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FAILURE PROBABILITY PREDICTION OF DIELECTRIC CERAMICS IN MULTILAYER CAPACITORS¹

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RECEIVED**AUG 13 1998****OSTI****ABSTRACT**

Dielectric ceramics in multilayer capacitors are subjected to manufacturing or service thermomechanical stresses which, if severe enough, will cause mechanical failure and perhaps subsequent loss of electrical function. Strength of monolithic ceramics is probabilistic in nature; however, probabilistic design of such electronic ceramic components generally has not been used by manufacturers and end-users of these components. To illustrate how probabilistic design may be utilized for small components, the present study demonstrates the applicability of an existing probabilistic life design computer code in the prediction of failure probability of a dielectric ceramic in an arbitrary multilayer capacitor. Issues involving the generation of representative strength and fatigue data for specimens at this small scale and the ultimate failure probability prediction of dielectric ceramics in multilayer capacitors are presented. Additionally, alternative means to generate a strength distribution as input for the probabilistic life design computer codes which are under consideration by the authors are discussed.

I. INTRODUCTION

Cracking of multilayer capacitors (MLCs) due to thermomechanical and residual stresses can occur during manufacturing or during service. This is problematic because mechanical failure may result in loss of electrical function. Multilayer capacitors are extensively used in high frequency circuits and switchmode power supplies [1]. They are subjected to thermal excursions which can produce tensile stresses sufficient for mechanical failure. The stress state and failure processes in MLCs are undergoing further scrutiny as the demand for thinner dielectric layers (and subsequent higher charge densities) increases. Understanding these stress states and identifying strength-limiting flaws are important in improving their reliability and optimizing their design.

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The mechanical integrity of dielectric ceramic materials used in MLCs has been investigated by a number of researchers. The fracture toughnesses are typically low (e.g., less than $\approx 1.8 \text{ MPa}\sqrt{\text{m}}$ [2-4]). These materials may undergo a phase change at their Curie temperature which affects their strength and fracture toughness [2, 5]. Some dielectric ceramics are susceptible to slow crack growth in humid environments [6] and to thermal shock [3].

The strength of monolithic ceramic materials is probabilistic and size-dependent. Existing probabilistic life design computer codes (e.g., NASA's CARES/LIFE [7] and AlliedSignal's CERAMIC/ERICA [8]) take these issues into consideration and predict the probabilistic mechanical reliability of ceramic (structural) components. Few citations were found where probabilistics were described and incorporated into the design or failure analysis of electronic ceramic components [9-10]. Although the strength distributions of some dielectric materials have been reported [3, 11], no citations were identified where such data were used to predict the mechanical reliability of a dielectric component.

The motivation of the present study was to perform a probabilistic design or failure probability demonstration on a dielectric ceramic component. The examined component was a BaTiO_3 margin in a MLC and is shown in Fig. 1. Several assumptions (mostly regarding the MLC geometry and thermoelastic properties) were made to facilitate the demonstration. The results were not intended to be quantitative or to be interpreted as such, rather, to demonstrate how they may be generated and used. Strain-free temperature in the MLC (and subsequent residual stress state) was the independent parameter while the failure probability was the dependent parameter.

II. PROCEDURES AND PROBABILISTIC ANALYSIS

Probabilistic life design or failure probability analysis of a ceramic component combines the strength distribution of the monolithic ceramic material comprising the component, finite element analysis of the component under the mechanical loading conditions of interest, and a multiaxial fracture criterion. In the present study, the failure probability of BaTiO_3 "margins" in a simple MLC were predicted by considering only residual stresses. AlliedSignal's tandem set of computer codes CERAMIC and ERICA [8] were used for this analysis. The design algorithm as applied in the present study is illustrated in Fig. 2, and the description of each constituent in Fig. 2 follows.

