Numerical and Semi-Analytical Methods for Micromechanical Modeling of Piezoelectric Polymer Composites and Nanocomposites for Thin Film Applications

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Motivation

- Multifunctional materials such as Piezoelectric Polymer Nanocomposites combine the properties of polymers such as light weight, flexibility with that of piezoceramics such as high electromechanical coupling to form materials suitable for applications in micro and nano sensors, actuators as well as self powered micro and nanodevices.
- The effective properties of polymer nanocomposites are greatly influenced by the properties of the individual constituents.
- Modeling and simulation plays an important role in predicting and designing material properties, and guiding experimental work such as synthesis and characterization.

Objective

- To calculate the effective elastic, piezoelectric and dielectric properties of piezoelectric polymer composites and nanocomposites using semi-analytical and finite element methods.
- To study the effect of critical parameters such as volume fraction , shape, orientation, distribution, matrix-reinforcement interphase on the effective electroelastic properties of piezoelectric polymer composites and nanocomposites.

Theory

- The governing equation of piezoelectricity

Divergence equations

$$\sigma_{ij,j} = 0$$

$$D_{i,i} = 0$$

Constitutive Equations

$$\sigma_{ij} = C_{ijmn}\varepsilon_{mn} + e_{nij}(-E_n)$$

$$D_i = e_{imn}\varepsilon_{mn} - k_{in}(-E_n)$$

Gradient Equations

$$\varepsilon_{mn} = \frac{1}{2}(u_{m,n} + u_{n,m})$$

$$E_n = -\phi_{,n}$$

where, $\sigma_{ij}, \varepsilon_{mn}, C_{ijmn}, e_{nij}, E_n, D_n, u_{ij}, \phi_n, k_{ij}$ are the stress, strain, elastic moduli, piezoelectric stress moduli, electric field, electric displacement, displacement, electric potential and dielectric moduli.

Material Properties

$$\sum_{Material} = \left[\begin{array}{cccccc|ccc} C_{11} & C_{12} & C_{13} & 0 & 0 & 0 & 0 & 0 & e_{31} \\ C_{12} & C_{22} & C_{23} & 0 & 0 & 0 & 0 & 0 & e_{32} \\ C_{13} & C_{23} & C_{33} & 0 & 0 & 0 & 0 & 0 & e_{33} \\ 0 & 0 & 0 & C_{44} & 0 & 0 & 0 & e_{24} & 0 \\ 0 & 0 & 0 & 0 & C_{55} & 0 & e_{15} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{66} & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & e_{15} & 0 & -k_{11} & 0 & 0 \\ 0 & 0 & 0 & e_{24} & 0 & 0 & 0 & -k_{22} & 0 \\ e_{31} & e_{32} & e_{33} & 0 & 0 & 0 & 0 & 0 & -k_{33} \end{array}\right]$$

Material	C_{11} (GPa)	C_{12} (GPa)	C_{13} (GPa)	C_{22} (GPa)	C_{23} (GPa)	C_{33} (GPa)	C_{44} (GPa)	C_{55} (GPa)	C_{66} (GPa)	k_{11} (nF/m)	k_{22} (nF/m)	k_{33} (nF/m)	e_{15} (C/m²)	e_{24} (C/m²)	e_{31} (C/m²)	e_{32} (C/m²)	e_{33} (C/m²)
SU8	5.02	1.42	1.42	5.02	1.42	5.02	1.8	1.8	1.8	0.0354	0.0354	0.0354	0	0	0	0	0
ZnO	209.71	121.14	105.36	209.71	105.36	211.19	42.37	42.37	44.28	0.0757	0.0757	0.0903	−0.480508	−0.480508	−0.567005	−0.567005	1.32044
PVDF	3.8	1.9	1.0	3.2	0.9	1.2	0.7	0.9	0.9	0.064	0.082	0.067	0	0	0.024	0.001	-0.027
PZT-7A	148	76.2	74.2	148	74.2	131	25.4	25.4	35.9	4.072	4.072	2.08	9.2	9.2	-2.1	-2.1	9.5

