Minimization of field enhancement in multilayer capacitors

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Abstract

Evidence has shown that capacitor failure can often be attributed to field enhancement that occurs near electrode tips. In this research, methods to minimize field enhancement have been investigated using a combination of finite element analysis and an evolutionary algorithm. Specifically, the two methods considered are (1) to modify the electrode structure and (2) to adjust the resistivity in the dielectric region surrounding the tip. Optimal electrode structures and resistivity profiles have been derived that result in a significant reduction of field enhancement. Interestingly, it is predicted that adjustment of resistivity can yield a much greater reduction with a relatively minor increase in conduction loss.

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1. Introduction

Failure of dielectric materials has been correlated to numerous mechanisms, including localized melting [1], electrolytic breakdown [2], the avalanche effect [3], and corona [4]. The probability of each of these mechanisms increases with the magnitude of the electric field in the dielectric. In fact, many researchers have experimental data showing that capacitor failures generally occur in regions of field enhancement surrounding defects (porosity) and electrode tips [5–7]. In general, field enhancement limits the energy density of a capacitor and shortens its lifetime [8,9].

In most commercial applications, electrodes are shaped (e.g., rounded [10]) to reduce the peak electric field. Rounding has been motivated by the analytical solution of the electric field in dielectrics. Analytical techniques can be used to show that a peak in the electric field magnitude will occur in the vicinity of sharp corners [11]. While effective, a large electric field magnitude (relative to the field in the bulk region) remains in rounded geometries. Limits of analytical techniques have prevented a more thorough investigation of alternative methods of reducing field enhancement. However, with advances in both computing power and numerical optimization approaches, such investigations are becoming more feasible.

In this research, a combination of numerical tools has been used to investigate alternative methods of reducing field enhancement. Specifically, an evolutionary algorithm (EA) has been coupled to a finite element model (FEM) to search for alternative electrode structures and alternative dielectric compositions that may lead to reduced field enhancement. The combination of an FEM and an EA is advantageous in that it is broadly applicable and relatively straightforward to implement. It has been found that nearly complete mitigation of field enhancement can be achieved with a relatively minor change in the resistivity of the dielectric material surrounding the electrode tip. Further, it is shown that reduction achieved through modification of the dielectric is more significant than that achieved by shaping of the electrode.

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2. Description of baseline capacitor

The baseline design studied is that of a multilayer capacitor composed of conducting metal electrodes and a dielectric material. A cross-sectional view of a single layer of the capacitor is shown in Fig. 1. As shown in the figure, rounding of the electrode was performed as part of the baseline design. In this research, the dielectric of the capacitor is modeled as a material with finite resistivity while the electrodes are modeled with zero resistivity. The permittivity is assumed to be homogenous. For the initial investigation, static conditions have been considered. The effect of proposed designs on transient performance is the subject of ongoing investigation. To model the electric field within the dielectric under static conditions, the scalar potential is used, wherein one can show [12]

$$\frac{1}{\rho(x,y)} \nabla V(x,y) = 0, \quad (1)$$

subject to the Dirichlet boundary condition

$$V(x,y) = v_0 \quad \text{on } \Gamma_0,$$
$$V(x,y) = v_1 \quad \text{on } \Gamma_1, \quad (2)$$

where $v_0$ and $v_1$ is the voltage applied to the electrodes bounded by $\Gamma_0$ and $\Gamma_1$, respectively. In (1) and (2), $V$ represents the scalar potential and $\rho$ the resistivity. The electric field is expressed in terms of the scalar potential,

$$\vec{E}(x,y) = -\nabla V(x,y). \quad (3)$$

The electric field obtained using finite element analysis (FEA) based on (1) for the case in which the resistivity is uniform in the dielectric is shown in Fig. 2. For this case, $\Gamma_0$ represents the boundary between the outer electrode and the dielectric and $\Gamma_1$ represents the boundary between the inner electrode and the dielectric. The values of $v_0$ and $v_1$ were set equal to 0 and 1 V, respectively. From Fig. 2 it can be seen that although the electrode is rounded, there remains a relatively large field enhancement at the electrode tip. The peak electric field is nearly 710 V/m, compared to a value of 250 V/m in the bulk region.

