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Effective Medium Theory of Nanodielectrics for Embedded Energy Storage Capacitors

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Contents

Introduction

- Capacitors are passive devices that store electrical charge because of charge separation between plates.
- Storing energy is a key issue in all electrical equipment.
- Passive components occupy about 70% of space on PCBs[1].
- Need for higher storage in compact space is increasing by the day.

1. R. K. Ulrich and L. W. Schaper, "Integrated Passive Component Technology," IEEE press, Wiley-Interscience, 2003.

Introduction

- Embedded Capacitors replace discrete capacitors in modern technologies like system in package (SIP) and system on chip (SOC)[2].

- Advantages - Miniaturization, increase component density and higher electrical performance [3].

- Applications of Embedded Capacitors include:




2. J. Lu, “High Dielectric Constant Polymer Nanocomposites for Embedded Capacitor Applications,” *Georgia Institute of Technology*, 2008.
3. S. K. Saha, “Nanodielectrics with giant permittivity”, Bull. Mater. Sci., Vol. 31, No. 3, June 2008, pp. 473–477.

Introduction

- Traditional ceramic capacitors cannot be used as embedded capacitors because of poor volumetric efficiency.

- Ceramic based dielectric material makes it hard to manufacture (reproducibility, stability and cost) and shows limited flexibility due to high ceramic loading.

- Polymer based dielectrics can be potential embedded capacitors because of their advantages and compatibility with PCB materials.

Background Theory: POLYMERS

- High processability, mechanical flexibility, electrical breakdown strength
- Low dielectric constant is a serious drawback for polymers to be used as embedded capacitors.
- This can be overcome by adding „fillers" to polymer matrix.
- Composites cannot be made with ceramic fillers of smaller size as their permittivity decreases with decrease in size[4].
- High loading of ceramic fillers in polymer defeat the purpose of composites.

4. J. Lu and C. P.Wong, "Recent advances in high-k nancomposite materials for embedded capacitor application," IEEE Trans. Dielectr. Electr. Insul.,vol. 15, no. 2, pp. 1322–1328, Oct. 2008.

Background Theory: METAL NANOFILLERS

- Metal nanoparticles are promising filler materials as low loading will suffice.
- They have interesting electrical, magnetic and physical properties[5].
- Metal-Polymer percolative composites are identified as strong candidates to realize high K[6].
- Nanoparticles based dielectrics have higher capacitance density because of small thickness of the film.

5. L. Nicolais and G. Carotenuto, Metal-Polymer Nanocomposites. John Wiley & Sons Inc.: Hoboken, NJ, 2005
6 . Yang Shen et al, "High Dielectric Performance of Polymer Composite Films Induced by a Percolating Interparticle Barrier Layer", Adv. Mater. 2007, 19, 1418–1422.

Background Theory: CAPACITOR

- Amount of charge stored in a capacitor is denoted by its capacitance.

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

C – Capacitance
K – Dielectric Constant
ε_0 – Permittivity of free space
A – Area of plates
d – Distance between plates

- Greater the value of K, greater the C value.

- Relationship between polarization, electric field and capacitance

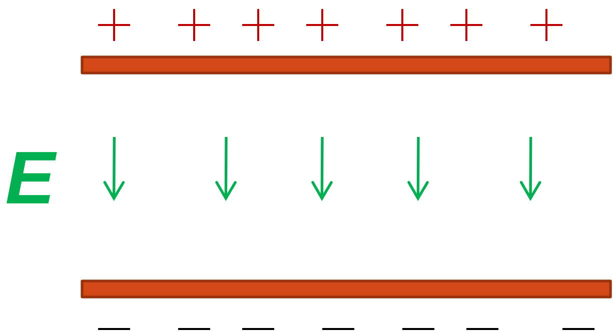
$$P = \varepsilon_0 \chi_e E_{effective}$$

where

$$\chi_e = K - 1$$

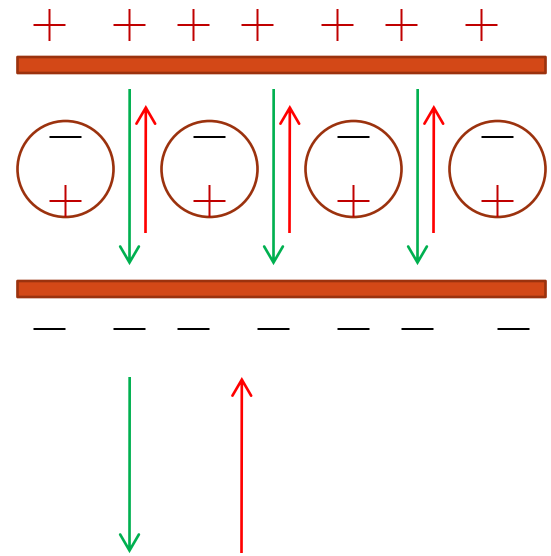
P – Dielectric Polarization
χ_e – Susceptibility
E – Electric field between plates

