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Investigation of Nanoparticle Size Effects on the Dielectric Properties of Functionalized Barium Titanate

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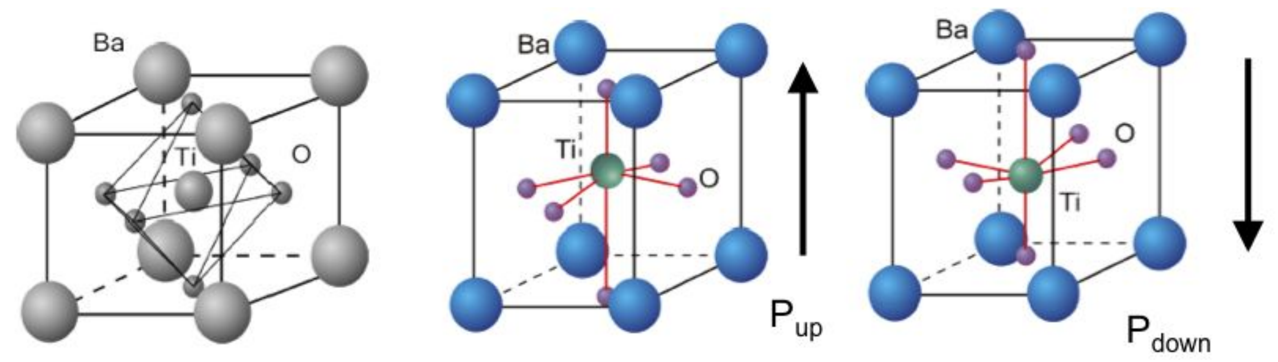
Background

Barium Titanate ($BaTiO_3$ or BTO) is a ferroelectric perovskite.



The electric dipole created by the displacement of the central titanium cation reverses in the presence of an external electric field. The reversal of the polarization allows BTO-containing materials to acquire a surface charge. Therefore, BTO has long been a favorite dielectric material for capacitors; it is ferroelectric at room temperature with an effective dielectric constant of ~5000 [1].

Motivation

The effective use of renewable energy sources, smart grids, and electrified vehicles is critically dependent upon the next generation of electrostatic capacitors and their promise for enhanced energy storage, power conversion, and power conditioning. Ceramic capacitors are ubiquitous in electronics and often contain BTO as a dielectric material, which has driven research into the dielectric properties of BTO.

Several studies have reported that the dielectric constant of BTO thin films increase with grain size up to 200 nm [2]. Dielectric constants were then found to plateau at grain sizes above 200 nm (Figure 1).

In contrast, results from research by Wada et al. showed that synthesis method and particle size both have an impact on the dielectric constant of BTO (Figure 2) [3]. Notably, drastic increases in dielectric constant were observed at small particle sizes (~60 nm).

Therefore, there is still debate as to how the ferroelectric properties of BTO change as a function of particle size and other physical properties.

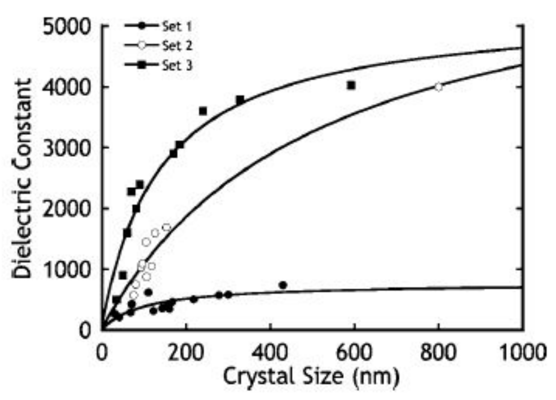


Figure 1. Results from a cross-study survey showing the impact of crystal size on the dielectric constant of BTO thin films.

