

**Department of Electrical and Computer Engineering**  
**Materials Engineering Program**  
**Center for Integrated Bio and Nano Systems**  
**9:00 a.m., Feb. 26, 2021**

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## **The digitization of materials and investigators**

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**Abstract:** In this talk, three different studies will be highlighted. The first will discuss how to increase the energy density of high dielectric constant capacitors. Results from experiments and simulations performed on a high energy density polymer matrix hybrid composite that features ferroelectric barium titanate nanoparticles and multi-walled carbon nanotubes (MWCNT) embedded in poly (vinylidene fluoride) (PVDF) provide important findings. The addition of the conductive MWCNT increases the charge storage ability of the matrix polymer by serving as a polarized charge transport phase for the ferroelectric nanoparticles. The development of conductive networks in the polymer matrix was prevented by establishing a uniform dispersion of the ferroelectric fillers that was achieved by a simple mixing method. The dielectric properties of the polymer matrix nanocomposites with hybrid fillers were optimized by taking advantage of synergistic effects between the charge storage effects of the ferroelectric phase and the charge transport effects of the conductive phase. The maximum energy density obtained, based on measured real permittivity and breakdown strength, was  $19.82 \text{ J cm}^{-3}$  while maintaining a low dielectric loss at 1 kHz. The reliable dielectric properties and flexibility make this hybrid composite potentially useful for flexible electronic devices and in electrostatic energy storage.

The second example will illustrate the importance of controlling the 3D arrangement of a second phase for achieving the electrical properties desired for EMI shielding or contact electrodes while minimizing cost. MWCNT/PMMA composites were fabricated using three different mixing methods (mechanical, solution, and melt mixing) which creates different arrangements of the carbon nanotubes that results in very different electrical properties. Specimens made by the three different mixing methods, which displayed the same electrical resistivity, were chosen for detailed TEM analysis. In all the specimens, the CNTs are found to be 12-15 nm of diameter while the length of the nanotubes varies. Selected area diffraction patterns indicate that the nanotubes in all three specimens are identical in phase and structure. TEM images reveal that the MWNT arrange themselves along the polymer boundaries in the mechanical mixed sample while they are evenly distributed throughout in the melt mixed sample with the formation of some micron sized agglomerates. The solution mixed samples did not show any distributed MWNT and instead all nanotubes form mostly agglomerates with different surface characteristics from those observed in the melt mixed samples. These results are in agreement with SEM and optical microscopy results obtained at higher magnifications.

The third study will describe the interesting microstructure that sol gel processed ITO thin films form during layered deposition. ITO films are ubiquitous in many optoelectronic applications because of its unique combination of high transparency and high electrical conductivity that many have attempted to replace without success. Our goal was to develop a patternable method of deposition that could be used for flexible electronics without requiring material waste.

We were successful in making excellent transparent films but we never achieved as high an electrical conductivity as we expected. In trying to determine the cause of the two order of magnitude lower conductivity, we conducted neutron reflectivity (NR) experiments for a series of spin coated samples deposited onto fused quartz substrates. Analysis showed that the films form a hierarchical structure where the topmost layer is always more porous than the underlying layers. Graphs of the neutron scattering length density plotted vs depth (thickness) of the multilayer films show that density increases as more layers are added. We found that NR was an extremely useful tool to connect the information obtained from non-contact AFM image results to the average density of the films and thus help explain some of the conductivity discrepancies.



**Short Bio:**

Prof. Gerhardt has been a faculty member at the Georgia Institute of Technology since January 1991. She was elevated to full professor in 2001 and chosen as the Senior Goizueta Faculty Chair in 2015. Prof. Gerhardt is the director of the Electrical Testing of Materials and Devices (ETMD) Center which conducts detailed experiments on all classes of materials as a function of frequency, temperature, voltage and atmosphere. Her group has done work for Arnold Magnetics, NanoResearch, Sandia National Laboratories and others and has assisted many research groups at Georgia Tech. In addition to the composite materials described above, her group also conducts research on the fabrication and characterization of thin films such as ITO and carbon nanotube thin films and relates their nanostructure to the obtained electrical and optical properties. She has been working on a monograph on dielectric and impedance spectroscopy for the last 10 years and hopes to complete this project within the next year. She is the author of over 200 peer reviewed publications and is a member of MRS, IEEE, ACeRS, Sigma Xi and other professional organizations. She was awarded the Friedberg Award at the 2017 MS&T conference in Pittsburgh. She is an ACeRS fellow and an IEEE Senior Member.

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