Background Theory: COMPOSITE CAPACITOR



$$E = \frac{V}{d}$$

V = voltage applied to the plates



$E_{effective} = E - E_{polarization}$

As $E_{effective}$ decreases, P and K increases

Background Theory: EFFECTIVE MEDIUM THEORY (EMT)

- Effective dielectric constant of medium is calculated with EMTs[9]. Few popular EMTs are

EMT Model	Formula
Maxwell – Garnett	$\varepsilon_{eff} = \varepsilon_h [\frac{1+2f(\frac{\varepsilon_i - \varepsilon_h}{\varepsilon_i + 2\varepsilon_h})}{1-f(\frac{\varepsilon_i - \varepsilon_h}{\varepsilon_i + 2\varepsilon_h})}]$
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	$\frac{\varepsilon_i - \varepsilon_{eff}}{\varepsilon_i - \varepsilon_h} = (1-f)(\frac{\varepsilon_{eff}}{\varepsilon_h})^{\frac{1}{A}}$

ε_{eff} - effective permittivity of the medium

ε_i - dielectric function of inclusion (filler)

ε_h – dielectric constant of host polymer

f – fraction of inclusion

A=0.5 for disks and 0.33 for spheres.

9. William M. Merrill, et al, "Effective Medium Theories for Artificial Materials Composed of Multiple Sizes of Spherical Inclusions in a Host Continuum", IEEE Transactions on antennas and propagation, vol. 47, no. 1, January 1999.

Background Theory: DRUDE THEORY

- Dielectric constant of size dependent Au nanoparticles[8] is

$$\varepsilon_i = \varepsilon_{free-electrons} + \varepsilon_{bound-electrons}$$

$$\varepsilon_i = 1 - \frac{\omega_{pf}^2}{\omega^2 + i\omega\gamma_f} + \frac{\omega_{pf}^2}{\omega_0^2 - \omega^2 - i\omega\gamma_b}$$

ω - frequency

ω_{pf} - plasma frequency $= 1.3*10^{16}$ Hz

Υ_f - size dependent damping factor $= 2.65*10^{14}$ Hz

Υ_b – bound electron damping term $= 2.4*10^{14}$ Hz

ω_0 - bound electron constant term $= 7*10^{15}$ Hz

8. A. E. Neeves and M.N.Birnboim, “Composite Structure for the enhancement of nonlinear-optical susceptibility”, J.Opt Soc. Am. B. Vol 6, No. 4, April 1989.

Background Theory: PERCOLATION THEORY

- Huge changes occur in physical and electrical properties for a critical loading of nanoparticles, known as percolation threshold, f_c[10].
- At loading above f_c , dielectric loses its insulating properties and becomes conductive.
- Power law describes properties of system at f_c

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

S is a constant of value 1

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

Simulation: SETUP

- A 2-step procedure is employed to calculate effective permittivity of the medium.
- First step is to generate an arrangement of nanoparticles in PVP matrix.
- Disks and spheres are randomly arranged for 2D and 3D modeling respectively.
- Number of fillers is chosen according to desired loading of nanoparticles.

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 PVP and Au 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.

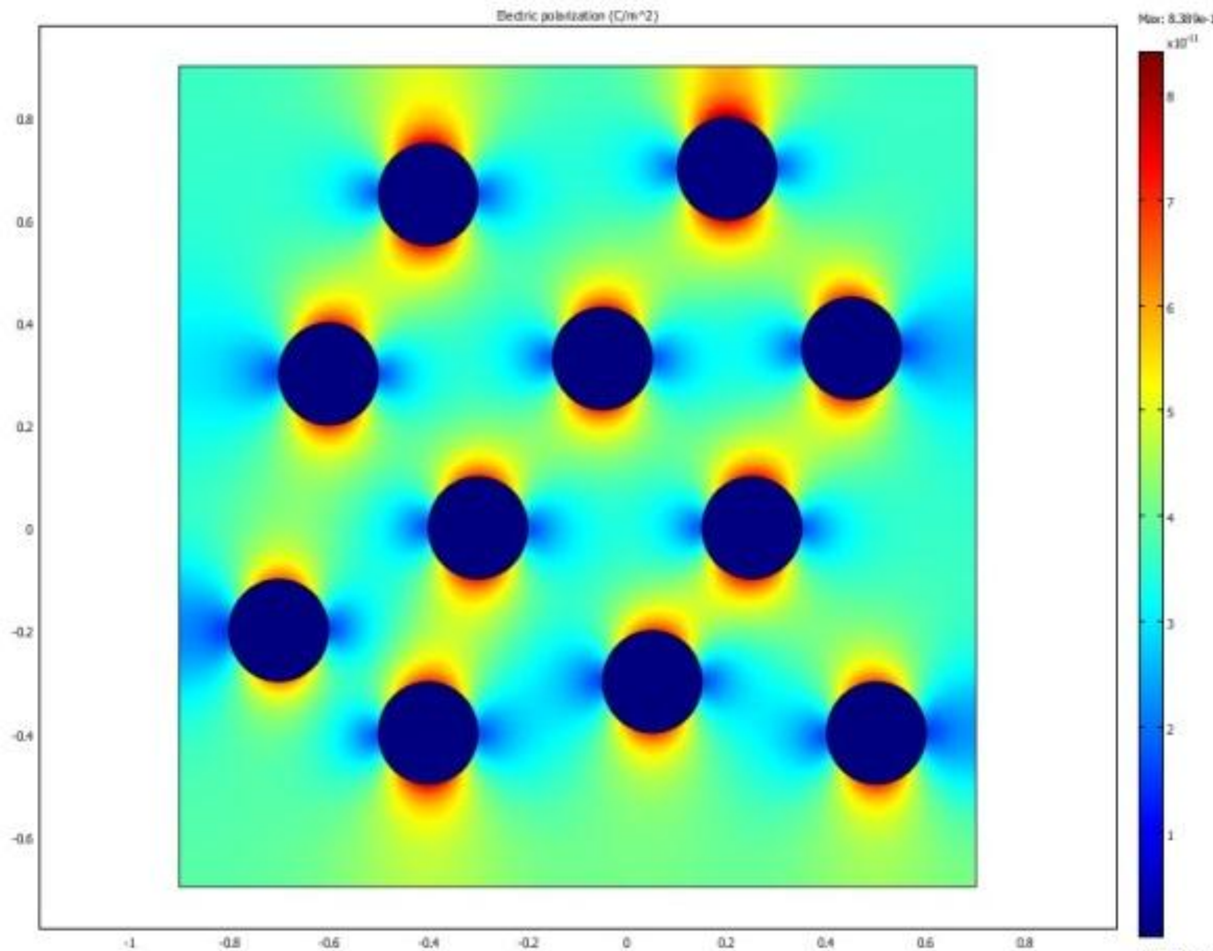
- Drude, EMT and Percolation theory expressions are defined as global expressions. Constants are also