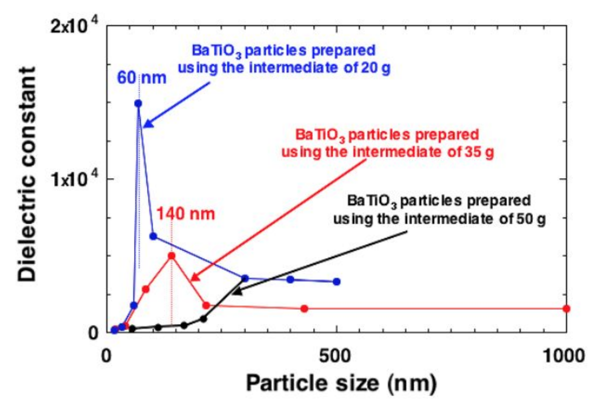


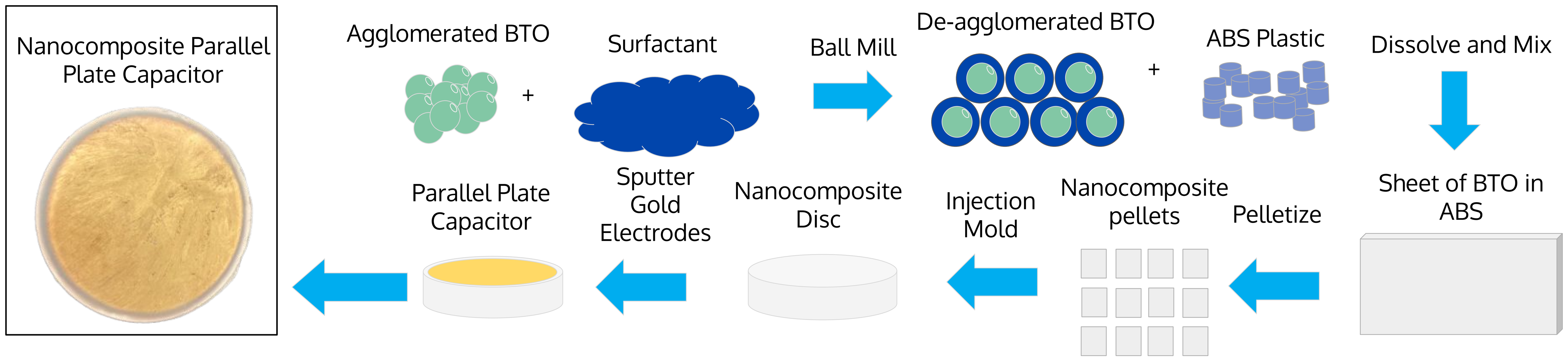
Figure 2. Results from an investigation into the effect of particle size and synthesis method on the dielectric constant of BTO particles

Project Goal

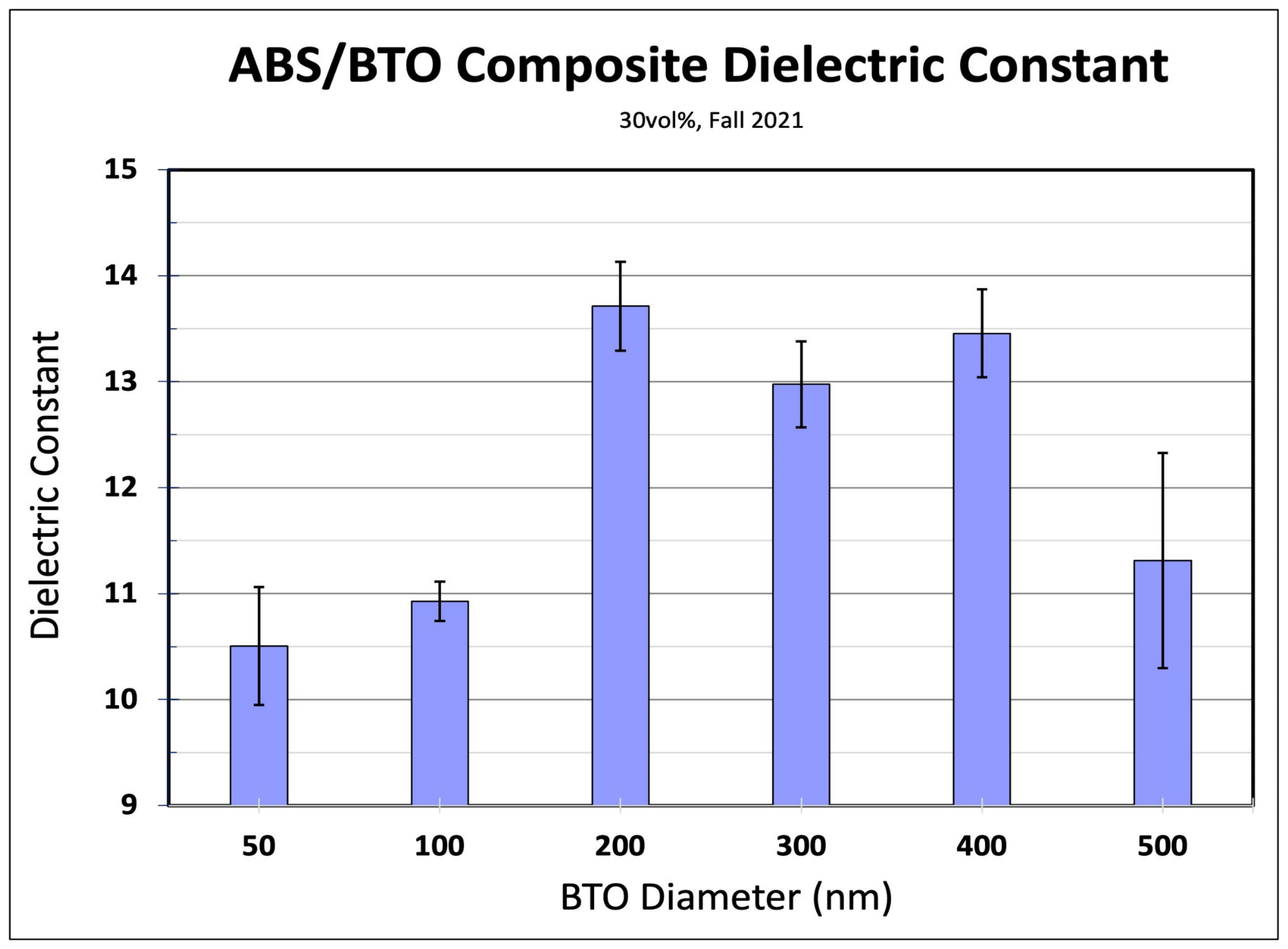
The goal of this project is to determine the impact of particle size on the dielectric constant of BTO. Achieving this goal involves:

1. measuring the dielectric constant of injection-molded polymer-matrix nanocomposites containing high volume loadings of BTO nanoparticles and
2. performing computational simulations of the nanocomposites using COMSOL.

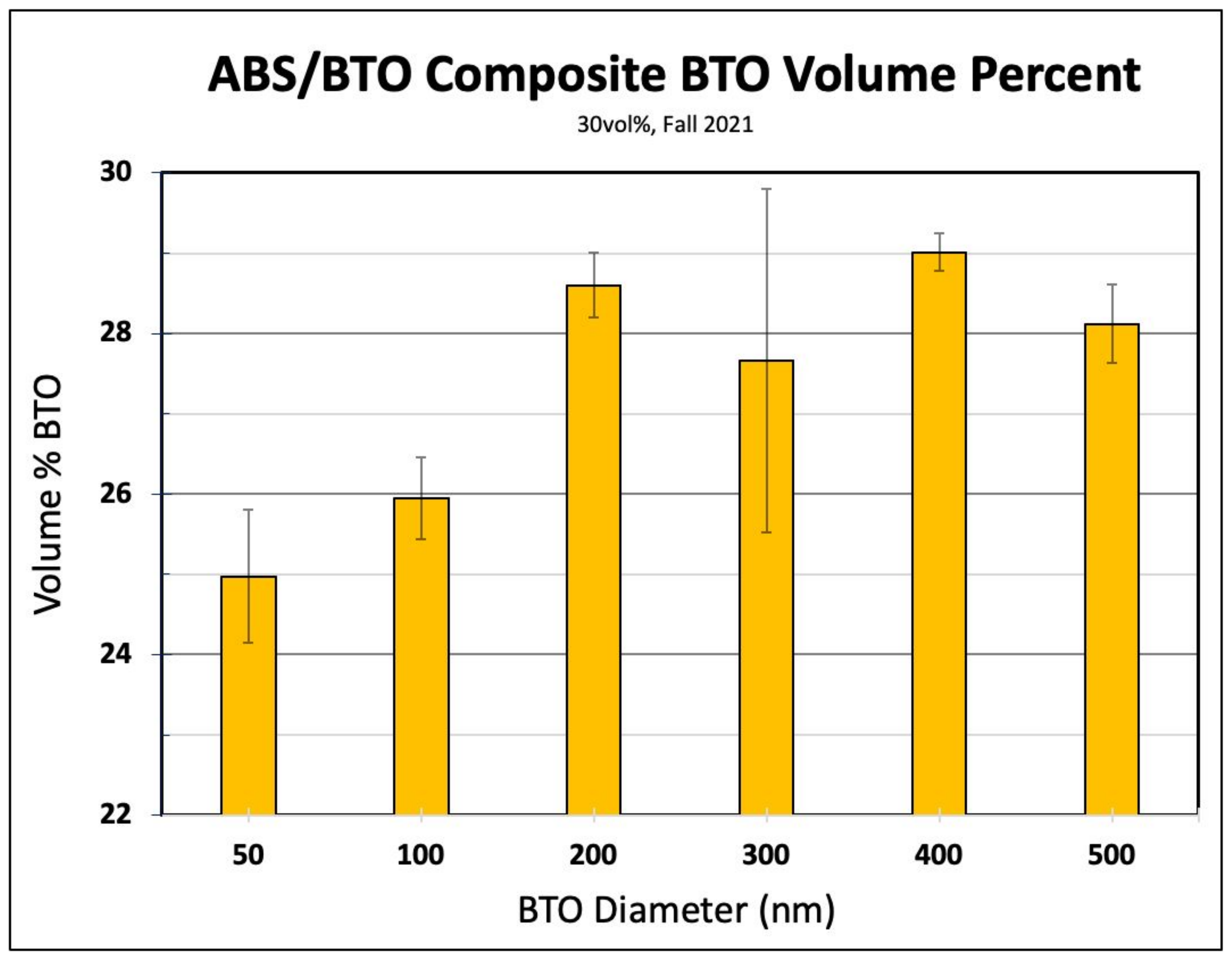
Fabrication



Experimental Results



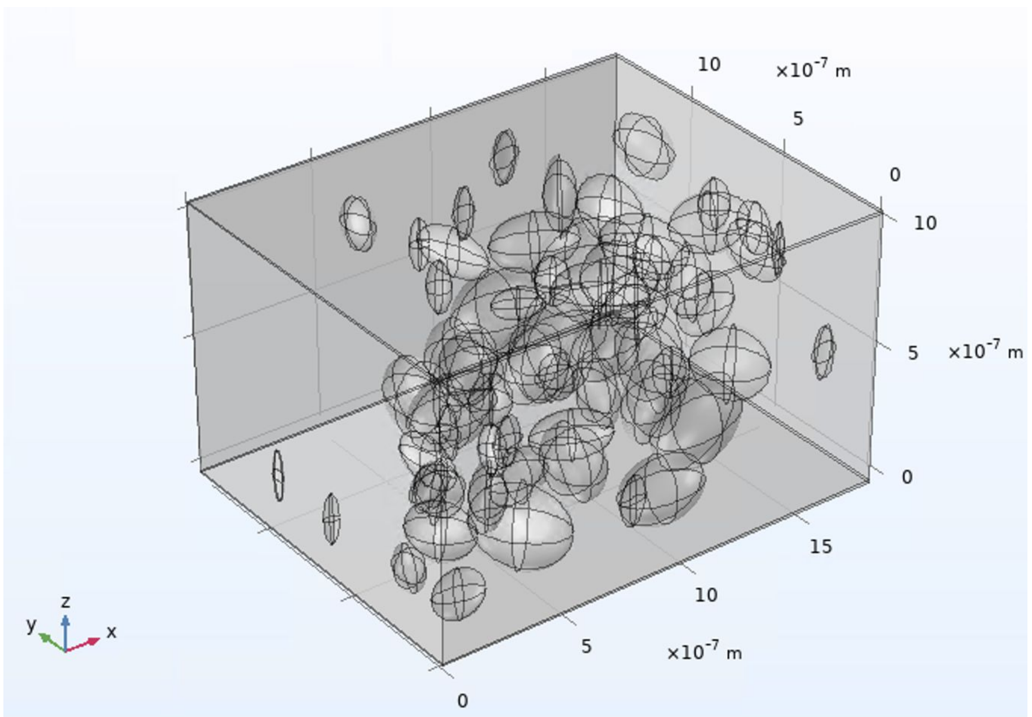
Mean Composite Dielectric Constant with 1 Standard Deviation Error



Mean Composite Volume Percent with N ranging from 3 to 5, with 1 Standard Deviation Error

Modeling

Computational models of nanocomposites were created using TEM images and an image processing pipeline that generated particle boundaries with the BTO volume percent present in the experimental sample. COMSOL Multiphysics was used to model the nanocomposite using the data extracted from the image processing pipeline. Using this model, a composite dielectric constant is calculated and compared with experimental values to investigate the electromagnetic properties of BTO.



13.06 volume percent BTO/ABS nanocomposite yielding a dielectric constant of 5.37

Future Work

Fabricate 50 volume% nanocomposites to get more reliable measurements and compare effect of volume loading on ε.

Use COMSOL model to find dielectric constant of the BTO.

Generate COMSOL models of 30 vol% composites for each nanoparticle size.

References & Acknowledgements

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[3] S. Wada et. al, "Origin of Ultrahigh Dielectric Constants for Barium Titanate Nanoparticles," J. Korean Phys. Soc., vol. 51, 2007.

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