Numerical Approach: Finite Element Analysis of 1-3 SU8/ZnO

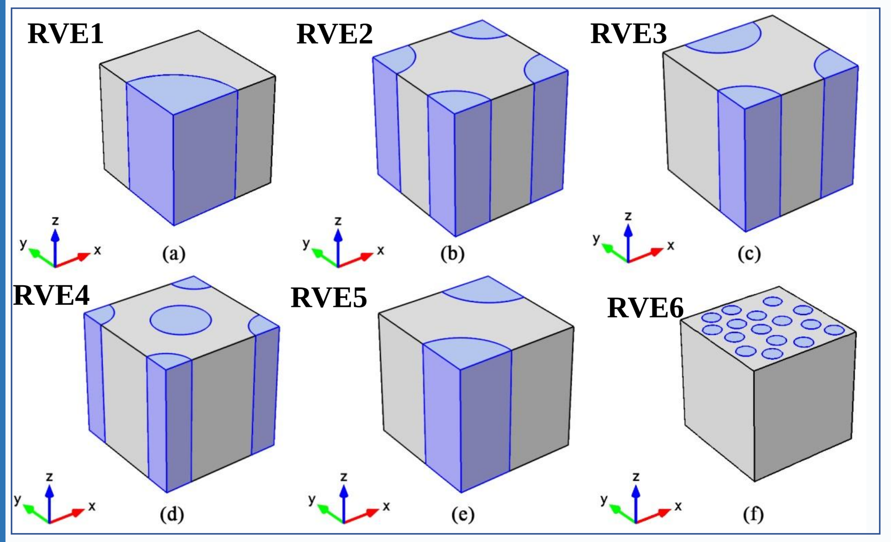

Fig 1: Six different types for SU8/ZnO RVEs

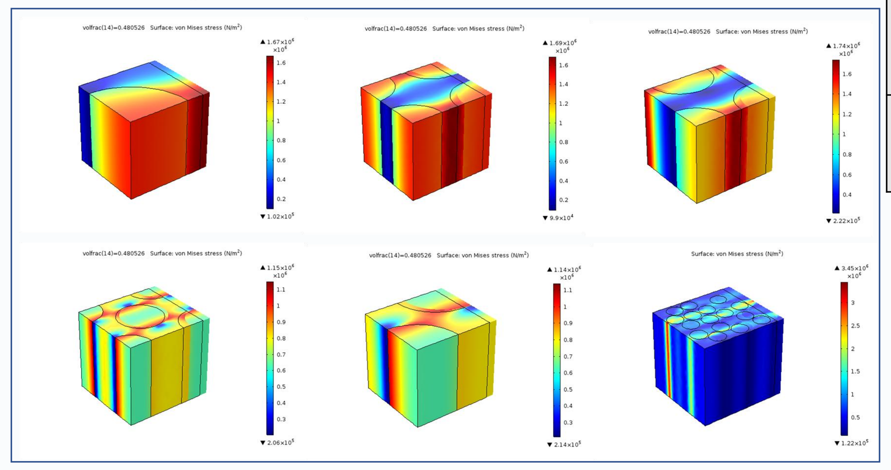

Fig 2: After applying boundary conditions for calculation of C_{11} and C_{12}

Kinematic Uniform Boundary Conditions

Property							Equations
E_3	$u=0$, $\varphi=0$	$u=h\varepsilon_{11}$, $\varphi=0$	$v=0$, $\varphi=0$	$v=h\varepsilon_{22}$, $\varphi=0$	$w=0$, $\varphi=0$	$w=h\varepsilon_o$, $\varphi=0$	$E_3 = \frac{\bar{\sigma}_{33}}{\bar{\varepsilon}_{33}}$
E_1	$u=0$, $\varphi=0$	$u=h\varepsilon_o$, $\varphi=0$	$v=0$, $\varphi=0$	$v=h\varepsilon_{22}$, $\varphi=0$	$w=0$, $\varphi=0$	$w=h\varepsilon_{33}$, $\varphi=0$	$E_1 = \frac{\bar{\sigma}_{11}}{\bar{\varepsilon}_{11}}$
e_{33}	$u=0$	$u=0$	$v=0$	$v=0$	$w=0$, $\varphi=0$	$w=0$, $\varphi=V_o$	$e_{33}^{eff} = -\frac{\bar{\sigma}_{33}}{\bar{E}_3}$
k_{33}	$u=0$	$u=0$	$v=0$	$v=0$	$w=0$, $\varphi=0$	$w=0$, $\varphi=V_o$	$k_{33}^{eff} = \frac{\bar{D}_3}{\bar{E}_3}$

