Improved prediction for failure time of multilayer ceramic capacitors (MLCCs): A physics-based machine learning approach

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ABSTRACT

Multilayer ceramic capacitors (MLCC) play a vital role in electronic systems, and their reliability is of critical importance. The ongoing advancement in MLCC manufacturing has improved capacitive volumetric density for both low and high voltage devices; however, concerns about long-term stability under higher fields and temperatures are always a concern, which impact their reliability and lifespan. Consequently, predicting the mean time to failure (MTTF) for MLCCs remains a challenge due to the limitations of existing models. In this study, we develop a physics-based machine learning approach using the eXtreme Gradient Boosting method to predict the MTTF of X7R MLCCs under various temperature and voltage conditions. We employ a transfer learning framework to improve prediction accuracy for test conditions with limited data and to provide predictions for test conditions where no experimental data exists. We compare our model with the conventional Eyring model (EM) and, more recently, the tipping point model (TPM) in terms of accuracy and performance. Our results show that the machine learning model consistently outperforms both the EM and TPM, demonstrating superior accuracy and stability across different conditions. Our model also exhibits a reliable performance for untested voltage and temperature conditions, making it a promising approach for predicting MTTF in MLCCs.

INTRODUCTION

Multilayer ceramic capacitors (MLCCs) have become essential components of modern electronics, powering a range of devices from consumer electronics to medical devices and automotive technologies. As part of the miniaturization trend in MLCC manufacturing, capacitive volumetric density of MLCCs has improved significantly because of reduced active dielectric layer thickness. However, the trend toward miniaturization raises concerns about reliability of MLCCs, particularly in terms of long-term operational stability at high temperatures and fields.[1,2] The majority of high capacitance MLCCs are based on $BaTiO_3$, which has superior dielectric properties, such as high permittivity, low dielectric loss, and the capacity to tailor properties over a wide temperature range.[3–6]There are two types of $BaTiO_3$-based MLCCs: those utilizing precious metal electrodes (PME) and those using base metal electrodes (BME). PME MLCCs employ Ag, Pt, Pd, and/or Ag–Pd alloys, all of which can be sintered in ambient air atmosphere.[3–6] In contrast, BME MLCCs employ Ni or Cu and must be sintered under low partial pressures of oxygen to prevent oxidation. These sintering conditions are typically reduced to $BaTiO_3$, and thus, a re-oxidation anneal is conducted at lower temperatures and partial pressure to minimize oxygen vacancies without oxidizing the metal electrodes.[7–12] Nevertheless, the cofiring of $BaTiO_3$-based MLCCs with Ni electrodes under low oxygen partial pressure conditions raises concerns about oxygen vacancies electromigration, which play a significant role in the degradation of insulation resistance in MLCCs and their breakdown eventually.

Highly Accelerated Lifetime Testing (HALT) is a traditional method to statistically investigate the reliability and lifetime of MLCCs.[13,14] In this method, MLCCs are exposed to much higher temperatures and voltages than those in normal operating conditions to accelerate the test. The lifetime of MLCCs under normal operating conditions can be extrapolated from the failure time of components measured by the HALT. The Eyring empirical model (EM) is frequently used to extrapolate HALT results to determine the mean time to failure (MTTF) of MLCCs under operating conditions, which can be expressed as

$$\frac{t_1}{t_2} = \left(\frac{V_2}{V_1}\right)^n \exp\left[\frac{E_a}{k_B}\left(\frac{1}{T_1} - \frac{1}{T_2}\right)\right], \tag{1}$$

where t, V, T, n, k_B, and E_a are the lifetime of MLCCs, applied voltage, temperature, the electric-field acceleration factor, Boltzmann's constant, and activation energy of mobility governing the degradation process, respectively. The voltage acceleration factor, represented by n, can be determined in PME MLCCs by conducting a statistical analysis on a limited number of tests. Typically, n is a constant and independent of temperature and applied voltage. However, in modern BME MLCCs, n is not a constant and is influenced by temperature and applied voltages, which can pose significant challenges in predicting the lifetime of MLCCs. Extensive testing is required to determine the non-linearities of n. It is also crucial to avoid driving accelerated lifetime tests to extremes that could induce multimode failures, as these do not reflect the normal operating conditions of the MLCCs.[14,15]