Simulation: SOLVERS and POST-PROCESSING

- Parametric solver sweeps frequencies from 1kHZ to 1peta Hz at constant loading.
- Parametric solver is also used at constant frequency when loading is varied from 0 to 1.
- Post-processing is used to create slice plots for 3D models and surface plots for 2D models.
- Global expression plots and data points values are acquired from post-processing.

Results: 2D MODELING

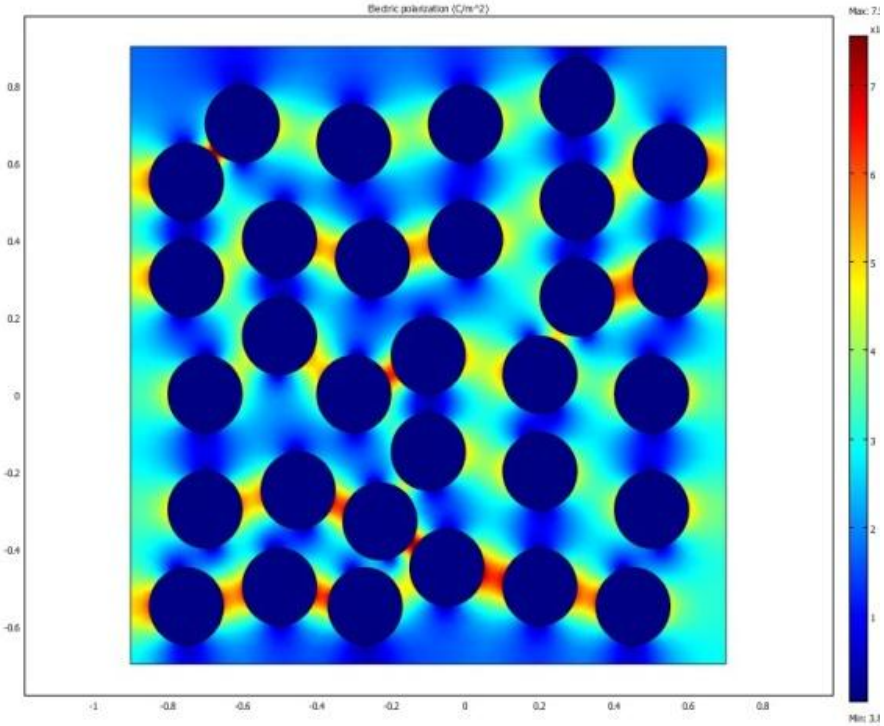
Additional polarization is created at surface of fillers in direction of electric field. With increase in net polarization, effective dielectric constant also increases as governed by equations mentioned in



