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Modeling and Simulation of Artificial Core-Shell Based Nanodielectrics for Electrostatic Capacitors Applications

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CONTENTS

INTRODUCTION

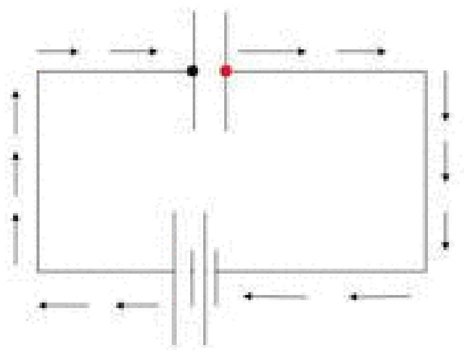
Prime Focus-Energy storage

- Growing demand for capacitors that can store a lot amount of energy and deliver it instantaneously [1].
- Polarizability of the dielectric plays an important role in the amount of charge stored.
- With increase in polarization, the electric field generated increases.
- Thus the charge storage or the capacitance increases as well.
- Passive components occupy about 70% of space in PCBs[2]
- Need for higher storage in compact size increases day by day

[1]J. Y. Li, L. Zhang, and S. Duchame, "Electric energy density of dielectric nanocomposites", Appl. Phys. Lett. 90, 132901, 2007.
[2]1. R. K. Ulrich and L. W. Schaper, "Integrated Passive Component Technology," IEEE press, Wiley Interscience 2003

INTRODUCTION

- A capacitor is an electrical component that contains two conducting plates separated by a dielectric.
- Uses
  - Energy Storage
  - Time delays
  - Tuned circuit



$$C = \varepsilon \frac{A}{d}$$

$$\varepsilon = \varepsilon_r \varepsilon_o$$

INTRODUCTION

Polymer Capacitors

- High processability, Mechanical flexibility, Electrical breakdown strength
- Compatibility with printed circuit board (PCB) technologies an low equivalent series resistance

Nano fillers

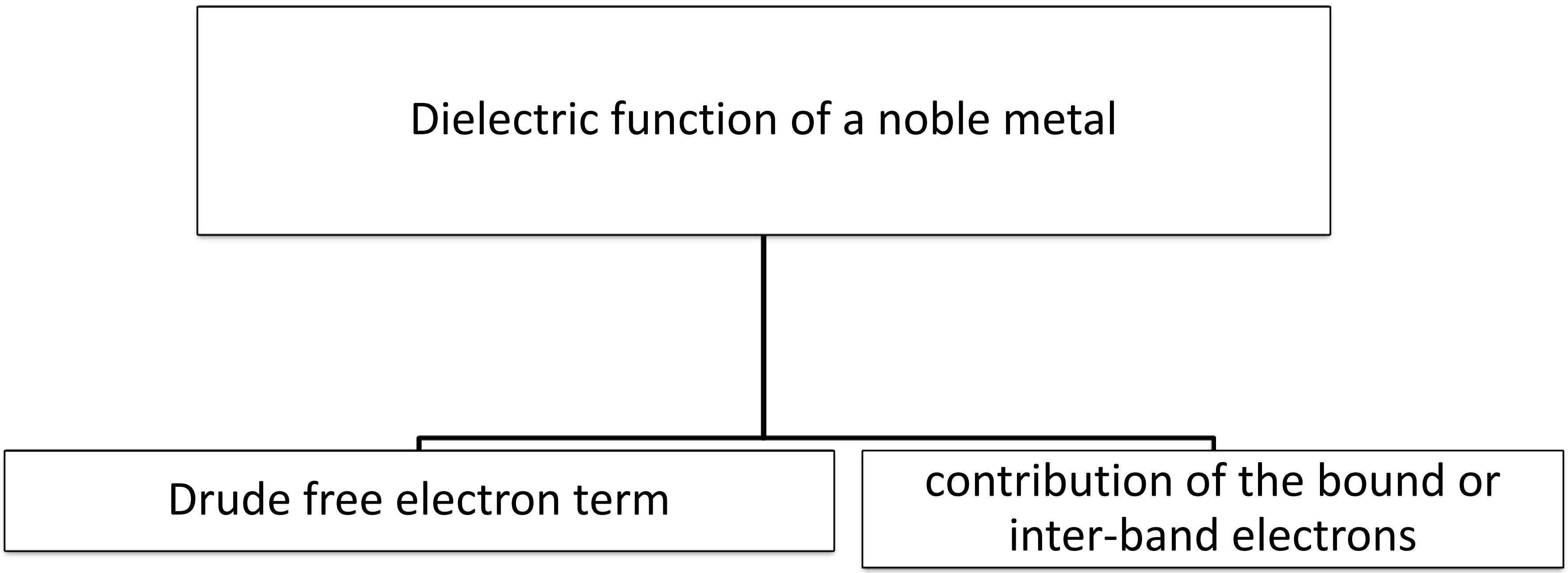
- Intermediate between that of molecules and of bulk material which enables to bridge the gap between molecular chemistry and surface science.
- Dramatic changes take place when the loading of these nano fillers in a polymer matrix reaches a particular threshold value, which is popularly called a percolation threshold [3].