Establishing an ‘optimal’ electrode structure equates to searching for the boundary surface geometry between the electrode and dielectric that minimizes the electric field enhancement at the electrode tips. Unfortunately, even for a relatively simple geometry with uniform resistivity, (1) is difficult to solve analytically. Herein, numerical methods described in the following sections are used as a tool to determine an optimal shape. In addition, numerical tools are used to establish an optimal nonuniform resistivity profile in the dielectric to minimize enhancement.

3. Numerical techniques

The solution of (1)–(3) to determine the electric field under alternative electrode and resistivity profiles was obtained using FEA. Specifically, the commercial package ANSYS [13] was used with PLANE67 elements. A representative mesh is shown in Fig. 3.

Coupled to the FEMs was an EA designed to search for optimal capacitor designs. EAs are stochastic algorithms loosely based upon the Darwinian theory of survival of the fittest [14]. They have been applied to numerous problems, including computer learning, game playing, neural network architecture development, computer security, and electric machine parameter identification and optimization. Fundamentally, in an EA structured for optimization, more ‘fit’ solutions evolve over time.

Numerous algorithms and methods fall under the umbrella of EAs, including genetic algorithms, evolutionary programming, and evolutionary strategies [14]. The basic steps for traditional EAs are shown in Fig. 4. To begin, a population of one or more members, generally referred to as ‘individuals’, is created. In this particular example an individual represents a capacitor design. Each individual of the population is composed of a set of genes (parameters). The individual is evaluated to establish its fitness (herein peak electric field in the dielectric). Once individuals are evaluated, a new population is created through reproduction, which includes recombination and mutation. Recombination is a method of combining the traits of indi-
individuals to create new offspring. Mutation is a means to vary the genetics of a population through the introduction of random changes in genes. The techniques used in recombination vary based upon the representation of the individual. If an individual is represented as a binary bit string, then a crossover algorithm is commonly used where an offspring is created using a portion of the bit string from each parent. In the case of a real-number representation, the genes of two parents can be averaged (weighted arithmetic mean) to obtain the genes of the offspring. In mutation, the genes of an individual are varied using a stochastic process.

If the individual is represented as a bit string, randomly selected bits may be complemented, or if the individual genes are represented as real values, the value may be scaled by a random number. Fitness of the offspring is evaluated and competition is used to select a subset of the population for survival in the next generation. The algorithm is terminated at a predetermined point, i.e., when a population member attains a desired fitness or a set number of generations have been executed.

For the research presented herein, the evaluation system is the FEM and the individuals of the population contain...
the distinct electrode structure or material properties of the dielectric. For reproduction, the parameters of the offspring are determined from parent parameters as

\[ P_{\text{offspring1}} = (aP_{\text{parent1}} + (1 - a)P_{\text{parent2}}) (1 + b), \]
\[ P_{\text{offspring2}} = ((1 - a)P_{\text{parent1}} + aP_{\text{parent2}}) (1 + c), \]

where \( P_{\text{offspring1}}, P_{\text{offspring2}}, P_{\text{parent1}}, \) and \( P_{\text{parent2}} \) represent the parameters for two offspring and two parents, respectively. The \( a \) is a weighting parameter and \( b \) and \( c \) are mutation parameters. The values of \( a, b, \) and \( c \) are uniformly distributed random numbers such that \( a \in [0, 1] \) and \( b, c \in [-0.001, 0.001] \). Distinct values of \( a, b, \) and \( c \) are obtained for each offspring pair.

In this research, an elitist strategy was used to select population members to survive to the next generation. More specifically, once the fitness measure is applied, a set number of the fittest members from the parent and offspring populations are selected to form the next generation’s population.

4. Minimization of field enhancement

4.1. Geometry of electrode tip

To determine an electrode geometry that minimizes enhancement, alternative capacitor designs were evaluated wherein the radius of the electrode tip was the gene used to establish the individuals of the population. A diagram of the defined radius is shown in Fig. 5. A population size of ten individuals was used for all generations.