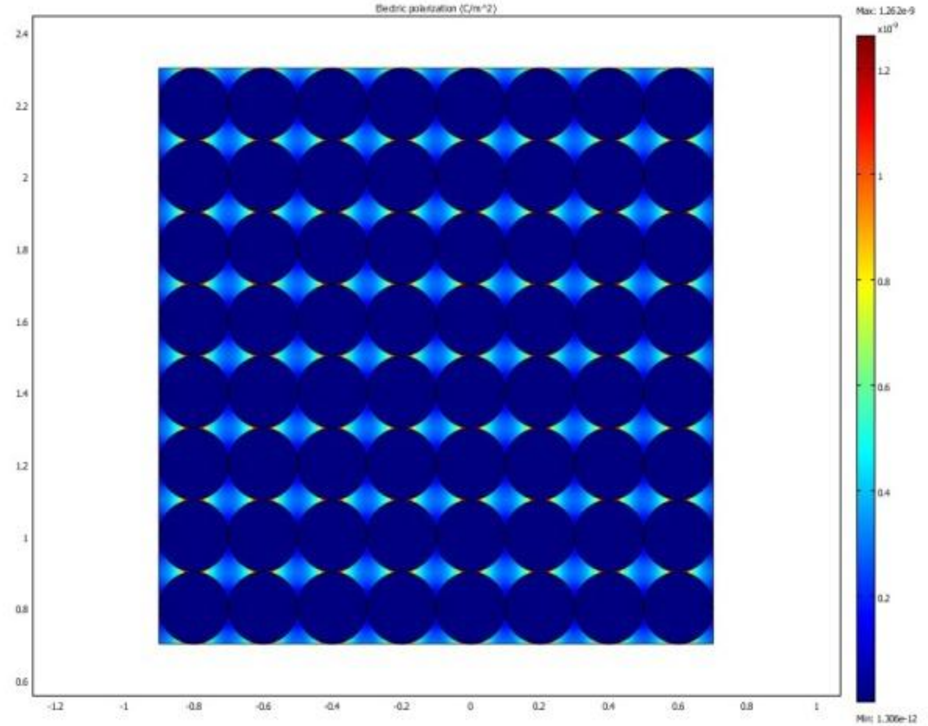
Electric polarization patterns in 2D nanodielectric with $f = 0.134$

Results: 2D MODELING

f = *0.38*



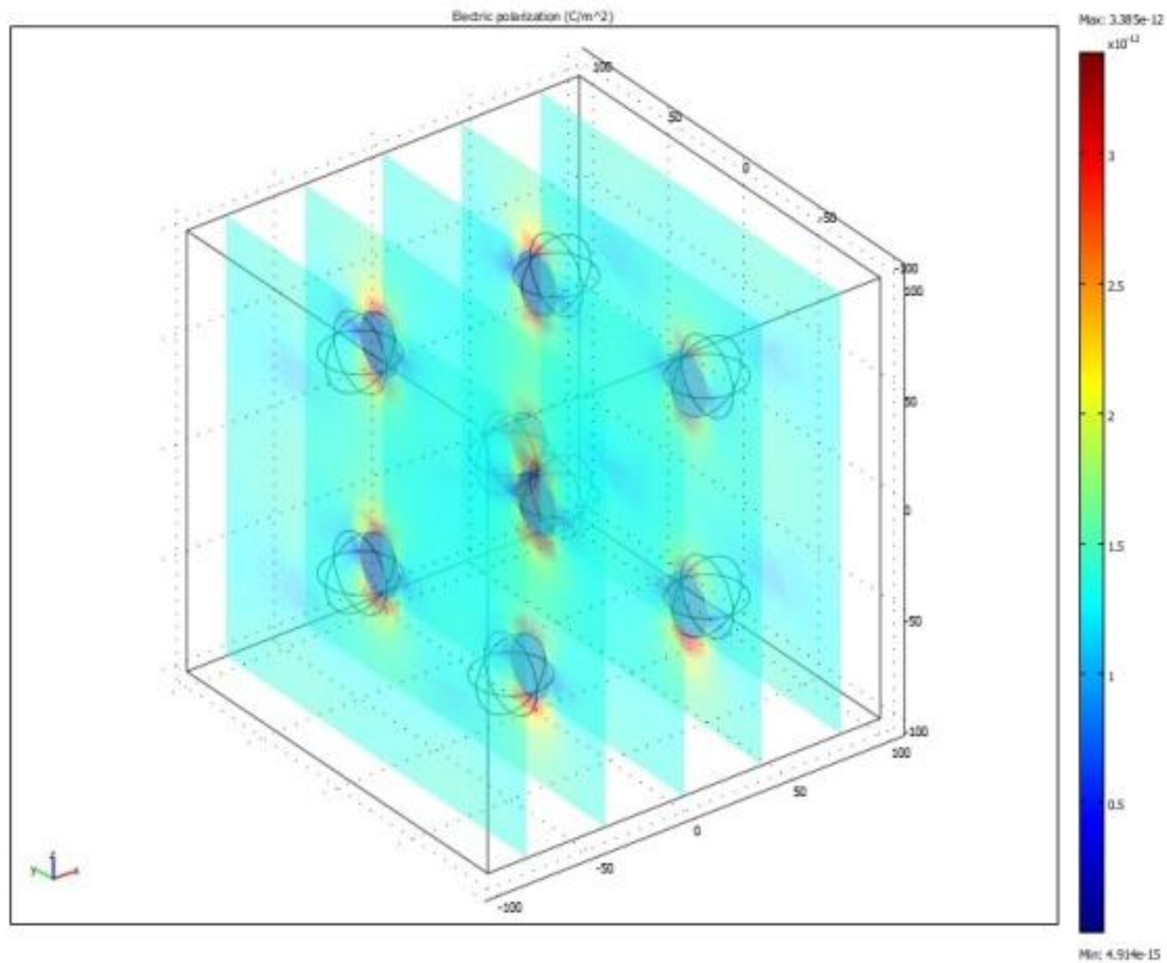
f = *0.78*



Effective dielectric constant increases with increase in loading of nanoparticles.