FEM Simulation

- Applied to the design process to decrease the development time and predict the output patterns, which saves time and production expense
- With advancements in computer technology, simulation of complex percolative systems like nanodielectric capacitors has become a reality
- Effective properties of the nano composites can be calculated using the Finite element analysis, available in COMSOL multi physics

[3]C. W. Nan, Y. Shen and Jing Ma, “Physical properties of composites near percolation”, Annu. Rev. Mater. Res. 2010. 40:3.1–3.21

Theoretical Framework: Drude Lorentz's Model



Theoretical Framework: Drude Lorentz's Model

- Due to additive nature of dielectric function, it can be represented as

$$\varepsilon_{bulk}(\omega) = \varepsilon_{free\text{-}electrons}(\omega) + \varepsilon_{inter\text{-}band\ electrons}(\omega)$$

- Size dependent dielectric function of Ag

$$\varepsilon_{bulk}(\alpha,\omega) = 1 - \frac{\omega_{pf}^2}{\omega^2 + i\omega\gamma_f} + \frac{\omega_{pb}^2}{\omega_0^2 - \omega^2 - i\omega\gamma_b}$$

where

ω	-	frequency	
ωpf	-	plasma frequency	$= 2.7*10^{16}$ Hz
ϒf	-	size dependent damping factor	$= 3.22*10^{13}$ Hz
ϒb	-	bound electron damping term	$= 1.088*10^{14}$ Hz
ω0	-	bound electron constant term	$= 7*10^{15}$ Hz

Theoretical Framework: Effective Medium Theory

- Modus Operandi

  "Choose a reference system with a known energy and concentrate on the energy difference" [4]

- Effective properties of the composite can be calculated by modeling the permittivity using the Effective medium theory and generalized effective medium theory or other similar mean field theories [5].
- Utilizes various properties of the resultant medium such as shape, size, fraction of inclusions, individual dielectric constants etc to calculate the effective permittivity.

[4]K.W. Jacobsen, P. Stoltze and J. K. Nørskov, Surf. Sci. 366, 394 (1996).
[5]C. W. Nan, Y. Shen and Jing Ma, "Physical properties of composites near percolation", Annu. Rev. Mater. Res. 2010. 40:3.1–3.21

Theoretical Framework: Effective Medium Theory

- EMTs are generally valid only for low volume fractions
- For higher values of fractions, the effective properties can also be determined using Percolation theory [6]
- Properties that are calculated using EMTs are dielectric constant and conductivity
- Different types of EMTs, each theory is more or less accurate under different conditions

[6]Aizenman, Michael; Barsky, David (1987), "Sharpness of the phase transition in percolation models", Communications in Mathematical Physics 108 (3): 489–526, Bibcode 1987CMaPh.108..489A