To overcome the limitations of the Eyring model, the tipping point model (TPM) was introduced based on a physical model that assumes the accumulation of a critical space charge density with oxygen vacancies at the cathode interface and considers local fields.[16] Consequently, the lifetime of MLCCs can be predicted as follows:

$$t_{crit} = \frac{\rho_{crit}}{a\vartheta Nq}\left[\exp\left(-\frac{E_a}{k_B T}\right)\sinh\left(\frac{qaE_{app}}{2k_B T}\right)\right]^{-1}, \tag{2}$$

where t and ρ_{crit} are the predicted lifetime and the critical space charge density at the cathode interface, respectively. a, ϑ, N, and q are jump distance, jump frequency, oxygen vacancy concentration, and oxygen vacancy charge, respectively. Based on the following equation:

$$\ln(t) = C(T) - \ln\left(\sinh\left(\frac{\beta E_{app}}{T}\right)\right), \tag{3}$$

by fitting the failure times in the ln-ln plot with a slope of −1, the values β and $C(T)$ can be determined, and the MTTF can be predicted. The β value reflects the local electric field that governs the rate-controlled process of developing the critical ionic space charge within a given microstructure as well as component design. The $C(T)$ value is the fitted data's intercept and includes terms such as diffusion activation energy, jump frequency, ionic hop distance, and mobile oxygen vacancy concentration. Morita *et al.*[15] modified the tipping point model by incorporating a depolarization field for low electrical field predictions considering the time-dependent development of the internal depolarization field. The basic assumptions of this approach consider that there is a critical accumulation of oxygen vacancy concentration in each BME MLCC that triggers the rapid increase in leakage current and ultimate failure of the MLCC design. The time between obtaining the critical oxygen vacancy concentration and breakdown failure is much shorter than the wear-out time. The Morita *et al.*[15] model considers that the space charge accumulation builds a small depolarization field that, with a low field application, has an effectively lower field and, thereby, longer lifetime than under higher fields. In previous articles, we demonstrate that the TPM outperforms the EM in terms of consistency and accuracy under different temperatures and electric field conditions.[17] We also demonstrate that relying solely on MTTF can be misleading due to the considerable variance in MTTF values.[18] As a result, rather than relying solely on MTTF, it is critical to estimate the lifetime distribution as a function of the testing variables.

Existing lifetime prediction models are heavily reliant on the availability and large quantity of experimental data. However, these can serve as an important starting point for developing a data-driven and physics-based machine learning approach for accurately predicting the lifetime of MLCCs at various temperature and voltage conditions. Machine learning techniques have been increasingly employed to predict the lifetime of electronic devices, providing valuable insights into their reliability and degradation mechanisms.[19–25] Orchard *et al.*[26] propose a particle filter-based prognostic approach for better uncertainty representation and management, enhancing accuracy, reducing uncertainty, and decreasing computational load using a feedback loop. Ng *et al.*[27] use machine learning for predicting battery states, address current model limitations, and highlight challenges for real-time battery management and optimization. Sawant *et al.*[28] review machine learning techniques for predicting capacitance and the remaining useful life of supercapacitors.

Despite the limited number of experimental data in MLCC reliability studies, machine learning techniques may be able to develop more accurate lifetime prediction models that do not rely solely on extensive experimental data but also capture the underlying physics of the failure mechanisms. Therefore, in this paper, we develop a more accurate physical-based machine learning model that can be used to expand the dataset in the absence of costly and time-consuming experimental data and later can be used to predict the variance of lifetime values, providing a more comprehensive estimate of the lifetime distribution.

METHODS

We initially utilize HALT to determine the MTTF of X7R MLCCs (EIA 1206 case size, 1 μF, and voltage rating of 50 V) under isothermal conditions at 135, 140, and 150 °C with a DC field ranging from 200 to 375 V. We declare each MLCC as failed when the leakage current exceeded 300 μA. Subsequently, to overcome the limitations of existing models, we employ the eXtreme Gradient Boosting (XGBoost)[29] method to develop a physics-based machine learning model (MLM), capable of accurately predicting the lifetime of MLCCs. We develop our model with two primary objectives: improving prediction accuracy for test conditions with limited data and providing predictions for test conditions where no experimental data exist, as demonstrated in Fig. 1.