Results: 3D MODELING

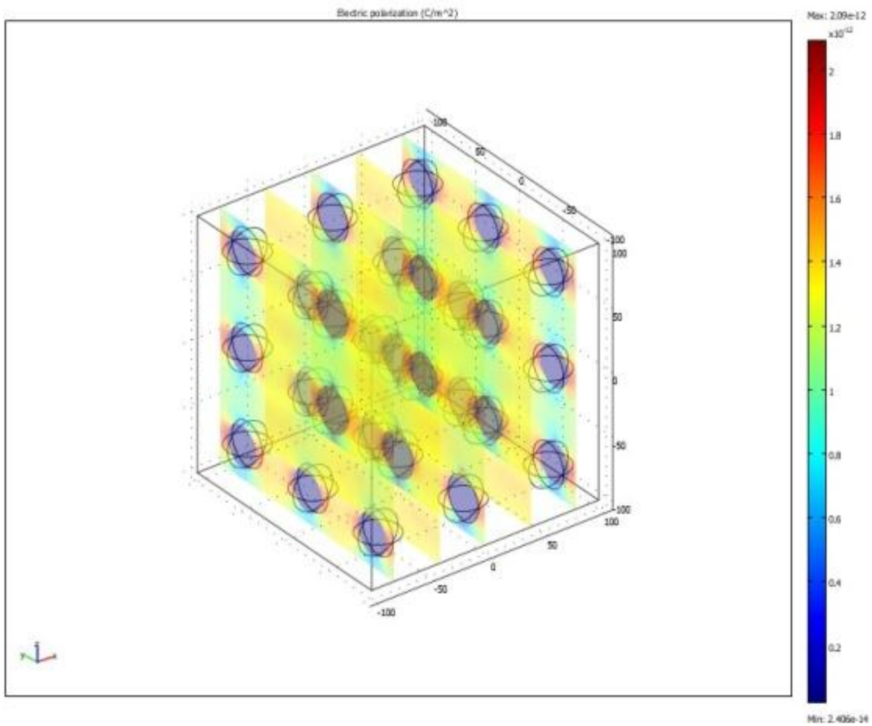
3D and 2D models follow same pattern of polarization increase when there is an increase in loading of nanoparticles.



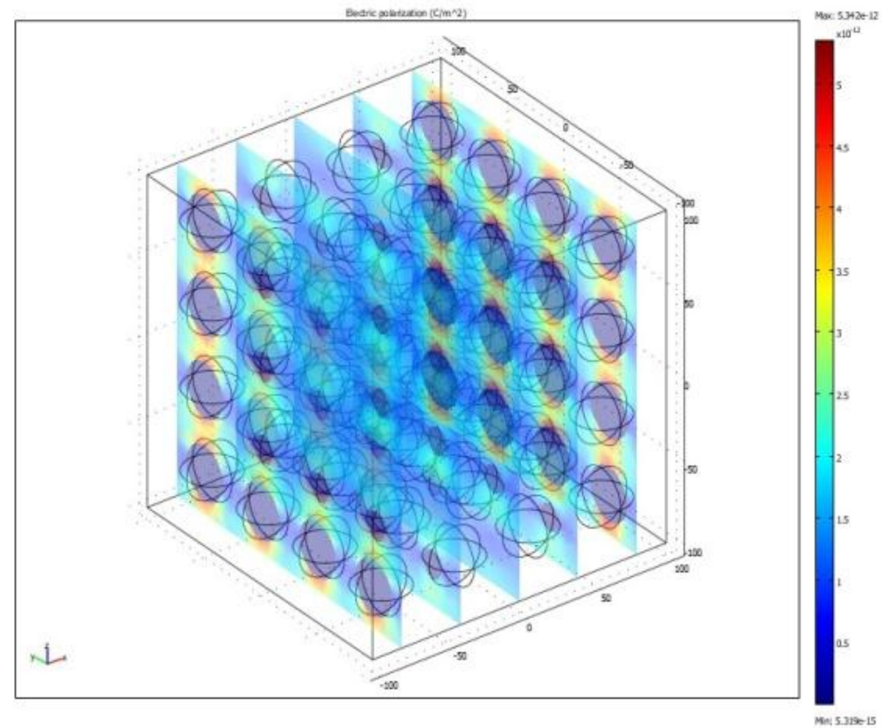
Electric polarization patterns in 3D nanodielectric with $f=0.022$

