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Synthesis and Modeling of Barium Titanate Nanoparticles in a Composite to determine Dielectric Constants

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Who we are

Todd Monson

Outline

Barium Titanate Colloidal Solutions and Composites

Composite Fabrication

Composite Dielectric Constant Measurement

Finite Element Modeling

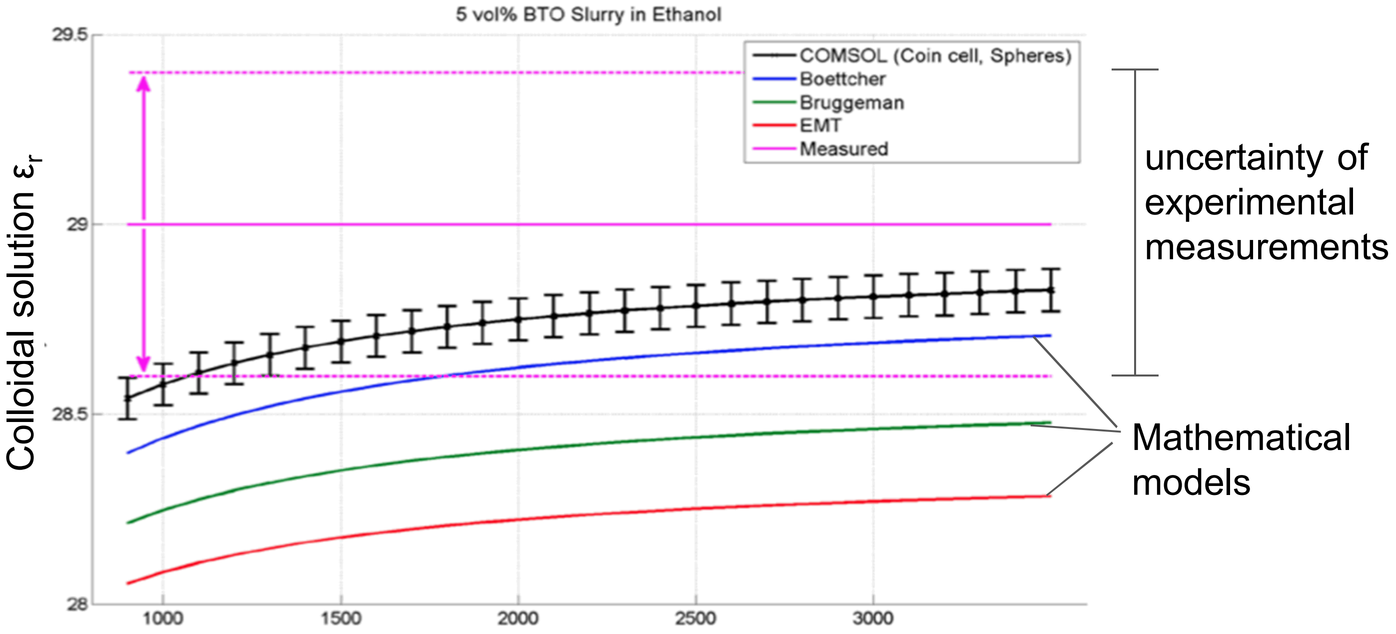
Matching Simulation with Experiment

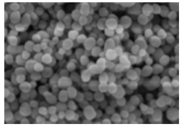
Surface functionalized particles

Conclusion

BTO Colloidal Solutions

Large uncertainty when extracting BTO dielectric constant (ε_r) from colloidal solution ε_r

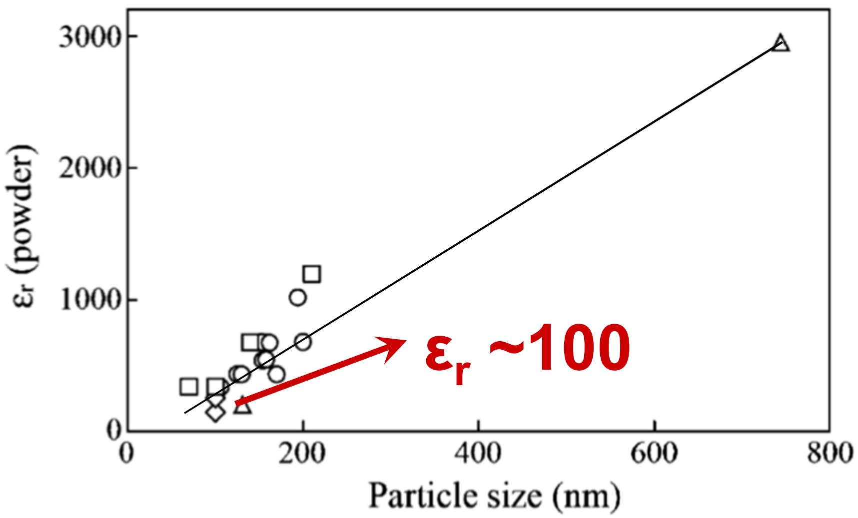




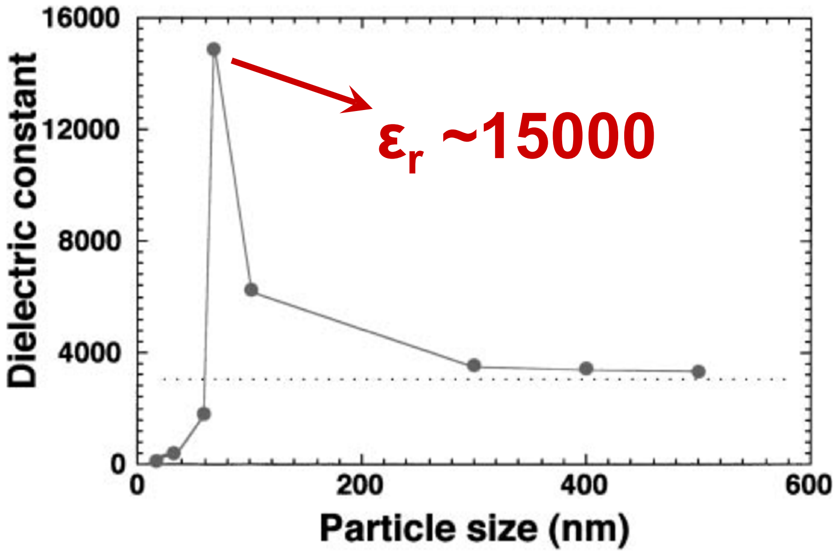
BTO ε_r

Puma et al. *Unpublished* (2014).