To accomplish the first objective of enhancing the accuracy of predicting MTTF at a specific temperature across various voltages,

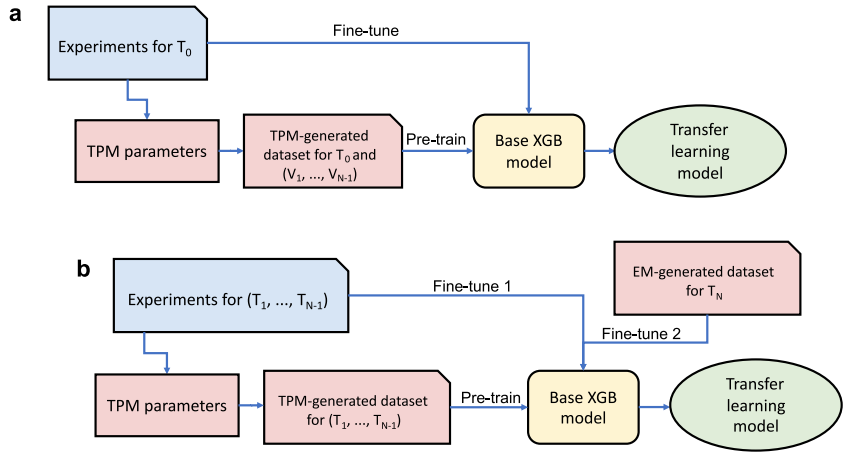

FIG. 1. (a) Enhancing the lifetime prediction of MLCCs based on a XGBoost model pre-trained on data generated by TPM for the consistent T_0. (b) Predicting lifetime of MLCCs for unseen experimental data for T_N.

we implement XGBoost models within a transfer learning framework. This approach allows us to address the limitation of TPM's accuracy caused by the limited availability of data. Initially, we determine TPM parameters [β and $C(T)$] by fitting to the MTTF experimental results obtained from HALT at a target temperature. Subsequently, we employ TPM to create a dataset at the specified temperature and varied voltage conditions. Then, we pre-train our XGBoost model on this dataset, creating a base model for predicting MTTF. The XGBoost parameters of the base model are collected for the transfer learning phase, during which we fine-tune the model using the experimental data employed to fit TPM parameters. This transfer learning approach is necessary because, during the pre-training phase, the base model is fitted to the dataset generated by TPM, leading to similar prediction errors. The errors introduced by TPM can be reduced by refining the MLM using the experimental data, resulting in enhanced model performance. It is important to note that instead of combining the experimental results and TPM-generated dataset, the experimental results are only introduced during the transfer learning stage. This process ensures that the model is exposed to the accurate data in the final step, rather than merely training on a single dataset containing a mix of TPM-derived and experimental data.

To achieve our second objective of providing predictions for untested voltage and temperature conditions, we employ both TPM and EM to estimate MTTF across various temperatures. The training phase consists of three steps: First, we pre-train the base model on a TPM-derived dataset based on temperatures (e.g., T_1 and T_2) for which experimental data are available, and thus, TPM parameters are known. Next, we fine-tune the base model on the experimental data available for T_1 and T_2, exposing the model to a dataset of higher accuracy. Finally, we fine-tune the model once more on the EM-derived dataset created for the target temperature, T_3. We employ EM because the use of TPM is restricted by the availability of data for the target temperature; $C(T)$ is temperature-dependent and cannot be predicted from other temperatures. In addition, to ensure accurate predictions by EM, it is crucial to use identical voltage values between the initial and target temperatures. This approach eliminates the impact of parameter n in the EM and prevents additional errors associated with it, which will be discussed in detail in the following section. Consequently, we assess the performance of the MLM on various voltages of the target temperature and compare it to the EM. In all instances, the XGBoost base model is trained by running a grid search cross-validation on the hyperparameters space shown in Table I.