The electrode design that yielded the minimum field enhancement is shown in Fig. 6. For this ‘optimal electrode’ design, the magnitude of the peak electric field is roughly 508 V/m. The radius is roughly 1.5 mm, or 24\% of the distance between electrodes. Using values of electric field calculated from the final EA population, the peak field as a function of radius was established and is shown in Fig. 7. From Fig. 7 it can be seen that the peak electric field versus radius has a parabolic behavior. Specifically, an initial increase in radius corresponds to a relatively sharp drop in peak electric field. However, as the radius continues to increase, the magnitude of the electric field begins to increase exponentially. The increase is due to the proximity of the electrode tip to its neighbor, i.e., the peak field is shifted from the electrode tip to the neighboring electrode.

4.2. Altering resistivity in bulk region

As an alternative to changing the electrode geometry, the resistivity in the region surrounding the electrode tip is considered. To investigate optimal resistivity profiles, several methods were considered. Specifically, as a first step, 14 rings were established between the electrode tip and neighboring electrodes. The rings are shown in Fig. 8.

In the first optimization approach using a nonuniform dielectric, it is assumed that the resistivity increases linearly from a specified starting value in the circle nearest the...
The starting resistivity represents the gene of the EA individuals. Using the EA with 10 individuals in the population, it was determined that the optimal starting resistivity is roughly 20% of the resistivity of the bulk region of the dielectric. The electric field and corresponding resistivity profile for the optimal design are shown in Fig. 9. From this figure, it can be seen that the peak electric field is 333.5 V/m, which is less than 50% of that seen in the base capacitor (Fig. 2). Interestingly, this reduction is much greater than that found by adjusting the electrode tip geometry (Fig. 6).

The peak field as a function of starting resistivity is shown in Fig. 10. To quantify the results, it is useful to highlight that the resistivity in the bulk dielectric material is $2.5 \times 10^{11} \ \Omega \text{m}$, while the resistivity of the electrode is assumed to be zero. From the figure it can be seen that the peak electric field initially decreases as the starting resistivity is reduced below that of the bulk region. However, as the resistivity is decreased below an optimal point, the peak field tends to increase (although the value remains well below that of the initial base capacitor). This results from a shifting of the peak field to the neighboring electrode. To illustrate, an example is provided in which the starting electrode tip to the resistivity of the bulk region in the outermost circle. The starting resistivity represents the gene of the EA individuals. Using the EA with 10 individuals in the population, it was determined that the optimal starting resistivity is roughly 20% of the resistivity of the bulk region of the dielectric. The electric field and corresponding resistivity profile for the optimal design are shown in Fig. 9. From this figure, it can be seen that the peak electric field is 333.5 V/m, which is less than 50% of that seen in the base capacitor (Fig. 2). Interestingly, this reduction is much greater than that found by adjusting the electrode tip geometry (Fig. 6).

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resistivity is set to zero (i.e., represented as an ideal conductor) and the final resistivity is set to the value of the bulk dielectric region. The resulting electric field and resistivity profiles are shown in Fig. 11. Therein, it can be seen that the position of the peak electric field has shifted from near the electrode tip (as it is in Fig. 2) to the outer edge of the transitional region nearest the neighboring electrode.

Prior to highlighting alternative designs, it is interesting to consider the number of generations and time required for the optimization approach. Specifically, in Fig. 12 the peak electric field for each of the 10 individuals of the EA population are shown for the first 12 generations. It can be seen that the population has converged to a peak electric field below 350 V/m by the sixth generation. Each of the fitness values takes roughly 7–8 s to compute. Therefore, the optimization required roughly 15 min using a 3.2 GHz single processor desktop computer.