BTO Colloidal Solutions in Literature



Tsurumi et al. *J. Am. Ceram. Soc.*, 89 [4] 1337-1341 (2006).



Wada et al. *Jpn. J. Appl. Phys.* Vol. 42 6188-6195 (2003).

Slide 5

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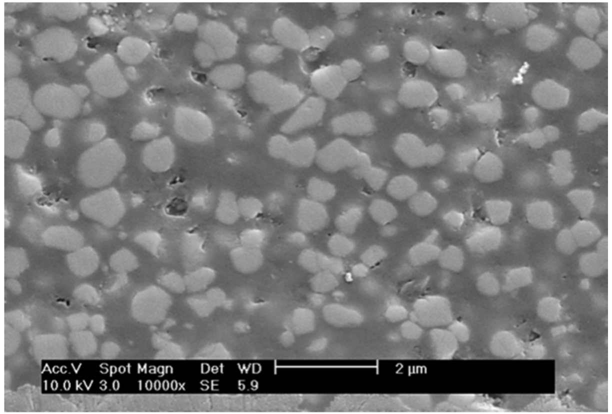
Kirklann Lau,

BTO Composites

BTO/epoxy Composite Films



Cho et al. *J. Mat. Sci.,* **16** 77-84 (2005).

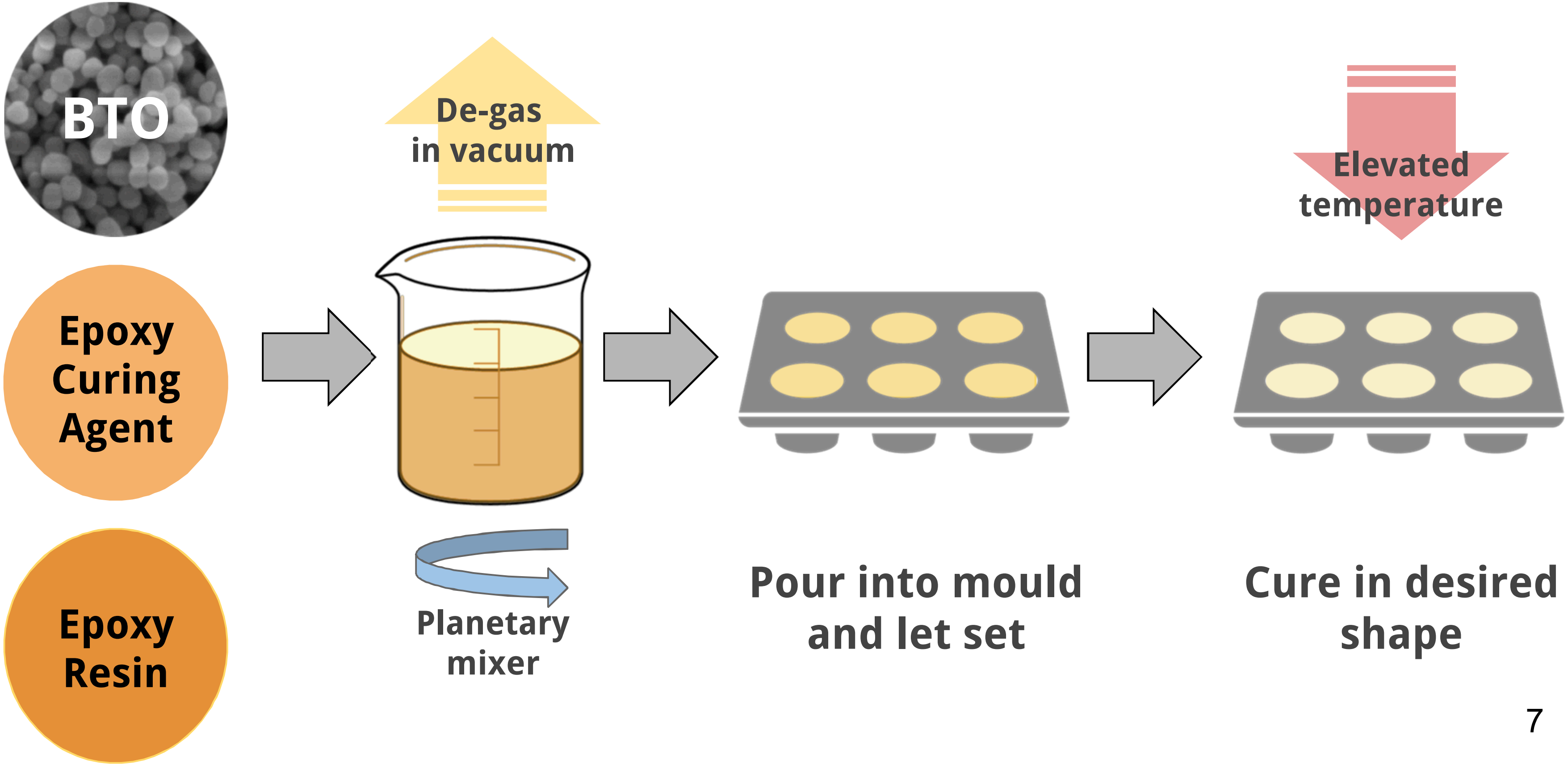
Jayasundere-Smith Equation

$$\varepsilon_{\mathrm{eff}} = \frac{\nu_p \varepsilon_p + \nu_c \varepsilon_c \left[\frac{3\varepsilon_p}{\varepsilon_c + 2\varepsilon_p}\right]\left[1 + \frac{3\nu_c(\varepsilon_c - \varepsilon_p)}{\varepsilon_c + 2\varepsilon_p}\right]}{\nu_p + \nu_c \left[\frac{3\varepsilon_p}{\varepsilon_c + 2\varepsilon_p}\right]\left[1 + \frac{3\nu_c(\varepsilon_c - \varepsilon_p)}{\varepsilon_c + 2\varepsilon_p}\right]}$$

