QUANTUM MODELING OF CAPACITOR ENERGY DENSITY

Adam G. Tournier, PhD
Associate Professor of Physics, McKendree University, USA

Abstract

Energy storage is necessary to power the technologies that sustain or global society. One of the devices utilized for the creation, storage, and delivery of electrical energy are capacitors. The basic physics of capacitors is discussed. The physical parts of the device are explained, and the separator film, which is the focus of this research, is modeled. By optimizing the polarization of the molecules in the separator film through quantum modeling of the electric displacement of the molecules, the dialectic constant of the material can be optimized. The dielectric constant is directly proportional to the energy stored in the capacitor. Increasing the dielectric constant will proportionally increase the energy stored in the capacitor, and increase the energy density of the device.

Keywords: Capacitors, Quantum Modeling, and Energy Density

Introduction

The energy needs of our global society are increasing. To effectively create, store, and deliver the energy needs of the future alternative materials must be found to augment the current methods and technologies utilized. Capacitors are one tool for the effective storage and delivery of energy to many technologies. To optimize current systems and support the creation of new technologies, higher density energy capacitors must be developed. Higher energy densities in capacitors allow fewer capacitors to be used, fewer recharging cycles for each device, and smaller size scale devises. Small size scale devices and longer capacitor life are keys to unlocking the energy needs of the future. This paper will examine one method for achieving increased energy density in film capacitors.

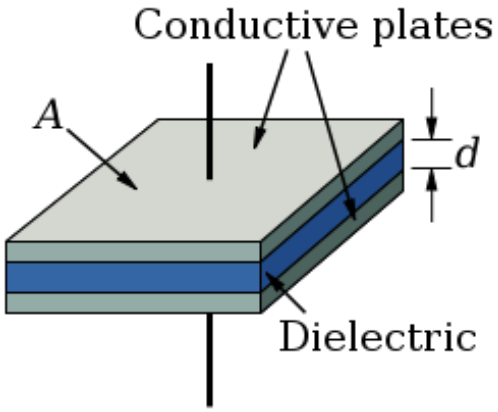
I.

Energy is a measure of a system's ability to do work. By finding new sources of energy, our society has developed technologies to improve the quality of our lives. The discovery of electricity and the delivery of this energy source created the increasing complexity we experience. These new technologies improve the quality of life, but have an ever increasing energy need. Our global society requires larger and more powerful energy sources to sustain current technologies foster the innovation required to discover new technologies, and industrialize the portions of our world that have not yet realized the gains of the twenty-first century.

The delivery of energy in an electronic system has two important factors. The first is how much energy a device can deliver. The total energy stored in a device is ultimately measured in Joules (J), but the industry standard is the Watt*Hour (W□h). A Watt (W) is a Joule per second (J/s), and a W□h is 3600 J. All electric storage devices have a limited number of Joules they can store and deliver. The larger the stored energy in a device the long the system will operate. The amount of stored energy per unit size is called the energy density of the device. An increase in energy density is the goal of this research. The second is the

rate at which the device can deliver its stored energy. This rate of energy delivery is measured in watts. Modern electronics are limited by the rate at which energy can be delivered from electric storage devices, and the limited energy density of the device.

The two main energy storage devices for electricity are capacitors and voltaic cells. Capacitors are the focus of this research. A capacitor is an arrangement of conductors separated by an insulator. This insulator is called a dielectric. In electronic circuits, the capacitor is usually two parallel conducting plates separated by a very thin film. Capacitance is a direct measure of the energy storage capacity of the device. The capacitance (C) of the device is given by $C = \kappa A\varepsilon/d$, where κ is the dielectric constant of the separator material, A is the cross sectional area of the plates, ε is the permittivity of free space, a constant, and d is the plate separation.

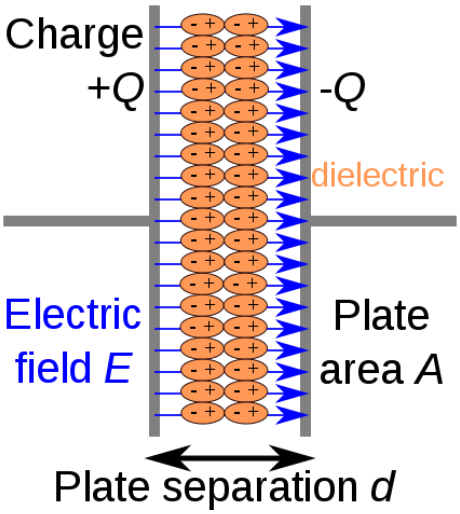


Despite the widespread use of polymer film capacitors in a large number of applications, this capacitor technology has not seen any major energy improvements over the past 40 years. Capacitors have not kept pace with the rapid advance in solid-state switching devices leading to a lowering of system efficiency while adding significant volume and weight to power electronics systems.