II.A. Strength Testing and Weibull Distribution Analysis

The flexure strengths of thirty BaTiO_3 specimen blanks were measured at ambient conditions (20°C , $\text{RH} \approx 55\text{-}60\%$). The average size of the grains within the blank was less than $1 \mu\text{m}$. To minimize the likelihood of edge-induced failures, the specimens were tumble polished to round their edges. The specimens had nominal dimensions of $6.3 \times 4.7 \times 1.1 \text{ mm}$, and were tested in three-point flexure using a 4 mm lower span. A cross-head displacement rate of 0.5 mm/min was used, and testing was performed in ambient air.

The two-parameter Weibull strength distribution was determined for the BaTiO_3 using AlliedSignal's CERAMIC computer code. The code uses maximum likelihood estimation to determine the Weibull modulus (m) and scaling

parameter (σ_0). These parameters represent the "material design data," and were used as input for the to-be-discussed failure probability prediction of the BaTiO_3 in a simple MLC.

II.B. Finite Element Analysis and Failure Probability Prediction

The stress field within BaTiO_3 margins in the MLC required finite element analysis (FEA) modeling in order to ultimately predict their failure probability. A cross-section view of a MLC in Fig. 1 shows these regions. Geometrical symmetry conditions were assumed about all three Cartesian planes, so a one-eighth model was developed which is shown in Fig. 3. Dimensions of the MLC were measured with an optical comparator and used as input for the FEA geometry. One of several MLC geometry simplifications was the consideration of only the exterior BaTiO_3 margins in the XZ plane; BaTiO_3 margins also exist in the XY plane on the exterior of MLCs, but they were not modeled in the present demonstration. Margin thickness was not an independent parameter in the present demonstration though it has been shown to affect mechanical strength in such systems [12]. The failure probability of the MLC margins at 20°C was determined for five different strain-free temperatures in the MLC: 120, 220, 320, 420, and 520°C. Because these strain-free temperatures were greater than 20°C, residual stress exists in the MLC at 20°C due to the thermal expansion mismatches between the four regions. Linear thermoelastic analysis was performed. Residual stresses reported for the BaTiO_3 phase transformation [5] were not considered in the present demonstration. The properties used in the model for each of the four regions shown in Fig. 3 are listed in Table. I. The elastic properties of regions #2 and #3 were calculated using a rule of mixtures using the ratios indicated in the caption of Fig. 3. Isotropic properties were assumed in this exercise; however, regions #2 and #3 are orthotropic in all likelihood.

Fig. 1. Polished cross-section of a MLC showing its margins. The failure probability of these were predicted in the present study.

Fig. 2. The probabilistic life design algorithm used in the present study.

Fig. 3. The finite element model used to determine the residual stress state in region #1. The BaTiO₃ margin is represented by region #1; region #2 is considered to have 80% BaTiO₃ and 20% electrode metal; region #3 has 90% BaTiO₃ and 10% electrode metal; and region #4 is a termination metal.

Table. I. Material Properties Used in the FEA Model.

Material or Region ID	Young's Modulus, E (GPa)	Poisson's Ratio, ν	Thermal Expansion Coefficient, α ($\times 10^{-6}/^{\circ}\text{C}$)
1 ("margin")	113	0.34	10
2	107	0.34	11.4
3	110	0.34	10.7
4	73	0.30	18

After the completion of FEA modeling, the stress output file was directly read into AlliedSignal's ERICA computer program to determine the stress gradient factor (which is a function of Weibull modulus) for the stress state in the BaTiO₃ margin and to introduce a multiaxial failure criterion. ERICA uses Evan's model [13] for the failure criterion, which has been shown to be analytically equivalent [14] to the often-used Batdorf's failure criterion [15-16].

In the final step, the failure probability of the BaTiO₃ margins were predicted for each of the five different strain-free temperatures. To do this, the stress gradient factor function for the BaTiO₃ margins was combined with the measured BaTiO₃ strength distribution using AlliedSignal's CERAMIC computer program.