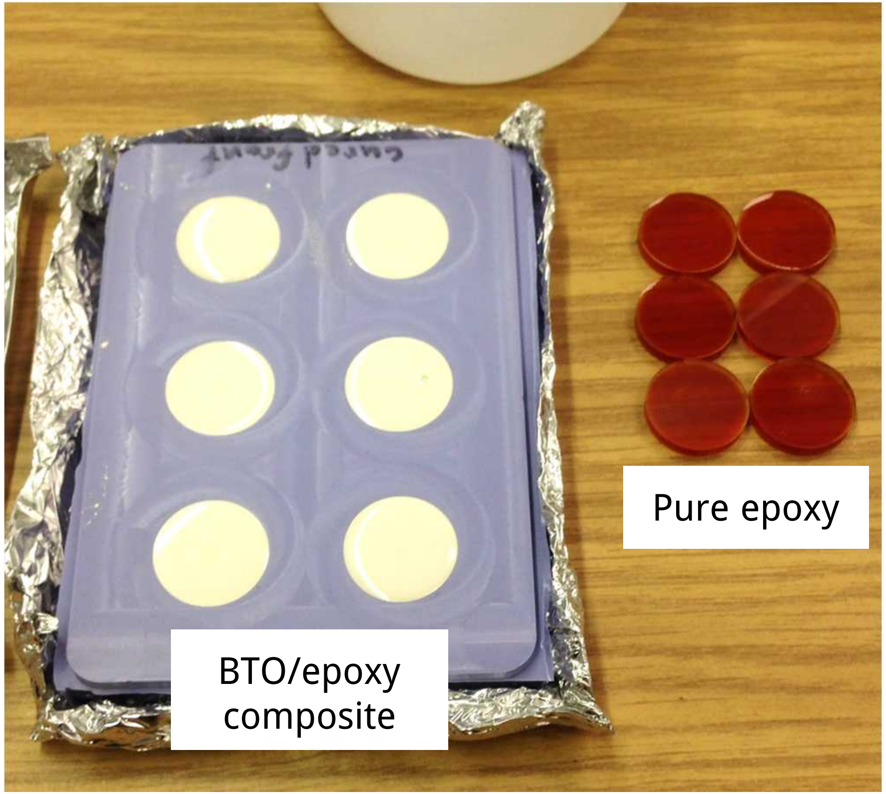
→ BTO ε_r

We fabricated similar BTO/epoxy composites and explore the validity of mathematical modeling to extract the BTO ε_r using finite element modeling

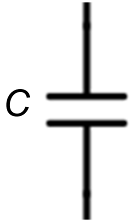
BTO Composite Fabrication



Composite Fabrication



Sputter electrodes



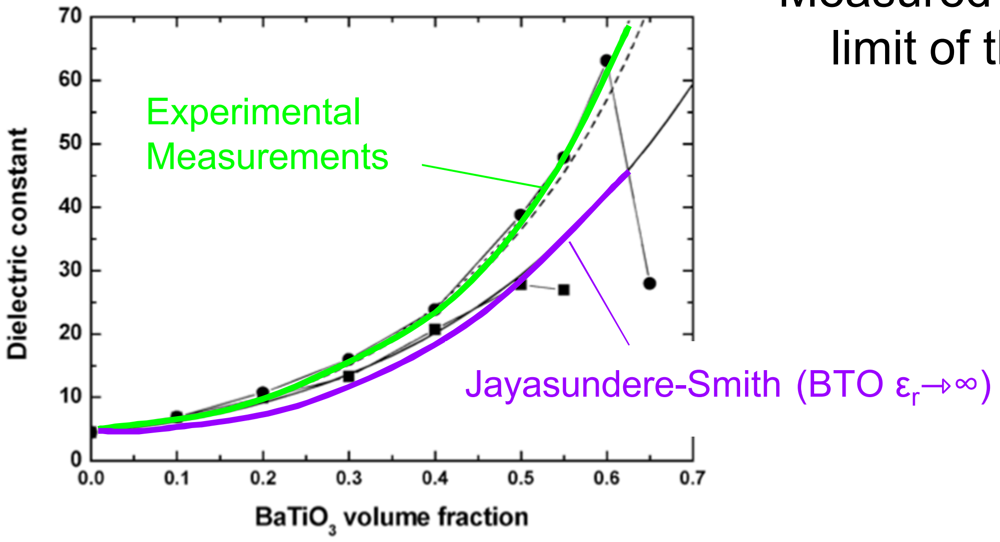
Measure *C* (capacitance meter or impedance spectroscopy)