To optimize modern capacitors one of the three physical parameters of the device must be altered. The area of the device could be made larger, but the ultimate goal of modern electronic is to scale to smaller sizes. The physical size of capacitors needs to decrease. Decreasing plate separation will increase energy density, as the capacitance is inversely proportional to the plate separation, and the separation is the thickness of the dielectric. Engineering thinner films will increase energy density. The third option is to increase the dielectric constant. This is the focus of this research. Through quantum modeling of the physical characteristics of the dielectric film novel films can be designed to achieve higher dielectric constants, and maintain dimensional stability under large voltage and temperature ranges.

William Whewell coined the term dielectric from dia-electric in response to a request by Michael Faraday.Dielectric films in capacitors are insulators, which do not allow free electron movement in the material. All of the electrons in the material are associated with specific nuclei. This binding leads to unique properties of the material when an external electric field is applied to the dielectric. Capacitors function by building an electric field between the plates of the device as electrons delivered by current flow through the rest of the circuits build on one plate of the capacitor. These excess electrons drive electrons from the opposite plate of the capacitor, creating charge separation between the plates. The electric field applies force to the electrons bound in the dielectric material forcing them to polarize. This polarization is the ability of the molecules of the dielectric to distort and counteract the charge separation on the capacitor plates. Increasing the energy stored in the electric field inside the capacitor. The dielectric constant is a measurement of the ability of the material to

be polarized. The larger the dielectric constant the more polarization the molecules are capable of. This leads to larger capacitance and a higher energy density in the device.



Increasing dielectric constant of a material can be accomplished by increasing the electric displacement of the molecules. As the electric field is applied to the dielectric the molecules are stretched, physically altered by the force of the electric filed. The orbits of the electrons in the material are altered creating a new distribution of the electron probability density for the molecule. The new distribution induces a polarized state for the molecule leading to the electrons spending more time by the positively charged plate of the capacitor. Analyzing the quantum states of the electrons in the molecule and determining how the field changes the probability density of their position will allow for the analytical calculation of the polarization of a single molecule of the dielectric material. Modeling the static dielectric constant for the material is the first step.

The second step of the process is to calculate the polarization of the molecule as a function of direction angle. As the material polarizes the orientation of the molecule can be changed. The vector direction of the molecular axis must be considered to derive a model for the dielectric constant of the molecule is three dimensions.The vector direction of the molecular axis may change as the field is applied leading to a contribution to the polarization separate from the changes to the electron probability density function. This three dimensional model must also consider how the molecules are bound to the rest of the bulk film and if there are any crystalline characteristics to the bulk film. Either of these factors will affect the orientation of the molecule with respect to the field, and in turn affect the polarization of the molecule.

The bulk film that is the real world material does not have the molecules oriented in a specific direction. An analysis of the orientation of the molecules of the bulk film must be considered. Using Transition Electron Microscopy (TEM) analysis a statistical model of the orientation of the molecule of the film can be created. By analyzing the bulk characteristics of the film a model can be created that will deliver an accurate calculation of the measurable dielectric constant of the film. Again, the inter-molecular forces due to coulomb forces or crystalline properties of the material must be considered in the statistical model of the bulk film.

Once an accurate statistical model for the bulk film of know materials is achieved, novel film design can be started. By utilizing the models of current films, new molecular orientations and compositions can be achieved and theoretically tested for increasing dielectric constant.

The most used film materials in capacitors are polypropylene (PP), with a market share of approximately 50%, and polyester (PE), with approximately 40% share. All other materials account for the remaining 10% share. This research will focus on initial models for PP and PE. Once accurate models are developed for these materials, novel film design can begin its theoretical stage. Followed by small-scale fabrication and experimentation of the novel films once stable molecular designs have been achieved.

Conclusion

Understanding the molecular characteristics of dielectric materials allows for the calculation of the polarization of the molecule through a quantum analysis of the probability density of the electron positions in the molecule. Once an accurate model of the probability density exists the polarization of the molecule can be modeled in three dimensions. With an analytical model of the polarization vector for the molecule a statistical analysis of the bulk material is necessary for the real dielectric constant of the film to be calculated. The quantum modeling of the molecules will require the cooperation of our Computer Science faculty and students. Senior thesis work from our undergraduate students will be used to accomplish the computer modeled quantum behavior and statistical analysis. The completion of these theoretical models will enable the design of novel compounds, which will be designed and manufactured in collaboration with The University of Missouri and Indiana State University.

References:

Bateman, Cyril, Understanding Capacitors, Electronics World, 1998.
Daintith, John, editor. Oxford Dictionary of Physics. New York: Oxford University Press, 2005.
Jackson, John David, Classical Electrodynamics, New York: Wiley, 1998.
Jacobs, F, Polypropylene Capacitor Film Resin, Passive component magazine, 2005.
James, Frank, editor, The Correspondence of Michael Faraday, Volume 3, London: The Institution of Electrical Engineers, 1996.
Von Hippel, Arthur, Dielectric Materials and Applications, New York: Technology Press of MIT, 1954.