Theoretical Framework: Effective Medium Theory

EMT Model	Formula
Maxwell – Garnett	$\varepsilon_{eff} = \varepsilon_h[\dfrac{1+2f(\dfrac{\varepsilon_i-\varepsilon_h}{\varepsilon_i+2\varepsilon_h})}{1-f(\dfrac{\varepsilon_i-\varepsilon_h}{\varepsilon_i+2\varepsilon_h})}]$
Symmetric Bruggeman EMT	$\varepsilon_{eff} = \frac{1}{4}[3f(\varepsilon_i-\varepsilon_h)+2\varepsilon_h-\varepsilon_i+\sqrt{(1-3f)^2\varepsilon_i^2+2(2+9f-9f^2)\varepsilon_i\varepsilon_h+(3f-2)^2\varepsilon_h^2}]$
Asymmetric Bruggeman	$\dfrac{\varepsilon_i-\varepsilon_{eff}}{\varepsilon_i-\varepsilon_h} = (1-f)(\dfrac{\varepsilon_{eff}}{\varepsilon_h})^{\frac{1}{A}}$

Where
ε_{eff} -effective dielectric constant of the medium

f - volume fraction of the filler

ε_i - dielectric constants of inclusions

E_h- dielectric constants of host

A =2 (disk fillers)
= 3(spherical fillers)

Theoretical Framework: Percolation Theory

- Concerns the movement and filtering of fluids through porous materials
- Distribution of minor phase in the microstructure of the composite, which depends in its shape, size, and orientation
- Percolation theory is one of the easiest mechanisms to model disordered systems because it has little statistical dependency

Theoretical Framework: Percolation Theory

- Significant when loading of minor phase of composite (fillers) reaches a critical value
- Substantial changes take place in the physical and electrical properties of the system, sometimes on the order of more than a hundred times
- This critical fraction of filler is called the percolation threshold, f_c.

Theoretical Framework: Percolation Theory

- A simple power law relation can be used to describe the changes in the properties in the system, near the percolation threshold [6]

$$\frac{K}{K_h} = |f - f_c|^{-s}$$

Where

K - effective dielectric constant,

K_h - dielectric constant of the host material

f - fraction of inclusions

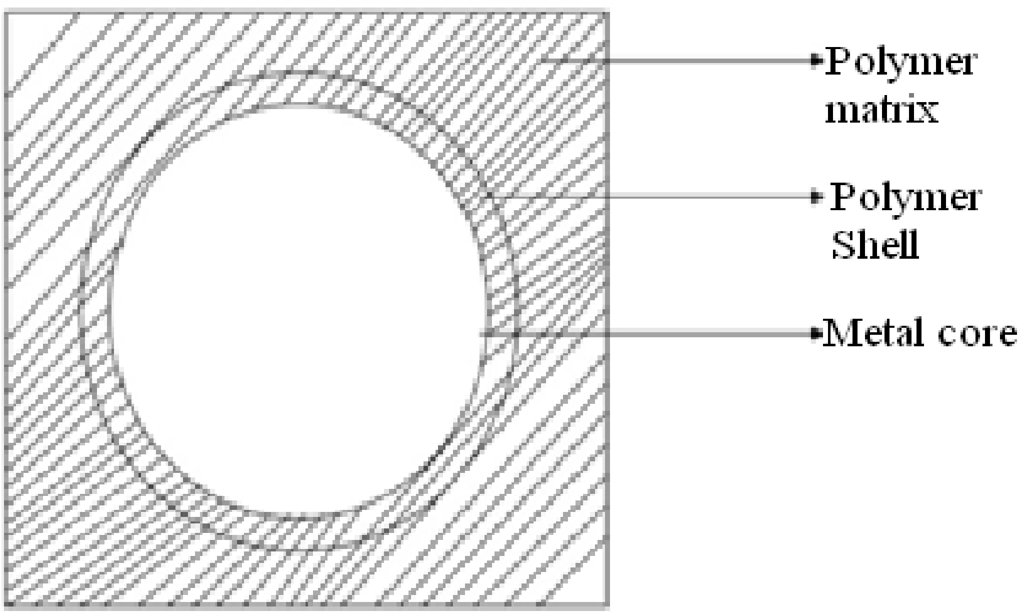
f_c - fraction of inclusions at the percolation threshold

$s = 1$

[6]Newman, M. E. J. (2005). "Power laws, Pareto distributions and Zipf's law". Contemporary Physics 46 (5): 323–351.