$$C = \varepsilon_0 \varepsilon_r \frac{A}{d}$$

Calculate composite ε_r

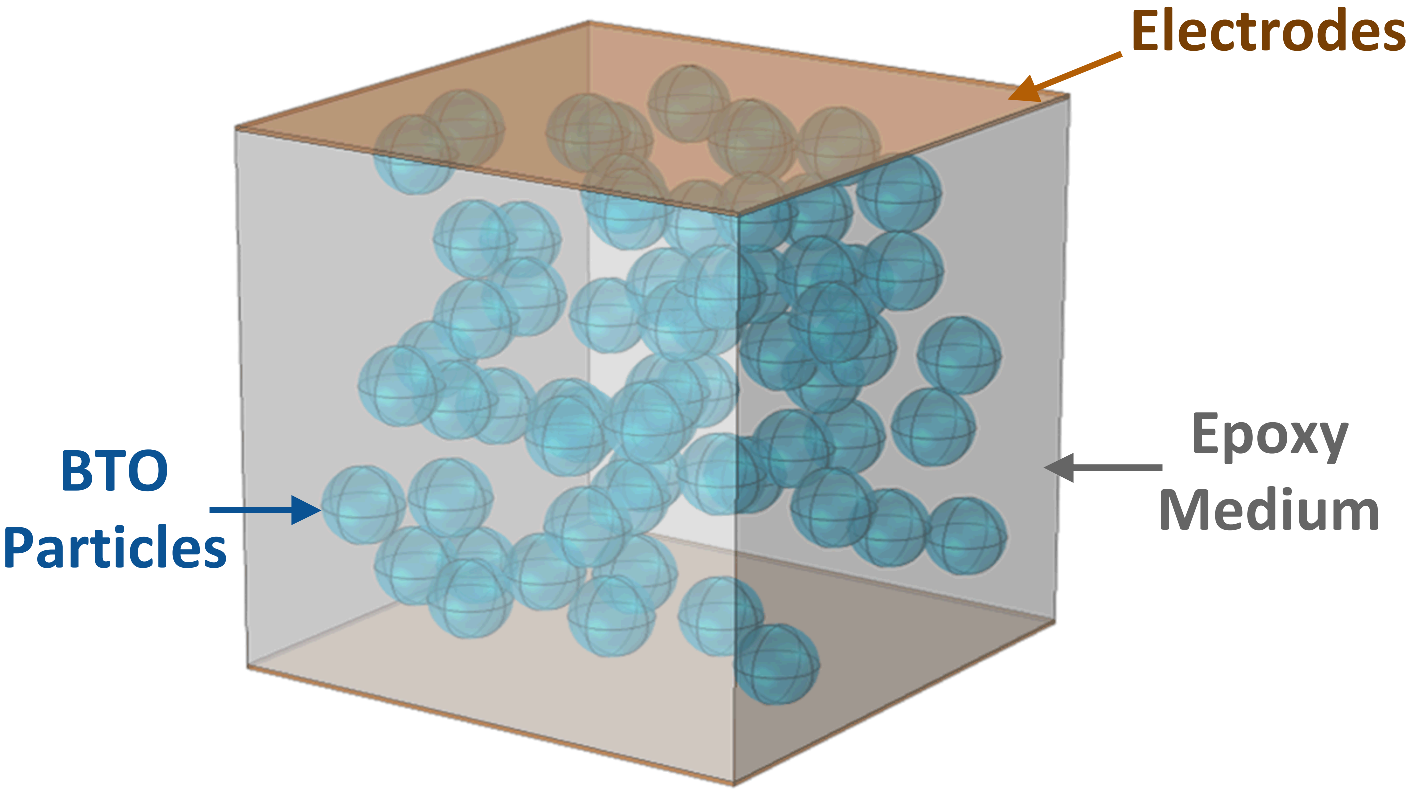
Composite Dielectric Constant

200nm BTO/epoxy Composite ε_r

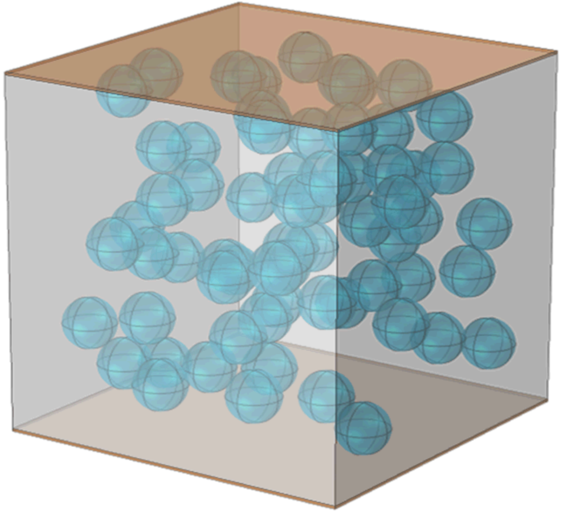


Measured composite ε_r is above the upper limit of the Jayasundere-Smith model

Finite Element Modeling



Finite Element Modeling



- Electric potential *V* applied to the simulated capacitor
- Surface charge *Q* is computed using