Results

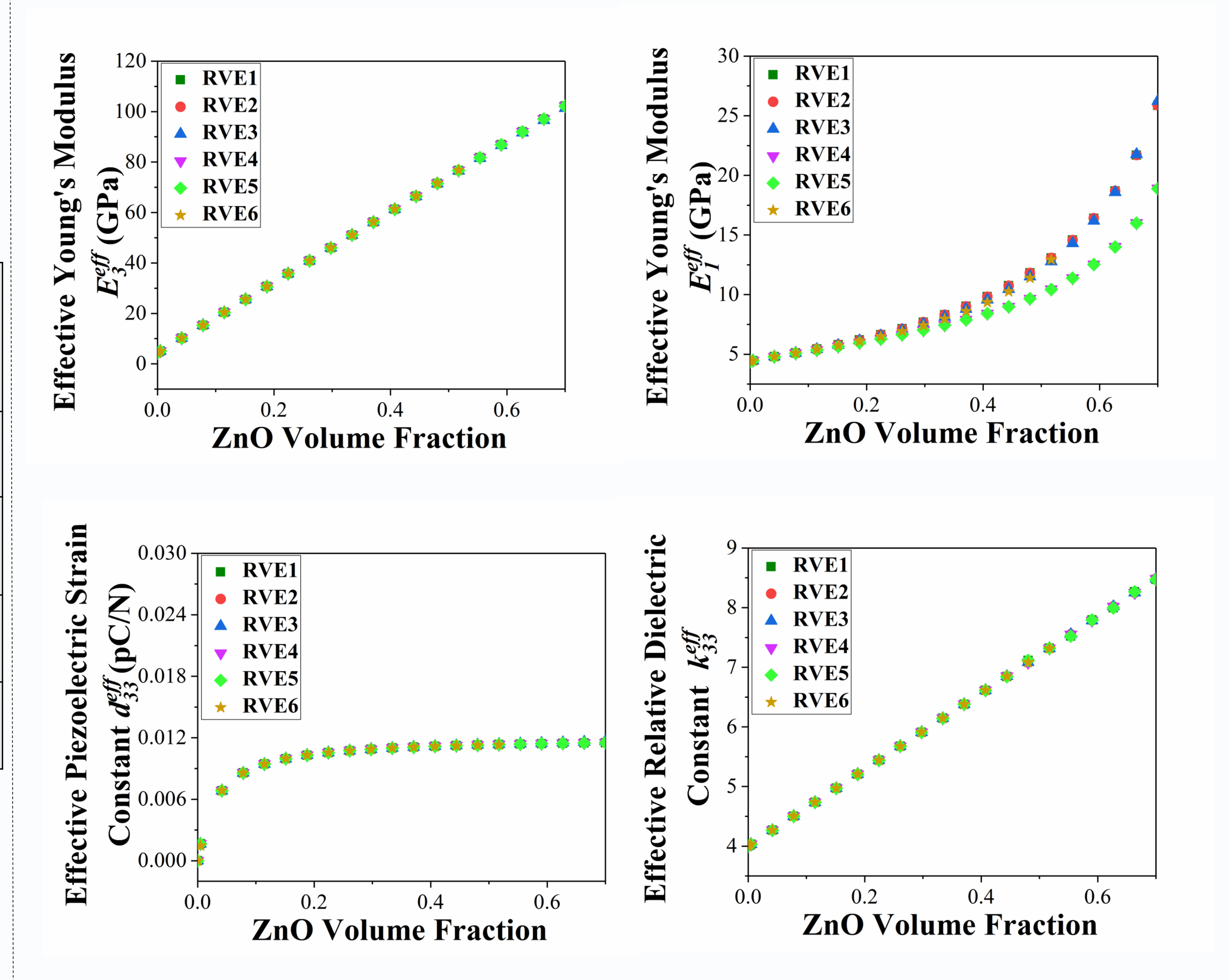

Fig 4: Graphs showing the change in effective elastic, piezoelectric and dielectric properties of the six SU8/ZnO RVEs with respect to volume fraction of the reinforcement.

Semi- Analytical Technique: Mori-Tanaka Approach PVDF/PZT-7A

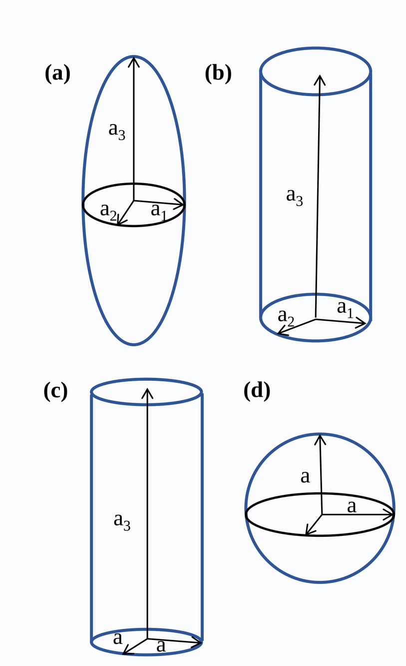

Fig 3: Types of reinforcements: (a) Ellipsoid (b) Elliptic Cylinder (c) Circular Cylinder (d) Sphere