To ensure positive MTTF values from the model, we apply a logarithmic transformation to the target MTTF. This transformation is a common technique used to address the issue of negative predictions or non-normality in the target variable. Specifically, we apply the natural logarithm transformation using the Python NumPy library's log function, which maps the original values of y to the log scale. After fitting the model using the transformed target variable, we obtain predictions by exponentiating the output of the model using the NumPy library's exp function. This procedure ensures that the predicted values are positive and can be interpreted as the exponentiated output of the model.

Finally, we perform feature engineering to extract relevant information from the raw data and improve the performance of the predictive model. Specifically, we generate a set of features based on the two primary variables of interest: V and T. These include various transformations of V and T, including V^2, V^4, $V.T$, $\frac{V}{T}$, LnV, LnT, $V.LnT$, and $T.LnV$. These transformations can help capture any non-linear or complex relationships between V and T and the response variable.

TABLE I. Hyperparameter grid space for XGBoost base model.

Hyperparameter	Range
`learning_rate`	`0.01, 0.1, 1`
`max_depth`	`3, 4, 5`
`n_estimators`	`100, 200, 500`

RESULTS AND DISCUSSION

To improve the accuracy of predicting MTTF for X7R MLCCs at a specific temperature across various voltages, we initially obtain MTTF data by conducting isothermal HALT under various DC field conditions. Subsequently, we use the linear least squares regression method to fit the experimental MTTF data at each temperature with the EM and TPM. Notably, at each temperature, we exclude the MTTF data associated with the target voltage condition and used the remaining MTTF data to calculate the EM parameter, n, and TPM parameters, β and $C(T)$. This is carried out to prevent data leakage while evaluating the MLM for the target voltage. Furthermore, the activation energy of these MLCC failures was previously calculated and reported to be 1.70 ± 0.30 and 1.66 ± 0.09 eV, respectively, using the EM and TPM.[17] However, we also prevent information leakage by only calculating the average activation energy of MTTF data that is used for training, excluding the target MTTF data. We use these calculated parameters to create our pre-training dataset, as well as make predictions using TPM and EM for final comparison.

For each target voltage, we use its corresponding TPM parameters to create a dataset for pre-training. Once the base model is created, we fine-tune the remaining experimental data, excluding the data point with the target voltage. Then, we evaluate the MLM against the target voltage and compare its performance to that of TPM and EM. The results are shown in Fig. 2. We use two evaluation metrics to compare the performance of the models. Specifically, we obtain the root mean square error (RMSE) and root mean square percentage error (RMSPE) scores, which are calculated as follows:

$$RMSE = \sqrt{\frac{1}{m}\sum_{i=1}^{m}\left(y_i - \hat{y}_i\right)^2}, \tag{4}$$

$$RMSPE = \sqrt{\frac{1}{m}\sum_{i=1}^{m}\left(\frac{y_i - \hat{y}_i}{y_i}\right)^2}, \tag{5}$$

where m represents the number of MTTF data points, and y_i and $\hat{y}_i$ denote the MTTF experimental value and the predicted MTTF of MLCC at the ith voltage and temperature condition, respectively. Both RMSE and RMSPE values are reported to provide a comprehensive assessment of the models' performance. RMSE measures the average squared difference between the predicted values and the actual values and provides an idea of how far, on average, the predictions are from the actual values. It is highly sensitive to large errors or outliers in the data. Because the differences between the predicted and actual values are squared, larger errors have a significant impact on the RMSE value. Consequently, a single large error can significantly increase the RMSE, even if the model performs well for the majority of the data points. RMSPE, on the other hand, is also sensitive to outliers; however, its sensitivity is affected by the magnitude of the actual values. For data points with large actual values, the percentage error might be small even if there is a significant absolute error. On the other hand, for data points with small actual values, a small absolute error can result in a large percentage error. Therefore, RMSPE is more sensitive to errors in the predictions for data points with smaller actual values. Moreover, since the RMSPE is expressed as percentage, it enables model comparison across datasets of different scales. This dual evaluation approach offers a better understanding of the performance of the prediction models in accurately estimating the MTTF of X7R MLCCs over a comprehensive range of voltages and specific temperature conditions. Table II shows the RMSE and RMSPE values for each predictive model at each temperature, where clearly demonstrates that MLM consistently outperforms other models.