Results: 3D MODELING

f=0.078



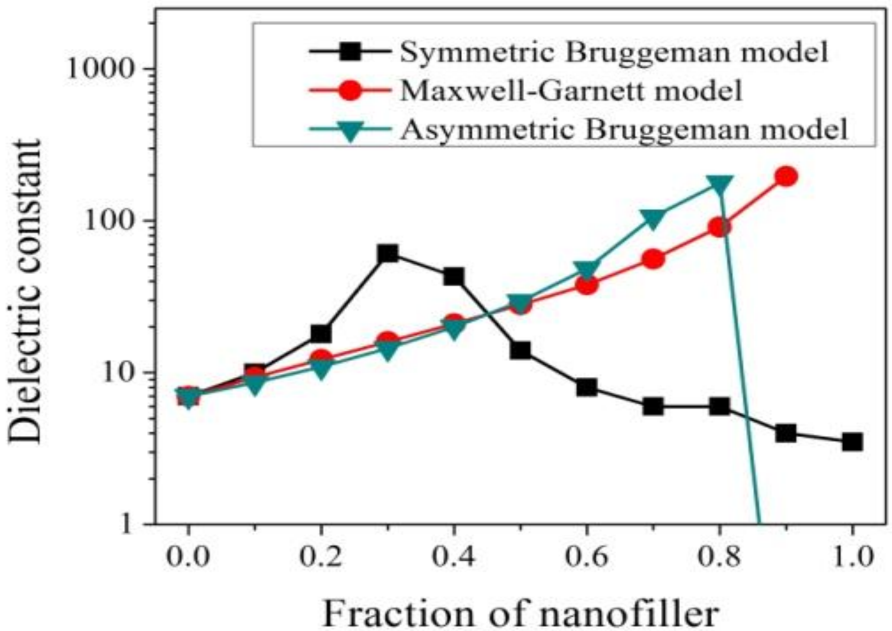
f=0.155



Effective dielectric constant increases with increase in loading of nanoparticles.

Results: K CALCULATION USING EMTS

- Effective dielectric constant of the medium is calculated using above mentioned EMT

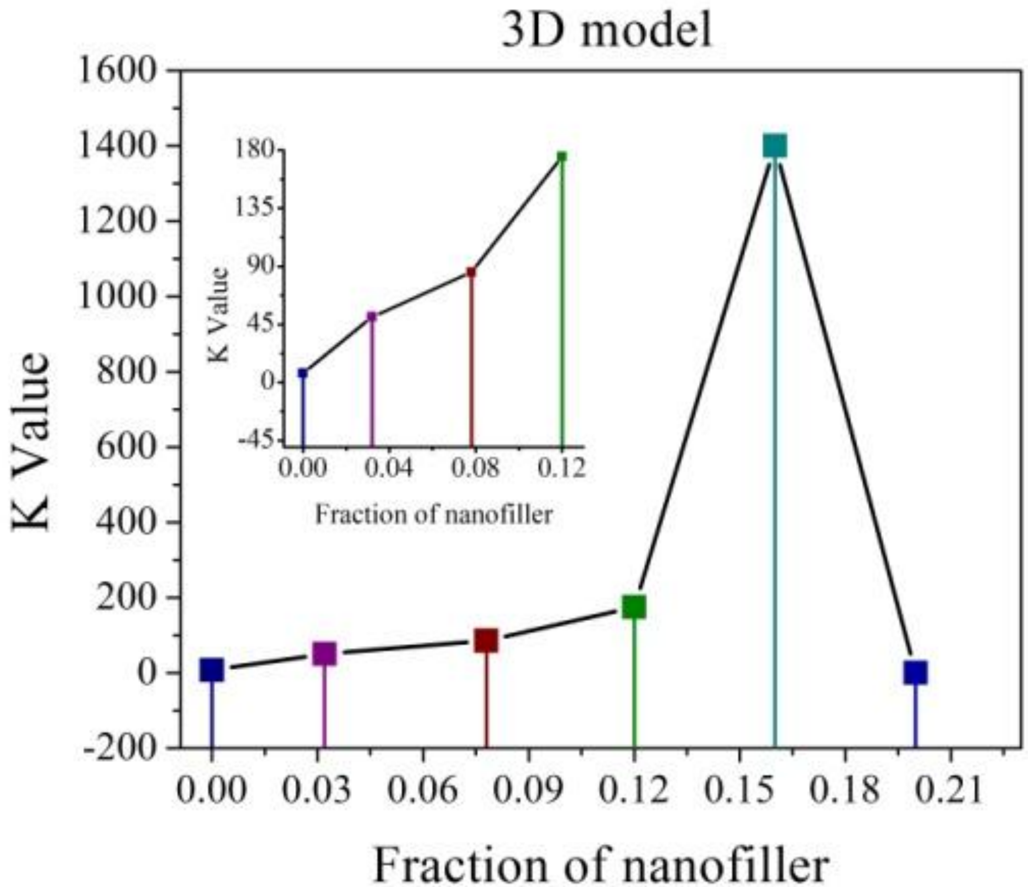


Real part of dielectric function of 2D composite calculated using various EMTs

- All EMTs predictions are close to each other at low loading.
- EMTs fail at high loading values because they ignore the inter-particle effects which are predominant at those values.