Determination of Eshelby Tensor

$$S_{MnAb} = \frac{1}{8\pi} F_{iJAb}(G_{inmj} + G_{imnj}), \quad M = 1,2,3$$

$$= \frac{1}{4\pi} F_{iJAb} G_{in4j}, \quad M = 4$$

Calculation of Dilute concentration Tensor

$$T = [(I + S(F^m)^{-1}(F^f - F^m)]^{-1}$$

Calculation of effective electroelastic matrix of the composite

$$F^{eff} = F^m + v^f\{(F^f - F^m)T[v^m I + v^f T]^{-1}\}$$

Results

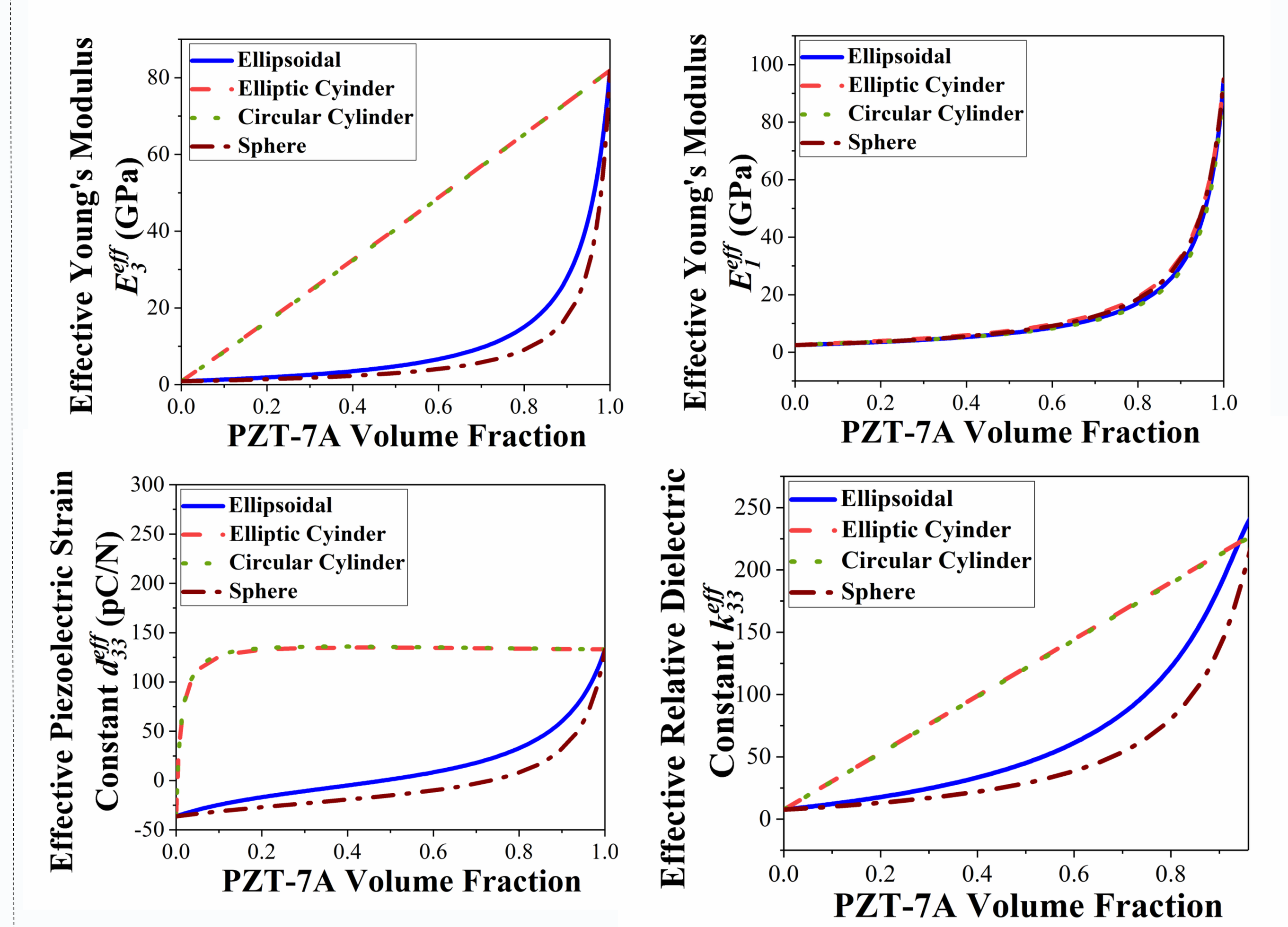

Fig 5: Graphs showing the change in effective elastic, piezoelectric and dielectric properties of the PVDF/PZT-7A composite different reinforcement geometries with respect to volume fraction of the reinforcement.

Observations/Conclusion

- The longitudinal elastic, piezoelectric and dielectric properties are insensitive to the distribution of fibers in the 1-3 composite system. However, the transverse properties do vary especially at higher volume fractions.
- The longitudinal electroelastic properties of elliptical and circular cylinder type reinforcement are exceptionally higher than ellipsoids and spherical types of reinforcements. However, the difference is inapparent in transverse direction.

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References

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