Simulation

Basic Model considered for simulation



Model of the Polymer-metal composite

Simulation : Settings

- AC/DC module – In plane electric currents model is used
- In sub domain settings, appropriate materials are selected from material library
- Conductivities and relative permitivities of PS and Ag are applied to the geometry
- Using boundary conditions, one face is set as input voltage while its opposite is ground
- Other faces are set to periodic condition
- Drude, EMT and Percolation theory expressions are defined as global expressions
- Constants are also declared

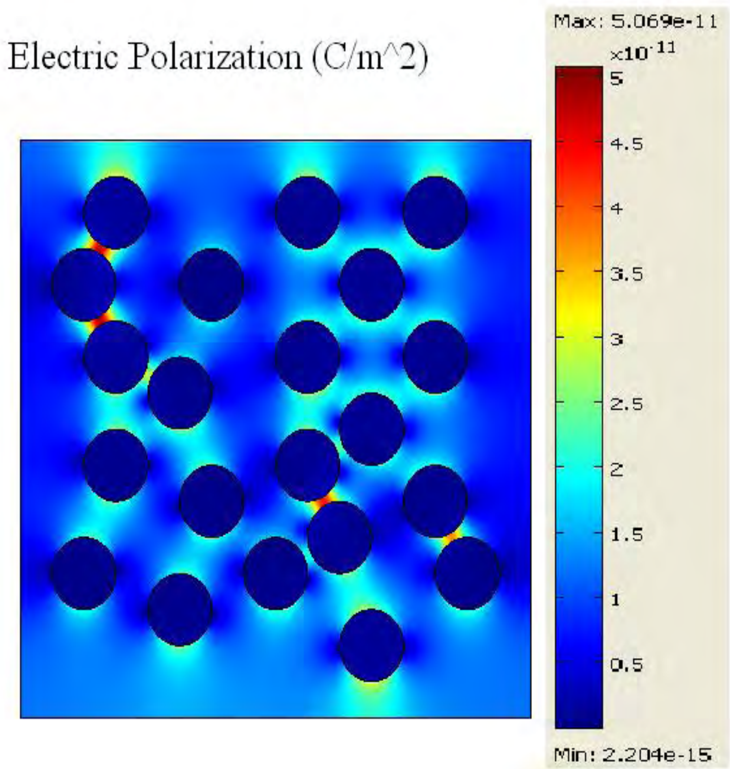
Simulation: Setup

- Separate geometries are drawn for each loading value in both 2D and 3D models.
- Number of fillers is chosen according to desired loading of nanoparticles.
- All 2D geometries have fixed area and 3D geometries have fixed volume for all loadings.

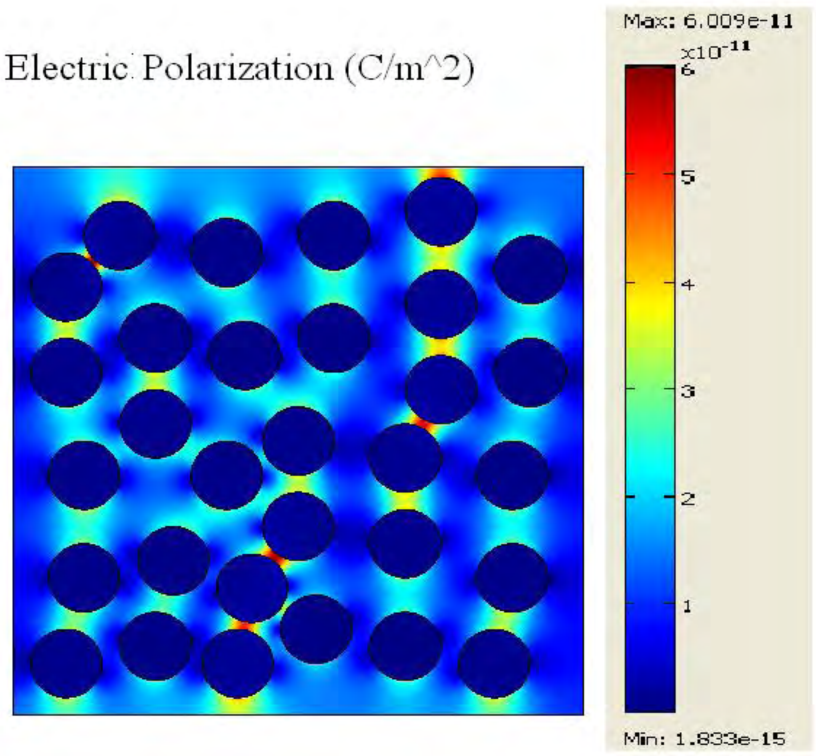
Simulation: Solver Parameters and Post processing