Results: K CALCULATION USING PERCOLATION THEORY for 3D MODEL

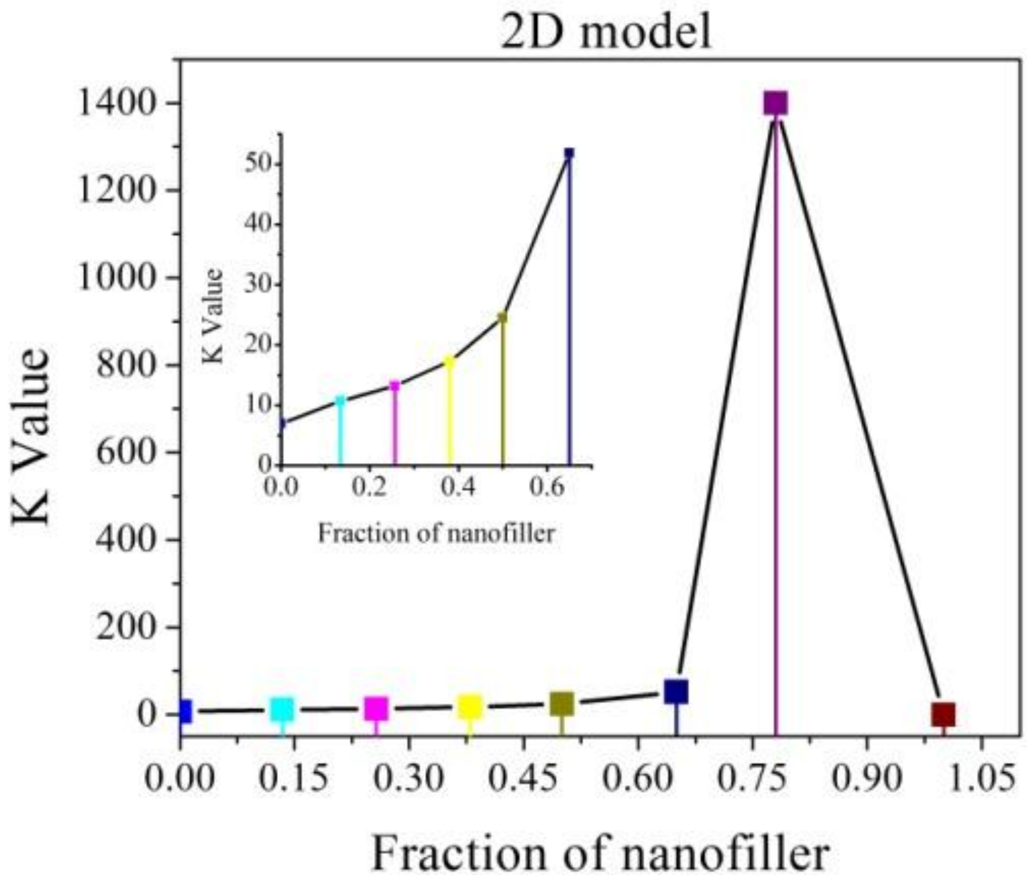
- Effective dielectric constant of the medium at f_c is calculated for 3D model.



Dielectric constant increases gradually with increase in loading. There is a sudden and huge increase in K value near percolation threshold

Results: K CALCULATION USING PERCOLATION THEORY for 2D MODEL

- Effective dielectric constant of the medium at f_c is calculated for 2D model.



An increase of magnitude 200 times is observed at *fc*. K value of polymer increased from 7 at *f*=0 to 1400 at f_c.