$$\nabla \cdot D = \rho_V \qquad E = -\nabla V$$

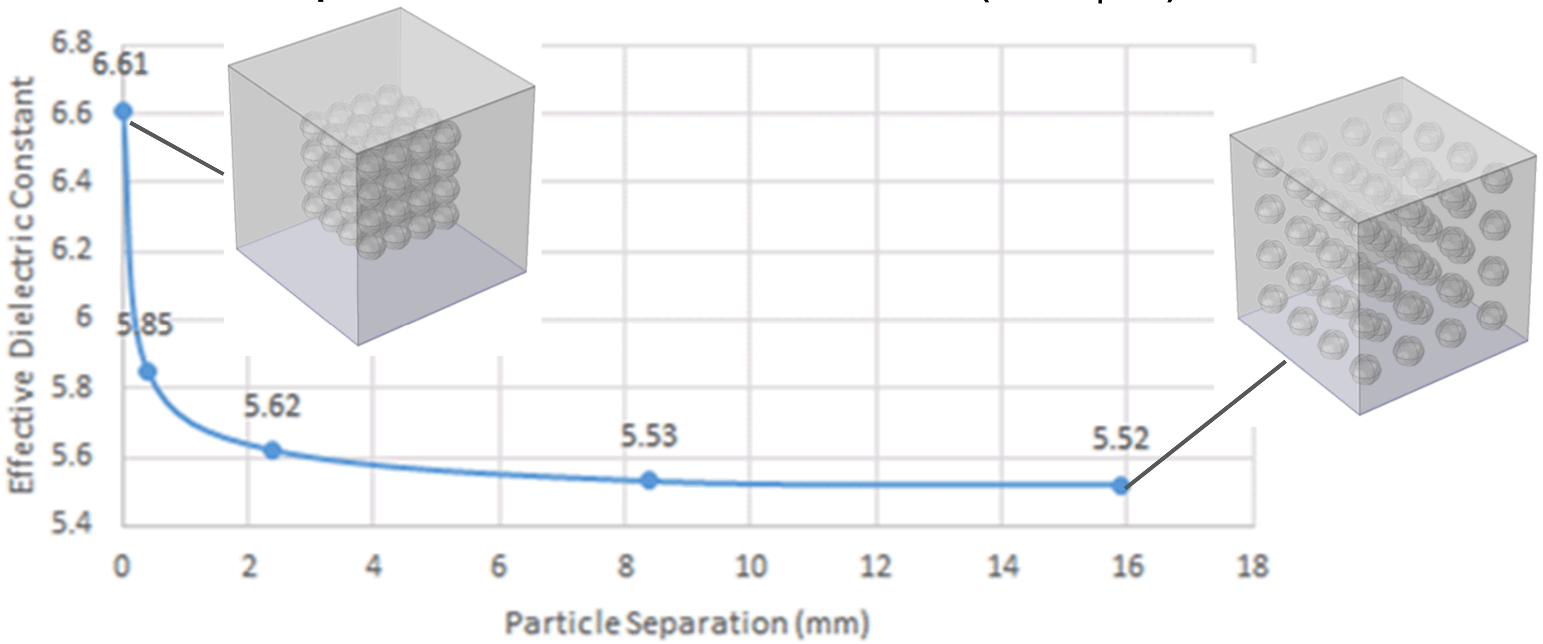
- Composite ε_r calculated using

$$C = \frac{Q}{V} = \varepsilon_r \varepsilon_0 \frac{A}{d}$$

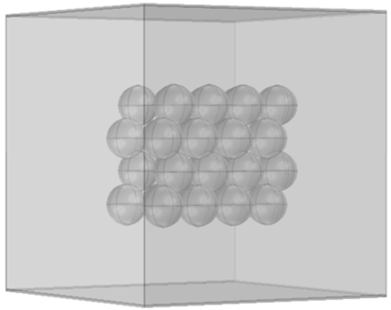
2 clutter, better suited to be said verbally
Kirklann Lau,

Effect of Particle Separation

Composite Dielectric Constant at 10 vol% (BTO $\varepsilon_r \rightarrow \infty$)

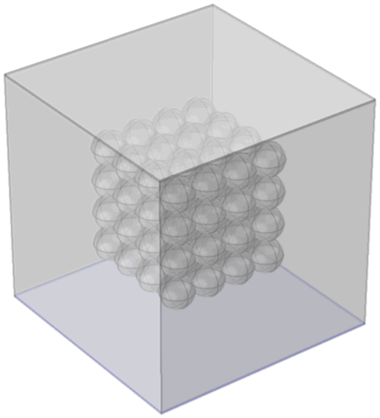


Effect of Particle Separation



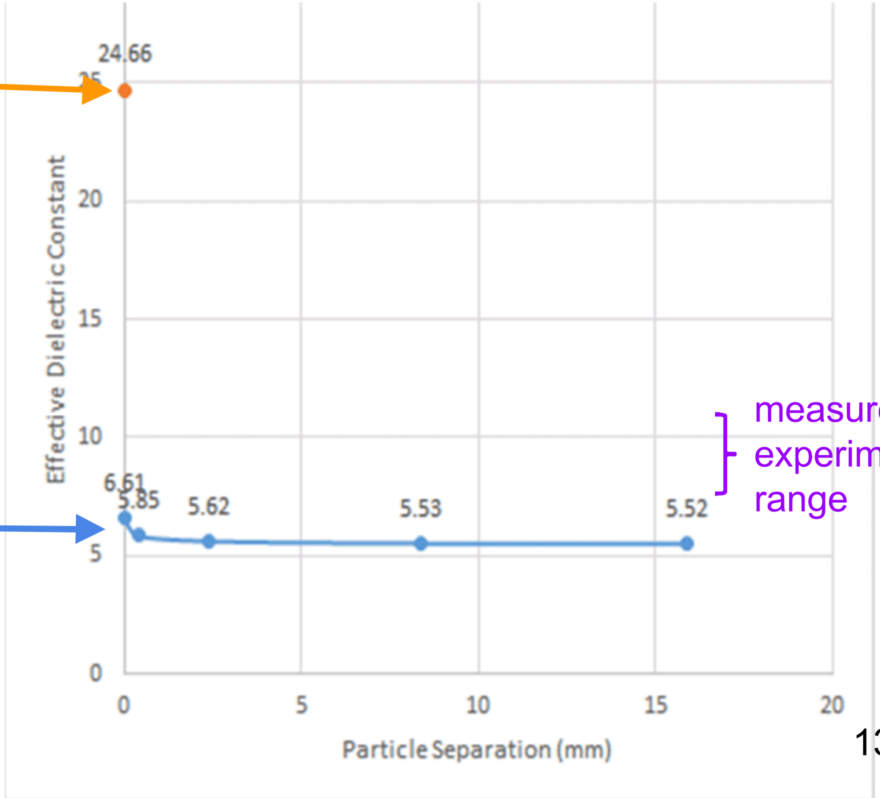
hexagonal close packed

Simulated
composite ε_r
up to ~24.66



cubic close packed

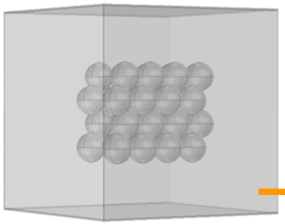
Composite Dielectric Constant at 10 vol% (BTO $\varepsilon_r \rightarrow \infty$)

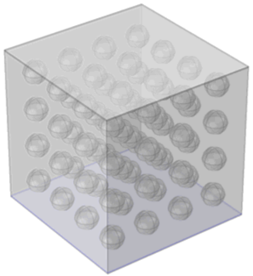


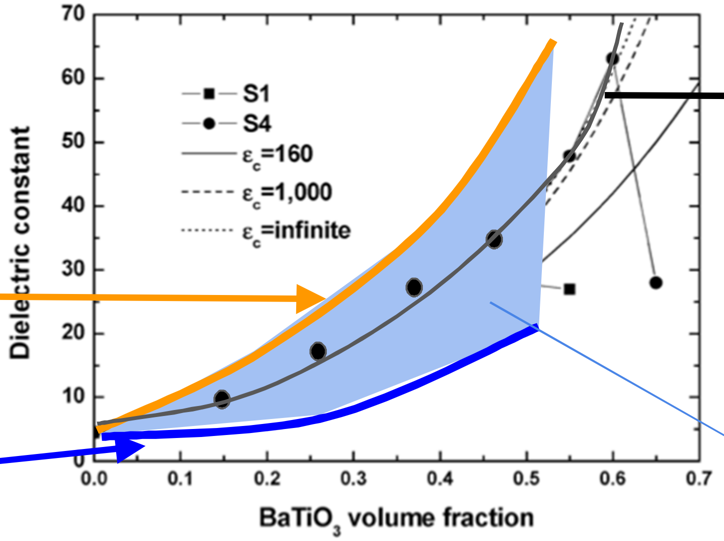
measured
experiment
range

Matching Simulation with Experiment

Graph of max separation to complete agglomeration with BTO $\varepsilon_r \rightarrow \infty$



