0)$ (Cont’d)

**Number of Zeroes**

\[
R(t = 0) = \left[1 - \left(\frac{\tilde{r}}{d}\right)^{\alpha}\right]^N = 1.00000
\]

**TABLE V.** Product level designator.

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Product level</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>non-ER</td>
</tr>
<tr>
<td>M</td>
<td>1.0 1/</td>
</tr>
<tr>
<td>P</td>
<td>0.1 1/</td>
</tr>
<tr>
<td>R</td>
<td>0.01 1/</td>
</tr>
<tr>
<td>S</td>
<td>0.001 1/</td>
</tr>
</tbody>
</table>

1/ FRL (percent per 1,000 hours).

**BX life to failure rate:**

- M: B1% life
- P: B0.1% life
- R: B0.01% life
- S: B0.001% life

**BX life to Reliability:**

- M: B1% life $= \eta \left\{ -\ln \left[ R(x_1\%) \right] \right\}^{1/\beta}$ where $R(x_1\%) = 0.99$
- P: B0.1% life $= \eta \left\{ -\ln \left[ R(x_2\%) \right] \right\}^{1/\beta}$ where $R(x_2\%) = 0.999$
- R: B0.01% life $= \eta \left\{ -\ln \left[ R(x_3\%) \right] \right\}^{1/\beta}$ where $R(x_3\%) = 0.9999$
- S: B0.001% life $= \eta \left\{ -\ln \left[ R(x_4\%) \right] \right\}^{1/\beta}$ where $R(x_4\%) = 0.99999$

**Number of zeroes represents the level of failure rate!**

**Note:** Some dopants such as Ca, Mg etc. may function as grain growth prohibitors. This criterion must be used carefully and for apple-to-apple comparisons only!
Summary and Future Work

- A general reliability model for BME capacitors has been developed, which consists of three parts:
  - A 2-parameter Weibull distribution
  - Two acceleration functions:
    - a power-law form for catastrophic failures
    - an exponential-law form for slow degradation failures
  - An empirical function that defines contribution of the structural/constructional characteristics of a MLCC, such as the number of dielectric layers $N$, dielectric thickness $d$, average grain size $\bar{r}$.
  - The capacitor chip size $A$ is found to not play a role in the reliability of a BME MLCC
- At $t=0$ the reliability model can be used as a construction analysis selection criterion for BME MLCCs that may be applicable to high-reliability applications
- For future work
  - Work closely with manufacturers to verify/improve the reliability model
  - Significant amount of life testing of BME capacitors
Acknowledgement

• NASA NEPP program for funding this work

• NASA GSFC Code 562 Parts Analysis Laboratory, for assistance in some electrical testing

• Dr. Henning Leidecker, the Chief Technologist for EEE Parts at GSFC, for valuable discussions

Thank you!

Questions?