Conclusions

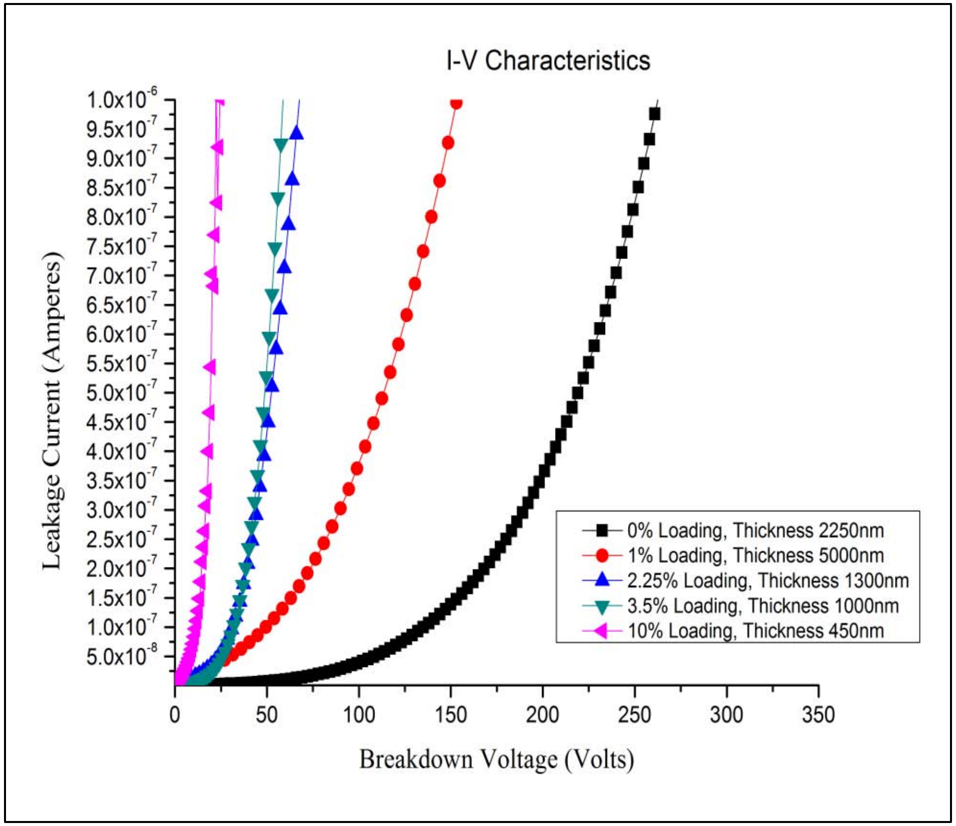
- Electric field and polarization patterns of 2D and 3D nanodielectrics are observed.
- At low loading, EMTs and Percolation theory predictions are close and both theories predict gradual increase in dielectric constant.
- EMTs fail at high loading but percolation theory takes in to account the metal-insulator nature of the composite and predicts huge increase in value of K at percolation threshold.
- At percolation threshold, K is determined as 1400, where as for a bare polymer this value is just 7.

Future Work

- This work will be extended other inexpensive metals such as Ag.
- Studies will be continued with particle of more complex structures, such as core-shell type.
- Comparison between analytical and empirical values will be carried out.

Preview of Empirical Results

- Nanoparticles are synthesis in our labs. Studies on PVP films were conducted.
- Parallel plate nanodielectrics are fabricated with different loadings of nanoparticles.

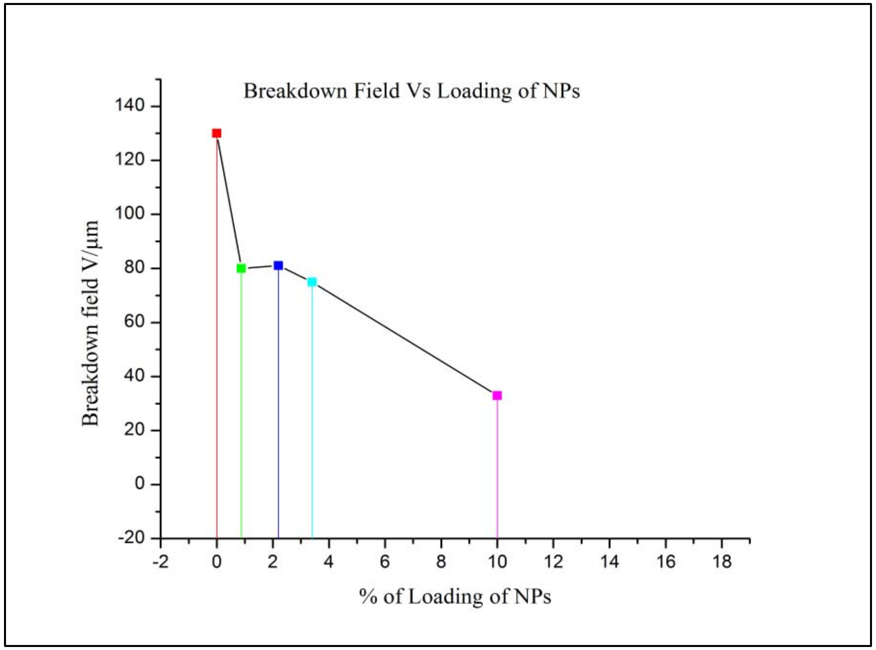


Loading of nanoparticles (by weight)	Loading of nanoparticles (by volume)	Breakdown field (V/µm)	Dielectric constant (K)
0	0	130	7
0.88	0.056	80	8.1
2.2	0.14	81	6.6
3.4	0.217	75	4.5
10	0.064	**33**	**20**

I-V Characteristics of nanodielectrics. Data used to plot the graph is tabulated.

Preview of Empirical Results

- SEM structural analysis, I-V characterization and capacitance measurements are carried out for fabricated devices.



Loading of nanoparticles (by weight)	Loading of nanoparticles (by volume)	Breakdown field (V/µm)	Dielectric constant (K)
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0.88	0.056	80	8.1
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3.4	0.217	75	4.5
10	0.64	**33**	**20**

Breakdown field of nanodielectrics Vs Loading of nanoparticles. Data used to plot the graph is tabulated.

With increase in loading of nanoparticles, breakdown field decreases and dielectric constant increases.

Questions?

Thank You