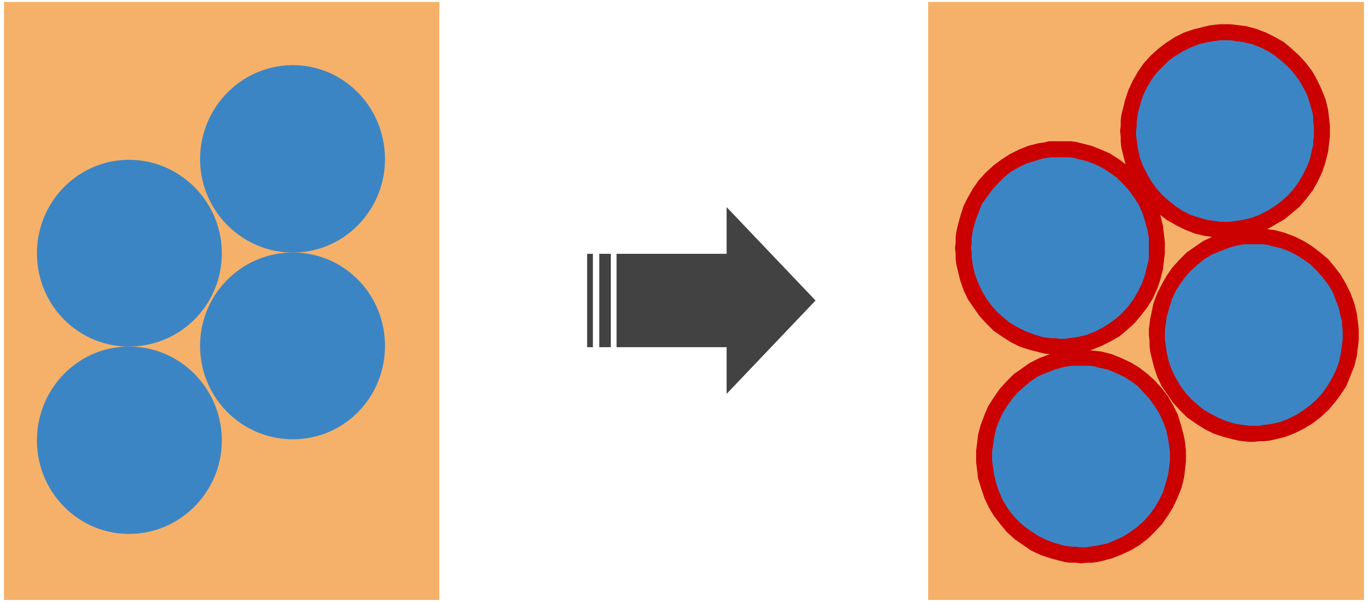




Measured composite ε_r lie within simulation range

COMSOL range from adjusting particle separation

Surface Functionalized Nanoparticles

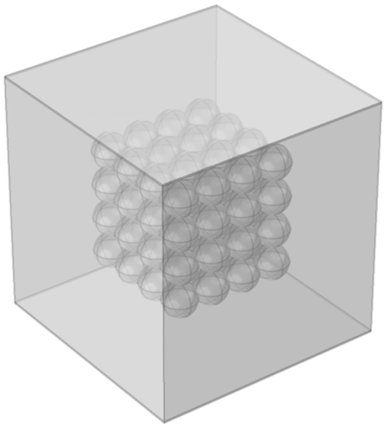


BTO Nanoparticles in an **Epoxy Medium**

Functionalized with a type of phosphonic acid (APPA)

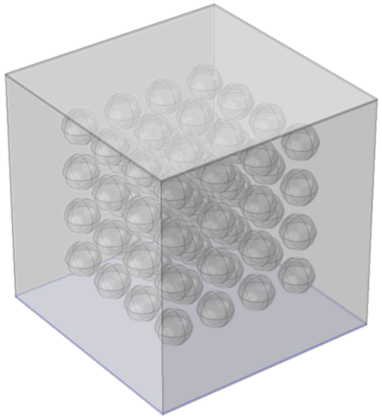
Surface Functionalized Nanoparticles

Non-functionalized



Composite ε_r = 7.30 ± 0.06

Functionalized



Composite ε_r = 6.93 ± 0.04

Conclusion

Composite dielectric constant is highly dependant on separation between particles

Jayasundere-Smith equation (and other mathematical models) cannot be applied to extract particle dielectric constants from thick (> 3mm) composites since they fail to properly account for agglomeration

COMSOL simulations can possibly provide insight on particle agglomeration within epoxy/BTO composites