III. RESULTS & DISCUSSION

III.A. Strength Distribution of BaTiO₃

The strength distribution measured with the BaTiO₃ blanks is illustrated in Fig. 4. The characteristic strength (σ_0) for this specimen and fixture type and size was 104.4 MPa and the Weibull modulus was 10.8. In comparison,³ diametral compression and four-point bending were used to measure the strength of a barium titanate ceramic [4], and strengths ranged from 18 to 82 MPa for diametral compression and 35-79 MPa for flexure. Preliminary optical fractography indicated that some of the BaTiO₃ specimens failed due to pores which were located at the flexure specimen's tensile surface. Such voids have been identified as the cause of some dielectric ceramic failure [17]. The appearance of the knee in the data shown in Fig. 4 suggests that more than one failure mode may be operative. Additionally, preliminary scanning electron microscopy indicates that the naturally occurring pores in the BaTiO₃ may be too small (taking into account the material's fracture toughness) to account for the measured low strengths. Thorough optical and scanning electron fractography is underway. Even though uncertainty existed regarding the identification of the dominant strength-limiting flaw in this BaTiO₃,

³ The test specimen geometry and loading condition in the present study are different than those in Ref. [4], so the reader is cautioned about making one-to-one strength comparisons among them.

material, a volume flaw⁴ was assumed to be the strength-limiting flaw in the material and MLC margin for the failure probability prediction exercise. The strength distribution data was then scaled to a unit volume subjected to uniform tensile stress in preparation for the actual failure probability prediction. The resulting scaling parameter was determined to be $\sigma_0 = 61.5 \text{ MPa} \cdot \text{mm}^{3/m}$ (where mm = millimeter and m = Weibull modulus).

III.B. Failure Probability of MLC

III.B.1. Finite Element Analysis

The residual stress state at 20°C in the MLC is a consequence of the thermal expansion mismatches of the various material constituents and their relative sizes. Examples of the σ_x , σ_y , and σ_z residual stress profiles are respectively shown in Figs. 5(a)-(c). Being that tensile stress in the BaTiO₃ margin is the prerequisite for any failure event, the σ_y stress state is of most interest as the σ_x and σ_z profiles are comprised primarily of compressive stresses. If the BaTiO₃ margin were to fail, then the arrow in Fig. 5(b) would indicate where the failure initiation location would likely be. The failure probability of the BaTiO₃ margins was subsequently determined using these FEA stress results with the measured BaTiO₃ strength distribution and AlliedSignal computer codes.

Fig. 4. Strength distribution of BaTiO₃ used as input to predict the failure probability of the BaTiO₃ margins. 95% confidence intervals indicated.

⁴ Edge, surface, and/or volume flaws could all have been considered and introduced into the analyses. However, such censorship requires thorough fractography which was deemed as unnecessary for the demonstration of the probabilistic life design exercise in the present study.

III.B.2. Failure Probability as a Function of Strain-Free Temperature

The failure probability prediction results show that the strain free temperature can significantly affect the failure probability of the BaTiO₃ margin. The failure probability as a function of stress and strain-free temperature is shown in Fig. 6. The failure probabilities clearly increase with strain-free temperature. There is essentially no failure predicted at 20°C when the strain-free temperature is 120°C. Failure probability of the BaTiO₃ margins is approximately 0.0095%, 0.7695%, 16.0285%, and 86.0849% when the strain-free temperature is 220, 320, 420, and 520°C, respectively. The 95% confidence intervals for these failure probabilities are listed in Table II. This exercise clearly supports a recognized fact that there is a very significant advantage in lowering the strain-free temperature in MLCs (even slightly if the strain-free temperature is already relatively low). Suggestions on how to facilitate the lowering of the strain-free temperature are outside the scope of the present study, but they qualitatively include using ductile and low-melting-temperature metals in the MLCs or choosing metals having values of thermal expansion coefficient in close proximity to that of the dielectric ceramic.