To consider further reduction of the peak field, a second EA was applied wherein each individual of the population has a set of 14 genes that represent resistivity values in the 14 concentric rings. The resulting optimal resistivity profile is shown in Fig. 13. Therein, concentric ring 1 is nearest to the electrode tip and the numbering proceeds outward toward neighboring electrodes. The optimal resistivity profile yielded a capacitor with a peak electric field of 272 V/m, which is only 9% higher than the field in the bulk region. The field and associated resistivity profile are shown in Fig. 14. Therein it can be seen that the field distribution is nearly uniform. For this study, convergence of the EA

Fig. 10. Peak electric field as a function of starting resistivity (assuming resistivity varies linearly from electrode tip).

Fig. 11. Results of a single parameter optimization where starting resistivity is set to zero and final resistivity is set to value of bulk region.
required over 500 generations (population of 10 individuals in each generation) and roughly 12 h to complete (3.2 GHz desktop).

For a final optimization approach, the concentric rings were subdivided into smaller regions that are herein referred to as concentric arcs. Each of the 50 concentric arcs, shown in Fig. 15, has an independent value of resistivity. Thus each individual is composed of 50 genes. The electric field and resistivity profile for the optimal design are shown in Fig. 16. For the optimal profile, the peak electric field was 267 V/m, or 7% greater than the electric field in the bulk region. As in the previous cases, the resistivity is a minimum at the electrode tip and increases into the bulk region. It is noted that the resistivity does change rather significantly as a function of the angular position. Despite the rather significant change with angular position, there is relatively little improvement compared to the capacitor design in which each ring has a uniform resistivity (Fig. 14). The optimization with 50 genes per individual (10 individuals in the population) required an estimated 10,000 generations to reach convergence. This required roughly 9 days of runtime (3.2 GHz desktop).
In theory, a more refined search could be applied wherein resistivity is considered in finer discretizations. However, as shown from this study, the time required to search for optimal designs increases dramatically. Moreover, comparison of the results of the concentric rings and the concentric arcs shows that such refinement may be unnecessary.

5. Discussion

The results in Section 4 point to a possible direction for reducing field enhancement, and thereby increasing power density of capacitors. However, it is noted that there are associated design tradeoffs. For one, changing the electrode structure or resistivity of a dielectric has the effect of increasing the conduction loss. To provide an estimate of the expected increase in loss the resistance of each of the capacitor designs was determined numerically based upon the ratio

$$R = \frac{V}{\int \vec{J} \cdot \text{ds}}$$

(5)

where $V$ is the applied voltage, $\vec{J}$ is the current density, and $\text{ds}$ is a two-dimensional surface surrounding the electrode in the middle of the dielectric. The resistance of the section of the baseline capacitor design (shown in Fig. 2) was numerically determined to be 31.1 MΩ.\(^1\) The resistance of the subsection, not the entire capacitor.

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\(^1\) The resistance calculated is that of a subsection, not the entire capacitor.
optimized capacitor designs with varying electrode radius (Fig. 6), and varying resistivity (Figs. 14 and 16) were 30.1, 29.8, and 30.3 MΩ, respectively. Comparing values, the resistivity is on the order of 5% less than the baseline design. Therefore, at worst one would expect a 5% increase in conduction loss.

In addition to loss, changing the electrode structure and introducing nonuniform resistivity in the dielectric would require additional material processing. At this time, practical methods of adjusting the resistivity of the dielectric to achieve the profiles observed in Figs. 9, 11, 14, and 16 are unknown. However, it is noted that doping of the dielectric to eliminate porosity has been used in [5]. Conceivably, controlled diffusion of dopant material through the dielectric, or a similar manufacturing process, could be used to achieve profiles similar to those determined herein. The profile of most practical interest is likely that shown in Figs. 13 and 14 due to its significant reduction in field enhancement and relatively simple resistivity profile.

6. Conclusions

Numerical techniques have been used to investigate new methods of reducing the peak electric field within a multilayer capacitor. Specifically, finite element-based models have been coupled with an evolutionary algorithm to search for electrode structures and dielectric resistivity profiles that minimize the peak electric field surrounding the tip. Using both approaches, significant reductions have been found that hold promise in greatly increasing the energy density of capacitors. Interestingly, designs in which the resistivity is adjusted yield a more significant reduction in the peak electric field compared to those in which the electrode tip structure is altered.

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References