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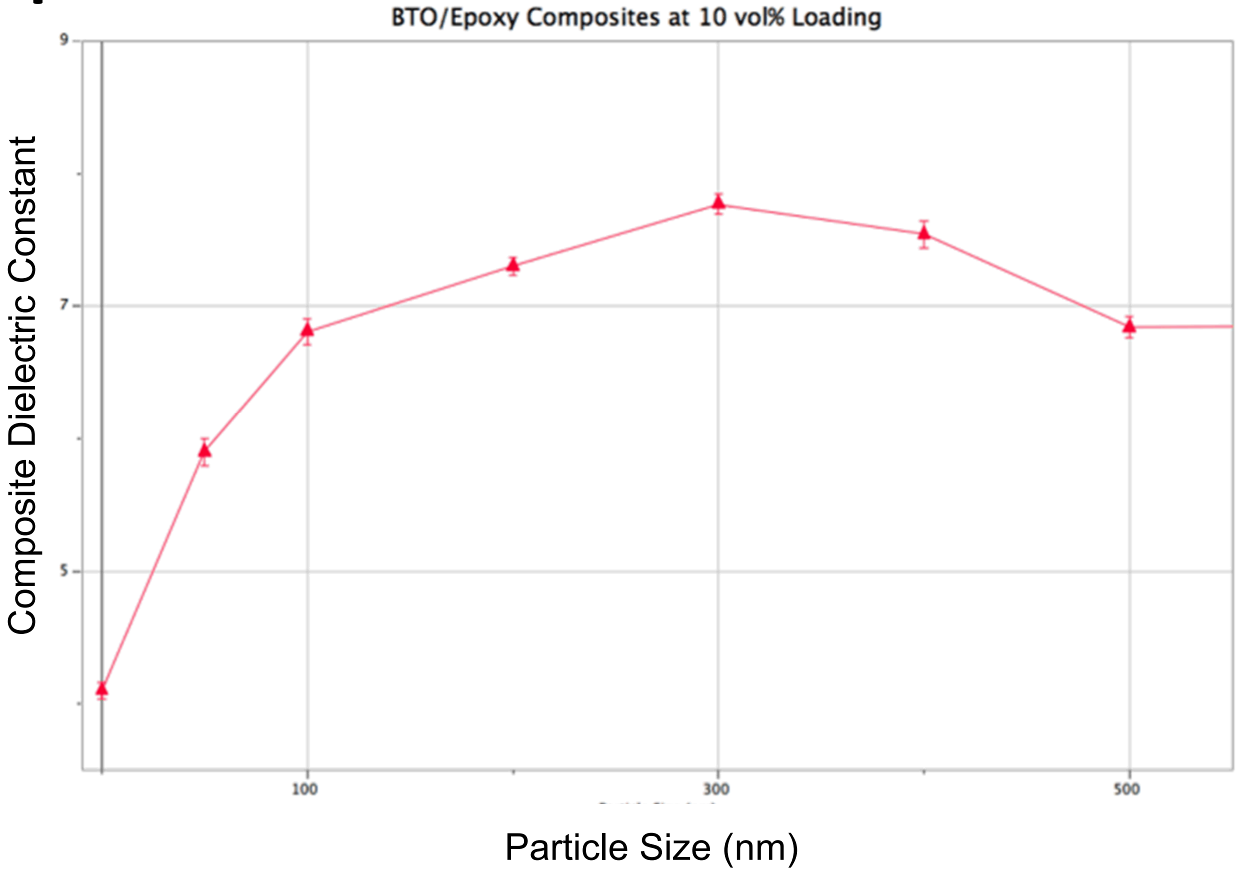
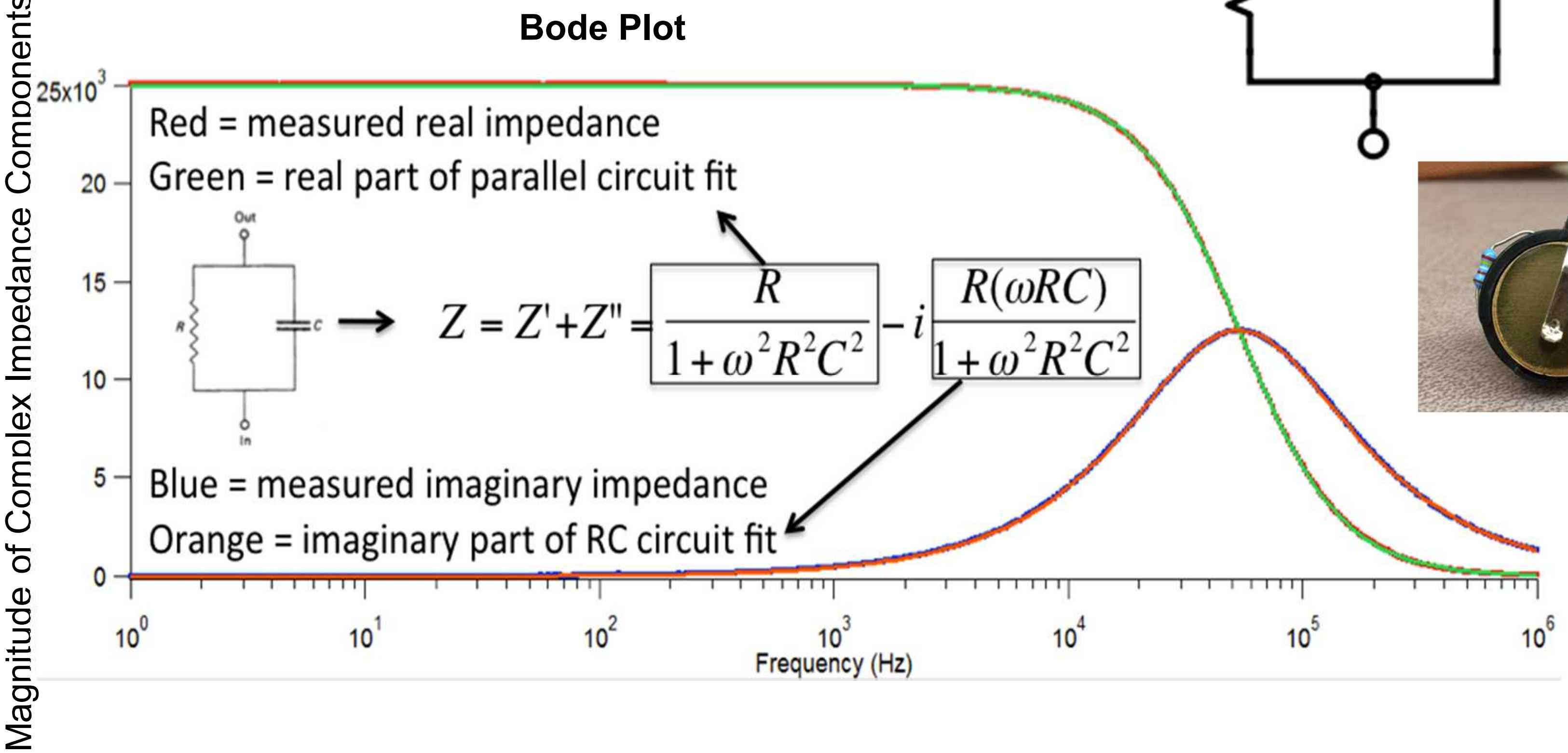
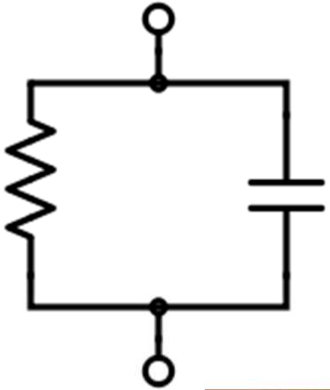
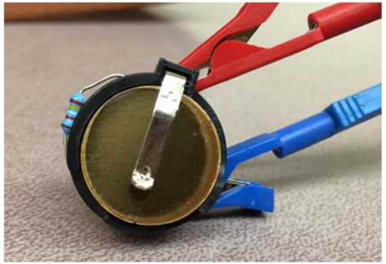
Composite Dielectric Constant vs. Particle Size