- Parametric solver sweeps frequencies from 1kHZ to 1peta Hz at constant loading.
- Post-processing is used to create isosurface plots for 3D models and surface plots for 2D models.
- Global expression plots and data points values are acquired from post-processing.

Results

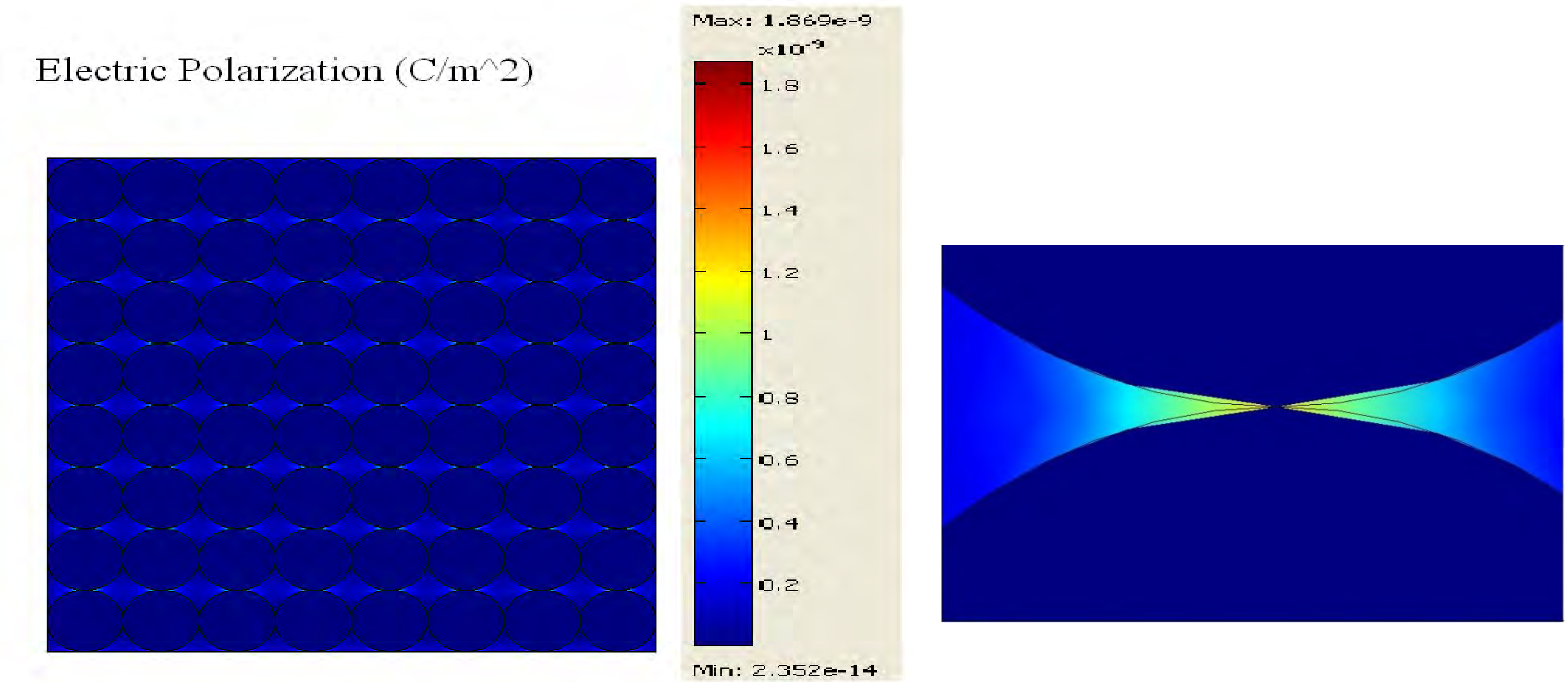


f=0.134