A coarsely-modeled MLC using several simplifying assumptions was used in the present study as a probabilistic life design exercise; however, this same algorithm is amenable for use for commonly used or realistic MLC mechanical tests or analyses. One common mechanical test in the MLC industry involves flexing an epoxy board which contains a solder-mounted MLC [18-19]. During this test the MLC is subjected to mechanical stress by the flexed board, and MLC failures are interpreted with respect to the amount of board flexure. Using the algorithm employed in the present study, probabilistics could be introduced into this MLC industry test to predict, for example, the failure probability as a function of board flexure, the amount of allowable flexure, etc. If realistic board flexures impart tensile stresses in the MLC sufficient to cause an unacceptable amount of failures, then the algorithm perhaps could be used in an iterative design-loop to alter the MLC design with the intent of reducing residual stresses: the thermal expansions may not be tailorable as desired in this instance, but the relative dimensions of the various ceramic and metal constituents in the MLC may indeed be. Additionally, the presently described algorithm may be used to predict the thermal shock susceptibility of MLCs, and perhaps be used as a guide to judge tolerable service thermal excursions.

IV. Closing Remarks and Future Directions

The validity of using strength data from large and perhaps independently processed BaTiO₃ to predict the mechanical reliability of small-sized BaTiO₃ constituents in MLCs is undergoing further scrutiny by the authors. A limitation of the above algorithm is illustrated by the following: by using the three-point flexure strength data described in *Section II.A.*, it is assumed that the mechanical properties and performance of these large-sized BaTiO₃ blanks are identical to that of the small-sized BaTiO₃ in the MLC. Although this assumption may be valid in rare circumstances, it probably is invalid in most. Consequently, strong interest exists to generate mechanical property data and/or flaw distribution data (and subsequent strength distribution data) for input in the probabilistic life prediction codes. This

Fig. 5. Example residual stress profiles at 20°C shown for (a) σ_x , (b) σ_y , and (c) σ_z when the strain-free temperature was 420°C.

Fig. 6. Failure probability at 20°C of BaTiO₃ margins in a MLC as a function of stress or strain-free temperature.

Table. II. Failure probabilities of MLC BaTiO₃ margins at 20°C with 95% confidence intervals.

Strain-Free Temperature (°C)	- 95% POF % (ppm)	Probability of Failure, POF, % (ppm)	+ 95% POF % (ppm)
120		0	
220	0.0019 (19)	0.0095 (95)	0.0419 (419)
320	0.5129 (5129)	0.7695 (7695)	1.1311 (11311)
420	7.6781 (76781)	16.0285 (160285)	37.7921 (377921)
520	38.3173 (383173)	86.0849 (860849)	100 (1000000)

could occur via micromechanical testing of the actual BaTiO₃ within the MLC, and would ensure that representative data is being generated with the actual material of interest.

Currently, at least two approaches are being explored by the authors to generate such micromechanical data for input in the probabilistic life design computer codes. The first involves the applicability of indentation-generated data using the analyses and models of Anstis *et al.* [20] and Chantikul *et al.* [21]. An advantage of this approach is that micromechanical data may be readily generated on the actual material in the electronic ceramic component. The disadvantage primarily involves the reconciliation of the strength distribution each produced by natural and artificially-produced flaws. Another technique being pursued involves the in-situ identification and determination of the flaw size distribution, and its conversion to a strength distribution. An advantage of this latter approach is that natural flaws are involved in the determination of the strength distribution. A disadvantage of this approach is confidently determining what the natural and strength-limiting flaw is. It is felt that these approaches, if successful, will greatly benefit and improve the probabilistic design algorithm for electronic ceramic components.

V. SUMMARY

Dielectric ceramics in multilayer capacitors are subjected to manufacturing or service thermomechanical stresses which, if severe enough, will cause mechanical failure and even perhaps subsequent loss of electrical function. The present study demonstrated the applicability of an existing probabilistic life design computer code in the prediction of failure probability of a dielectric ceramic in a multilayer capacitor. Issues involving the generation of representative strength and fatigue data for specimens at this small scale and the ultimate failure probability prediction of dielectric ceramics in multilayer capacitors were described.

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