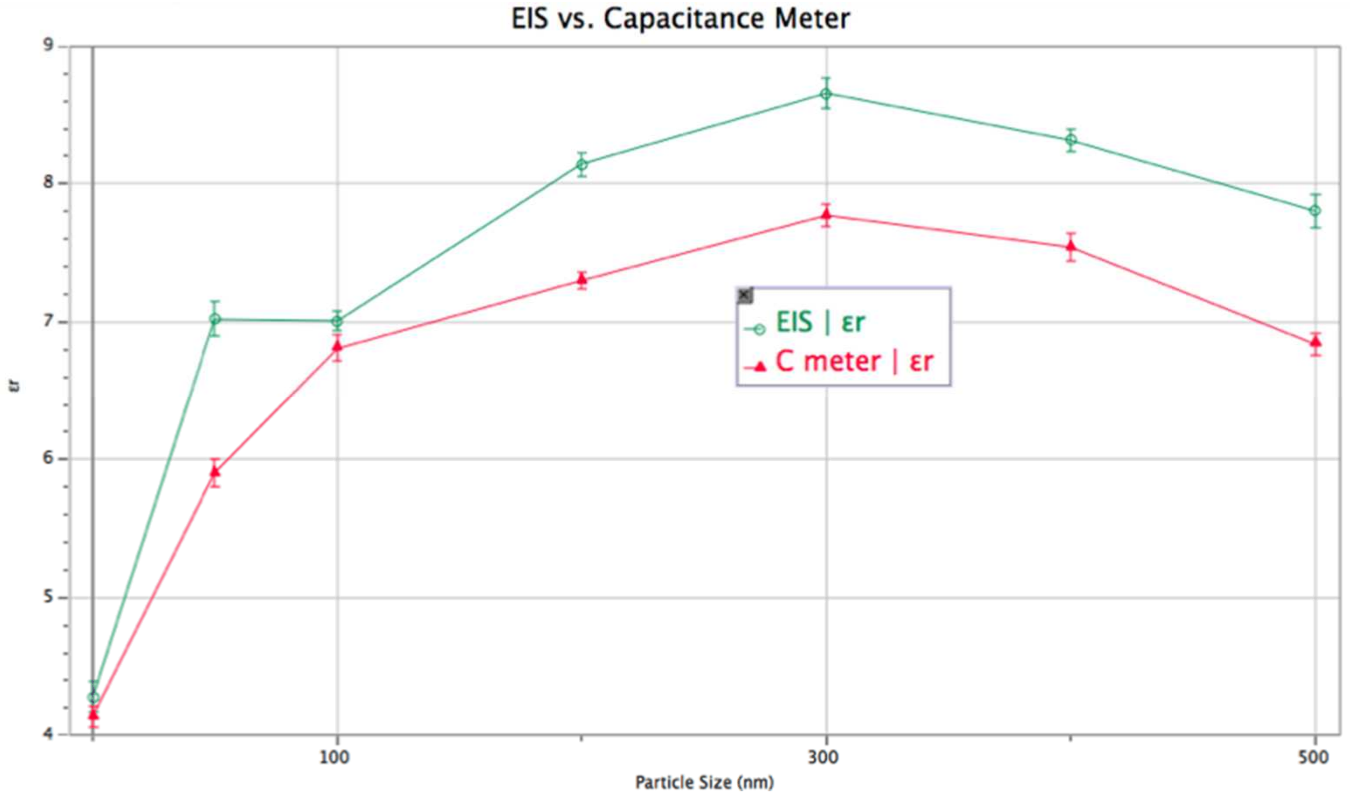
Impedance Spectroscopy







Impedance Spectroscopy vs. Capacitance Meter



EMT Equations

$$\delta_p = \frac{(\varepsilon_{mx} - \varepsilon_{md})(2\varepsilon_{mx} + \varepsilon_p)}{3\varepsilon_{mx}(\varepsilon_{md} - \varepsilon_p)}$$

$$\frac{\varepsilon_p - \varepsilon_{mx}}{\varepsilon_p + \varepsilon_{md}} = (1 - \delta_p)\left(\frac{\varepsilon_{mx}}{\varepsilon_{md}}\right)^{\frac{1}{3}}$$

$$\varepsilon_{mx} = \frac{\varepsilon_{md}(1 - \delta_p) + \varepsilon_p \delta_p \left(\frac{3\varepsilon_{md}}{\varepsilon_p + 2\varepsilon_{md}}\left(1 + \frac{3\delta_p(\varepsilon_p - \varepsilon_{md})}{\varepsilon_p - 2\varepsilon_{md}}\right)\right)}{(1 - \delta_p) + \delta_p \left(\frac{3\varepsilon_{md}}{\varepsilon_p + 2\varepsilon_{md}}\left(1 + \frac{3\delta_p(\varepsilon_p - \varepsilon_{md})}{\varepsilon_p - 2\varepsilon_{md}}\right)\right)}$$

$$\frac{\varepsilon_{mx} - \varepsilon_{md}}{\varepsilon_{mx} + 2\varepsilon_{md}} = \delta_p\left(\frac{\varepsilon_p - \varepsilon_{md}}{\varepsilon_p + 2\varepsilon_{md}}\right)$$