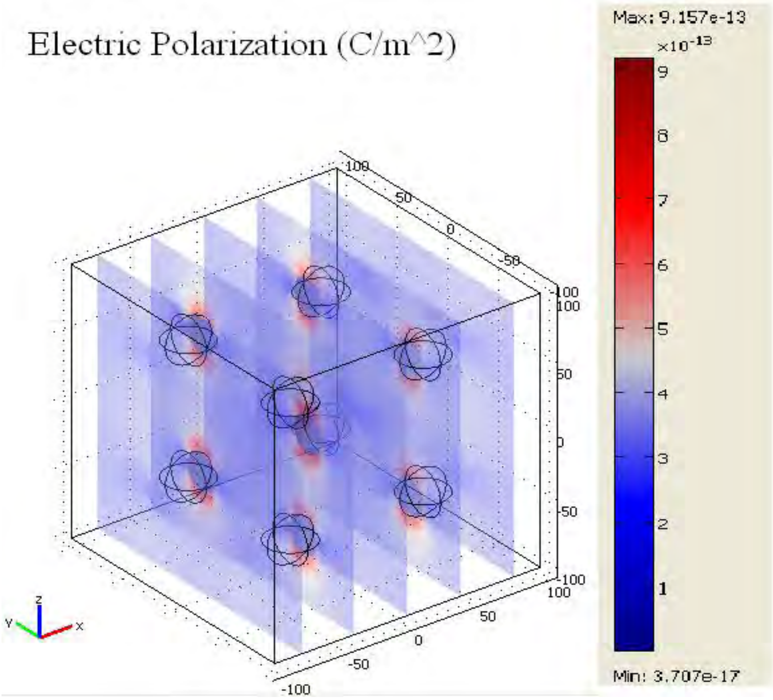
f=0.38

Results

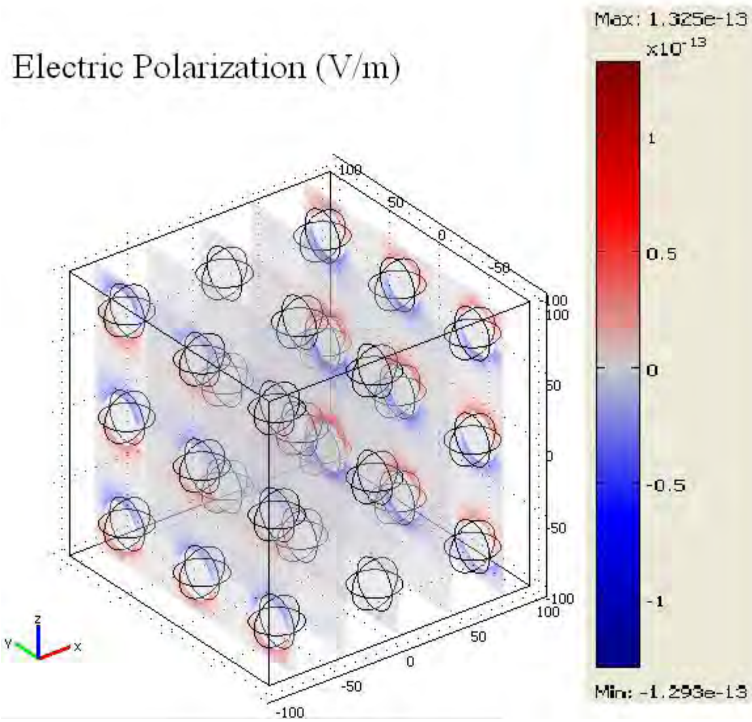


f=0.78

Results

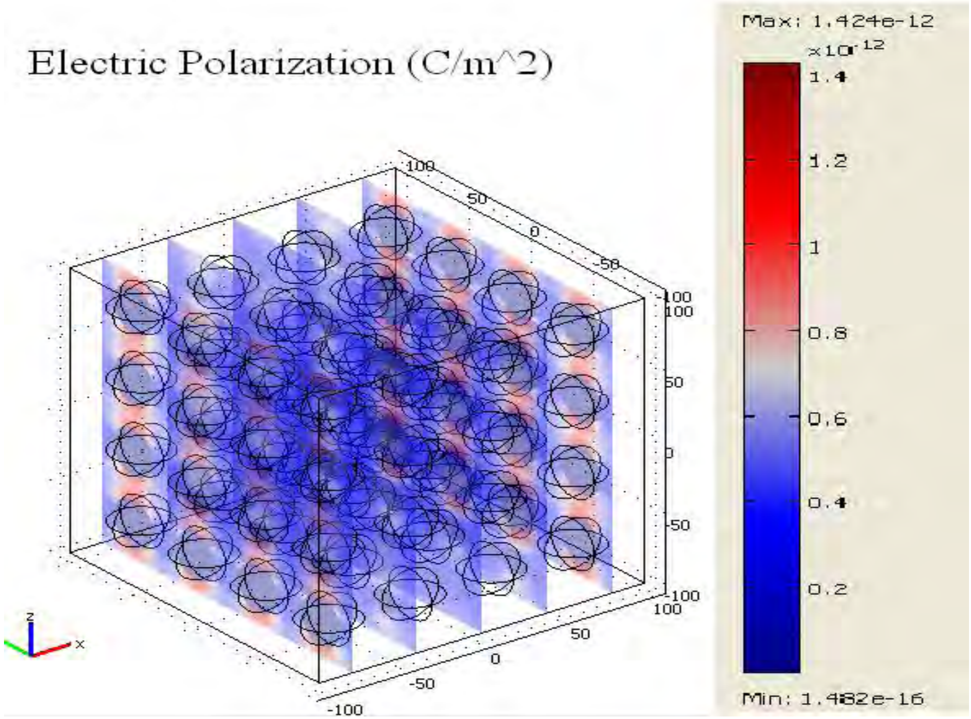


f=0.022



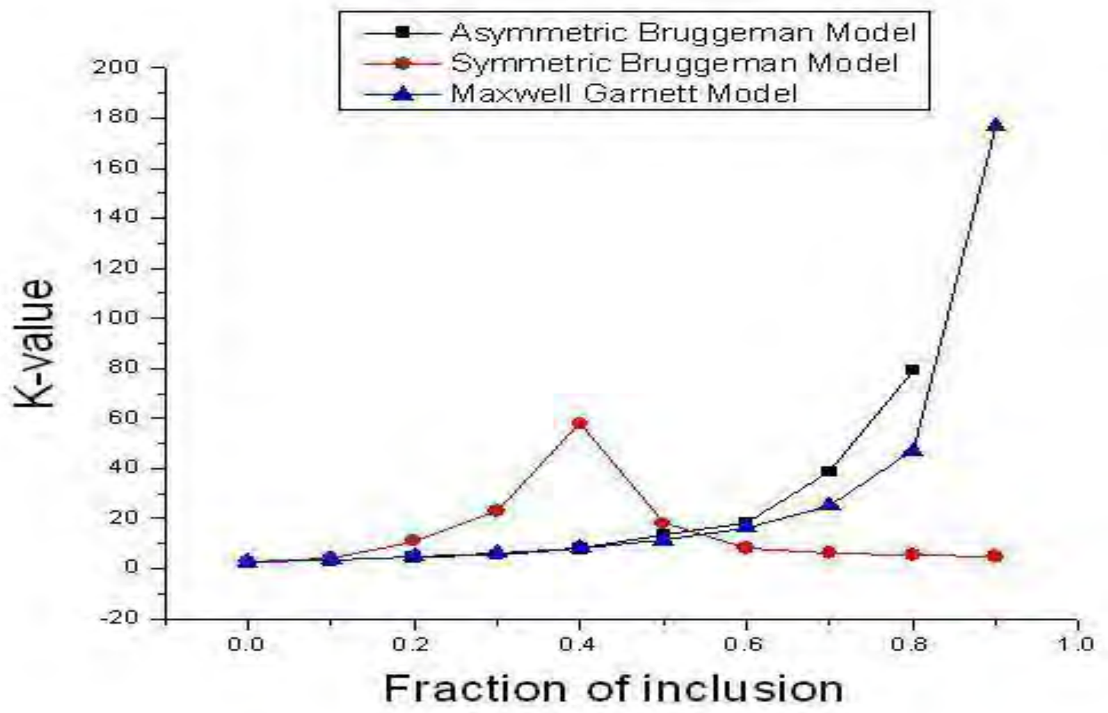
f=0.078

Results

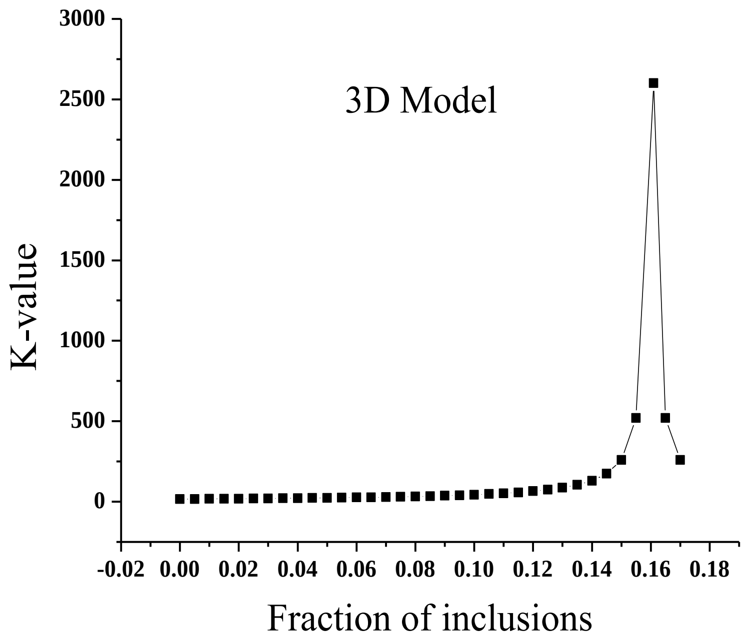


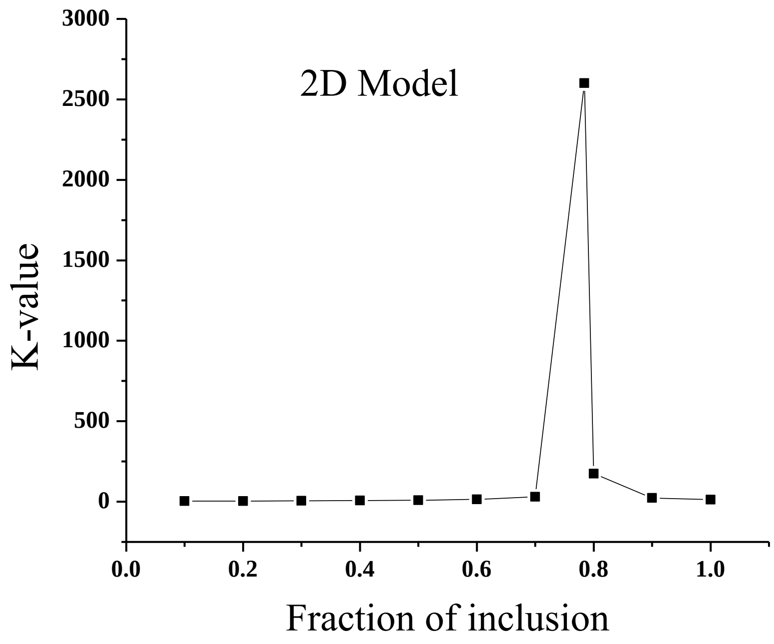
f=0.78

Results: K Value calculation using EMTs



Results : K value calculation using Percolation theory





Conclusion

- Electric field and polarization patterns of 2D and 3D nanodielectrics are observed.

- At low loading, EMTs and Percolation theory predictions are close and both theories predict gradual increase in dielectric constant.

- EMTs fail at high loading but percolation theory takes in to account the metal-insulator nature of the composite and predicts huge increase in value of K at percolation threshold.

- At percolation threshold, K is determined as 2600, where as for a bare polymer this value is just 2.6.

Acknowledgements

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Questions?


Thank You!