A deeper look into the error analysis of predicted MTTF values for all models reveals that the error is more significant for the largest voltage conditions at each temperature, where the conditions are more aggressive, and the failure mechanism may have changed. Consequently, the RMSPE score is specifically decreased for smaller values of MTTF under such aggressive conditions since a small error in predicting a small true value can result in a large percentage error (e.g., see RMSPE for TPM at 140 °C). This suggests that under extreme conditions, models may struggle to predict failure times accurately. In such conditions, however, the MLM model outperforms the EM and TPM models. The average percentile error and standard deviation of MTTF predictions for EM, TPM, and MLM

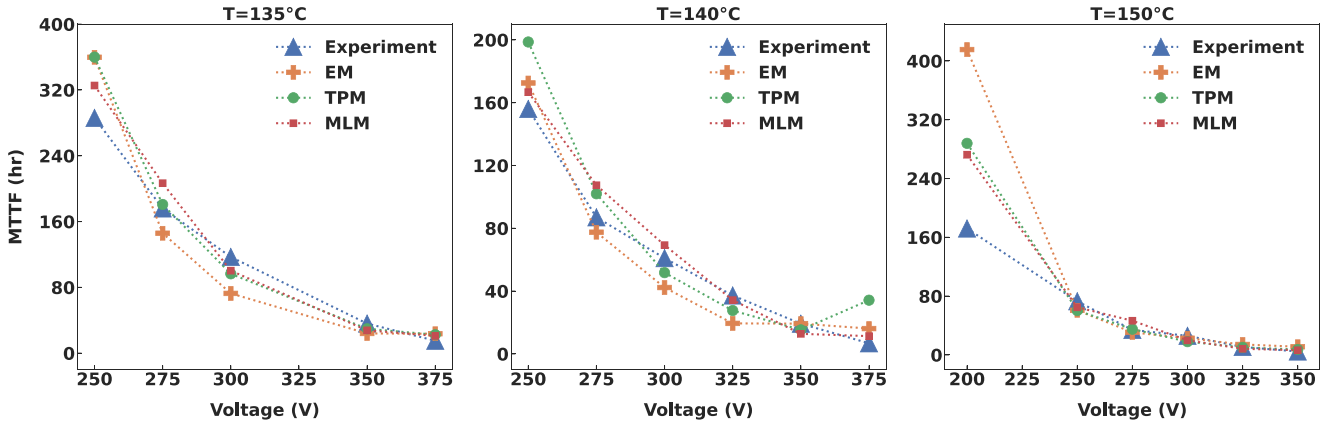

FIG. 2. A comparison of MTTF predictions from the EM, TPM, and MLM for BME X7R MLCCs at the consistent temperature T_0 under different dc bias conditions, with experimental MTTF data .

TABLE II. RMSE and RMSPE values for MTTF predictions made by EM, TPM, and MLM for BME X7R MLCCs at constant temperature T_0 under different dc bias conditions with experimental MTTF data.

	RMSE			RMSPE (%)		
Temperature (°C)	EM	TPM	MLM	EM	TPM	MLM
135	41.3	34.7	24	36.6	27.0	23.4
140	13.7	22.3	10.6	61.5	167.0	33.0
150	99.6	47.7	41.5	82.8	39.1	34.9

models are 45 ± 46, 47 ± 91, and 27 ± 17, respectively. These findings highlight the superior performance of the MLM in predicting MTTF values, particularly under extreme voltage conditions, as well as its stability across different temperature and voltage conditions, as its accuracy does not change significantly with possible changes in the failure mechanisms.

The large variation in error when predicting MTTF values using the EM may be attributed to their sensitivity to the number of experimental data points used for fitting and failure mechanism. As previously demonstrated, the values of n (electric-field acceleration factor) and E_a (activation energy) in the EM can vary significantly depending on the selection of data points. In addition, since the closest voltage condition to the target condition is used to predict the MTTF values with the EM model, the reported errors may represent the minimum possible errors. If the farthest voltage condition is selected, the errors increase significantly by a factor of n. This implies that the accuracy of the EM model can be influenced by the availability and representativeness of experimental data used for model fitting, and it is highly dependent on the proximity of the data used for prediction to the target condition, and the model's performance may deteriorate when extrapolating to conditions further away from the fitted data. However, the large variation in error observed when predicting MTTF values using the TPM can be primarily attributed to the dominant failure mechanism. This was demonstrated by excluding the most aggressive condition (largest voltage conditions) at all temperatures. In this case, the average percentile error and standard deviation of MTTF predictions for EM, TPM, and MLM models change to 31 ± 33, 21 ± 15, and 22 ± 13, respectively, which resulted in a significant reduction in the average percentile error and standard deviation of MTTF predictions for TPM. Moreover, it is worth noting that despite previous findings, $C(T)$ values in TPM are not merely a function of temperature but also found to be dependent on the applied voltage and sensitive to the selection of data points, which further contributes to the variability and potential inaccuracy of TPM predictions. These outcomes highlight the limitations of TPM and EM and emphasize the need for a more robust and accurate approach for predicting MTTF values, such as MLM. The MLM demonstrates superior precision and consistency in a wide range of conditions, and its strength lies in integrating a physics-based methodology, using TPM and EM as foundational models, with the incorporation of transfer learning. This innovative coupling of strategies introduces a data-centric approach, providing the model with a novel resilience against probable failure mechanisms and variability in testing conditions.

To investigate the performance of the MLM model in providing predictions for untested voltage and temperature conditions, we use a similar approach for training the MLM. First, the base model is pre-trained on a TPM-generated dataset from available test conditions. Next, the model is fine-tuned on the available experimental data. Finally, we fine-tune the model once more on an EM-generated dataset using shared voltage conditions. As mentioned before, the shared voltage condition constraint is to avoid exponential error introduced by the factor n. We use the same considerations as we did for the previous objective, to avoid information leakage. The performance of MLM and EM is evaluated against experimental data, as shown in Fig. 3. Subsequently, the RMSE and RMSPE values for each prediction model at each temperature are reported in Table III. The results clearly demonstrate that MLM consistently outperforms EM in terms of accuracy. One of the limitations of EM is its dependence on the existence of data with the same voltage when making

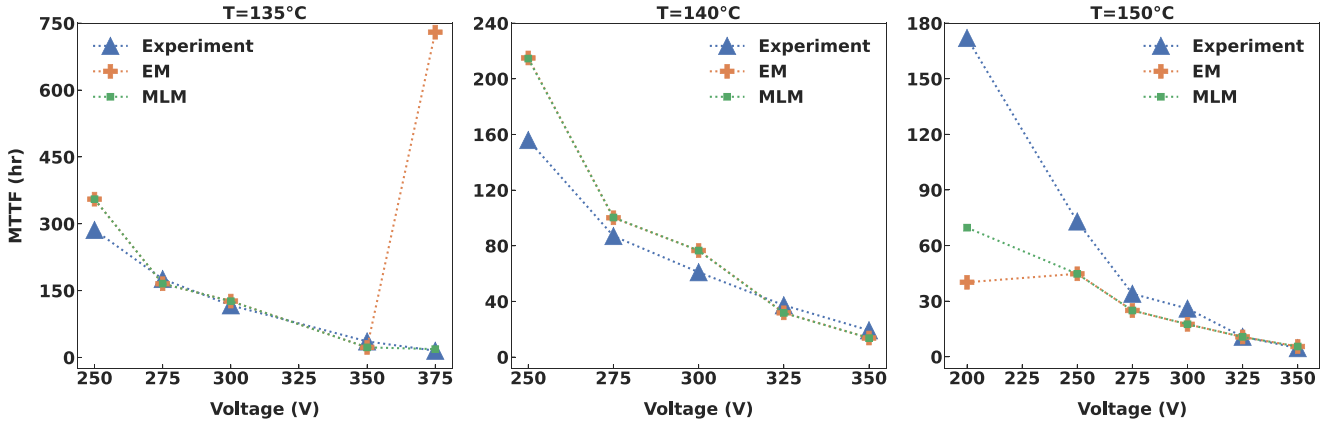

FIG. 3. A comparison of the MTTF predictions from EM and MLM for BME X7R MLCCs at unseen temperature T_N under different dc bias conditions with experimental MTTF data . For T = 140 °C, all voltage conditions are already available from previous tests on temperatures other than 140 °C, thereby making the performance of MLM and EM of equivalent accuracy. For 135 and 150 °C, not all voltage conditions are available from previous experiments, leading to large errors on those points by EM.

TABLE III. RMSE and RMSPE values for MTTF predictions made by EM and MLM for BME X7R MLCCs at unseen temperature T_N under different dc bias conditions with experimental MTTF data.

	RMSE		RMSPE (%)	
Temperature (°C)	EM	MLM	EM	MLM
135	321.2	32.1	2100	23
140	28.1	28	25.9	25.9
150	55.3	43.6	39.8	34.5

predictions for different temperatures. If the voltages for which the data points are generated are not shared between the initial and target temperatures, average values of n should be used. Choosing an inaccurate value for n leads to poor prediction performance because of the exponential error introduced by the first term in the EM. This is evident when comparing EM performance across the three test conditions. For T = 140 °C, all voltages are shared between the training and testing data; therefore, the performance of MLM goes hand in hand with that of EM, with a minor improvement. However, for the other two temperatures, not all voltages are shared, and EM shows poor predictive performance on those conditions (see Fig. 3 for T = 135 °C at 375 V and for T = 150 °C at 200 V). Therefore, to ensure accurate predictions with EM, it is crucial to use shared voltage values between the initial and target temperatures. In contrast, the MLM model, which is not reliant on specific assumptions about parameter n, consistently demonstrates superior accuracy compared to the EM model, as clearly demonstrated in the results.

SUMMARY AND CONCLUSION

In this study, we present a physics-based machine learning model (MLM) based on the XGBoost method for predicting the mean time to failure (MTTF) of multilayer ceramic capacitors (MLCCs) under various temperature and voltage conditions. The MLM employs a transfer learning framework to overcome data limitations and provides accurate predictions even for untested conditions. Unlike the heavy reliance of existing lifetime prediction models, such as the Eyring model (EM) and the tipping point model (TPM), on the availability and quantity of experimental data, the MLM uses transfer learning to leverage the underlying physics from those models and adapt to existing data to make reliable predictions. The MLM demonstrates greater accuracy and stability across varied test conditions, capturing complex patterns with limited data. This contrasting with the performance of EM and TPM, which are considerably sensitive to the end points and have shown to introduce large prediction error at those extreme points. However, despite the relative abundance of data in our study, the size of the data is generally small, which hinders a more thorough validation of our model. Further research and validation are needed to improve the performance of the proposed model and distinguish possible dominant failure mechanisms based on limited experimental data in each regime. In addition, our approach focuses solely on voltage and temperature as main features. Incorporating additional stress factors, such as mechanical stress and humidity, could further improve the model's predictive capabilities. Finally, despite data constraints, our physics-based approach guarantees accuracy at least on par with EM and TPM. We contend that as long as conventional models can be utilized, our MLM can augment their accuracy, delivering superior performance and stability. This paper focused merely on predicting the MTTF. We have argued that one needs to consider the entire distribution for the lifetime of MLCCs to achieve a valid reliability estimate. The next phase of our ongoing work would be to predict the variance of the distribution as a complementary factor for thorough reliability analysis.

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AUTHOR DECLARATIONS

Conflict of Interest

The authors have no conflicts to disclose.

Author Contributions

P.Y. and A.S. contributed equally.

Pedram Yousefian: Conceptualization (lead); Data curation (lead); Visualization (supporting); Writing – original draft (equal); Writing – review & editing (equal). **Alireza Sepehrinezhad**: Conceptualization (supporting); Software (lead); Visualization (lead); Writing – original draft (equal); Writing – review & editing (equal). **Adri C. T. van Duin**: Writing – review & editing (equal). **Clive A. Randall**: Funding acquisition (lead); Supervision (lead); Writing – review & editing (equal).

DATA AVAILABILITY

The data and source code that support the findings of this study are available at the Zenodo repository (https://doi.org/10.5281/zenodo.7943453) and source code developed openly at the GitHub repository (https://github.com/asepehri93/MLCC-LifeTime-Prediction).[30]

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