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Multiscale Design of Piezoelectric PLA/$BaTiO_3$ Composites for Electrically Active Bone Grafts

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INTRODUCTION & AIM

Piezoelectric scaffolds for bone regeneration

Bone is an electromechanically active tissue, where **mechanical loading can be associated with local electrical signals involved in remodeling and regeneration**. Piezoelectric scaffolds aim to reproduce this coupling, supporting the design of bioactive bone grafts with both structural and stimulatory functions [1-2].

PLA/$BaTiO_3$ composites and computational design

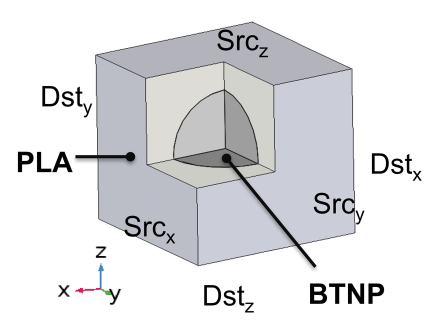
Barium titanate ($BaTiO_3$, BT) is a high-permittivity piezoelectric ceramic previously explored in polymeric scaffolds for tissue engineering applications [3]. When dispersed in biodegradable PLA-based matrices, BT can introduce electromechanical functionality while preserving processability. However, the **effective response strongly depends on microstructural features** such as filler content, particle distribution, and matrix properties. Therefore, FEM-based computational homogenization is used here to link PLA/BT microstructure to **effective elastic, dielectric, and piezoelectric properties**, supporting the rational design of electrically active bone graft materials.

METHOD

FEM-based RVE homogenization

1. RVE periodicity

Cubic representative volume element with $BaTiO_3$ inclusions embedded in a PLA matrix



Mechanical and electrical cell periodicity

$$\begin{cases} u_{dst} = u_{src} + e_{avg}(r_{dst} - r_{src}) \\ V_{dst} = V_{src} + E_{avg}(r_{dst} - r_{src}) \end{cases}$$

Linear piezoelectric constitutive law

$$\begin{cases} D = d\,\sigma + \varepsilon^T E \\ \varepsilon = s^E \sigma + d^T E \end{cases} \quad \textit{Strain-charge form}$$

2. Homogenization procedure

Mechanical load cases

- 6 independent mechanical deformation cases while average electric field equal to 0:

$$\begin{cases} \varepsilon_{xx} = 0.01, \varepsilon_{yy} = 0.01, \varepsilon_{zz} = 0.01, \gamma_{yz} = 0.01, \gamma_{xz} = 0.01, \gamma_{xy} = 0.01 \\ \langle E_j \rangle = 0 \end{cases}$$

Electrical load cases

- 3 independent voltage steps while mechanical constrained RVE

$$\begin{cases} E_x = 1, E_y = 1, E_z = 1 \\ \varepsilon_{xx} = \varepsilon_{yy} = \varepsilon_{zz} = \gamma_{yz} = \gamma_{xz} = \gamma_{xy} = 0 \end{cases}$$

Homogenized elasticity tensor

$$C_{ij}^{eff} = \frac{\langle \sigma_i^{(j)} \rangle}{\langle \varepsilon_j \rangle}$$

Homogenized piezoelectric tensor

$$e_{ij}^{eff} = \frac{\langle D_i^{pz,(j)} \rangle}{\langle \varepsilon_j \rangle}$$

Homogenized dielectric permittivity tensor

$$\varepsilon_{ij}^{eff} = \frac{\langle D_i \rangle}{\langle E_j \rangle}$$

3. Geometry and material properties

RVE geometry

- Spherical $BaTiO_3$ inclusions
- Particle/cell size varied to control microstructural architecture
- Filler v/v% : 5, 10, and 15

Material assumptions

- PLA matrix: linear elastic, isotropic
- $BaTiO_3$ filler: linear piezoelectric, anisotropic
- Perfect particle–matrix bonding
- Small-strain regime
- $BaTiO_3$ polarization axis aligned with the *z*-direction

Explored parameters

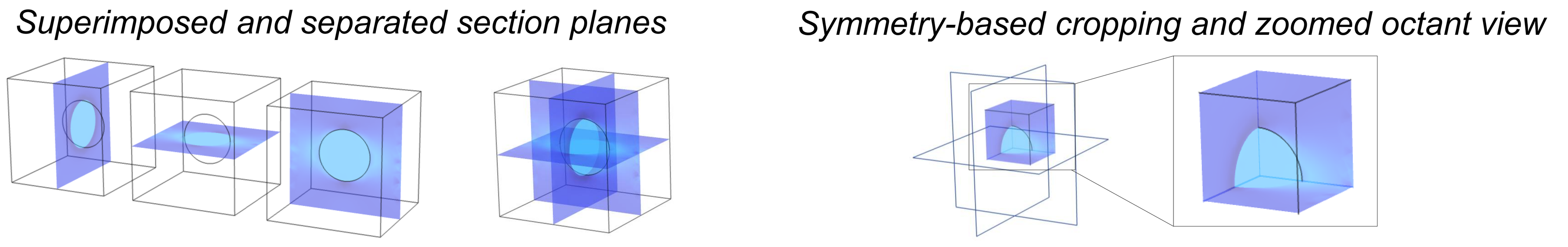
- Matrix elastic modulus
- $BaTiO_3$ volume fraction

Comsol Multyphysics 6.0

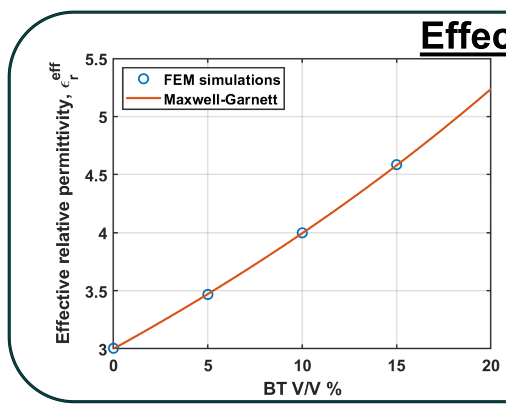
RESULTS & DISCUSSION

3D FEM visualization workflow

Superimposed and separated section planes — *Symmetry-based cropping and zoomed octant view*

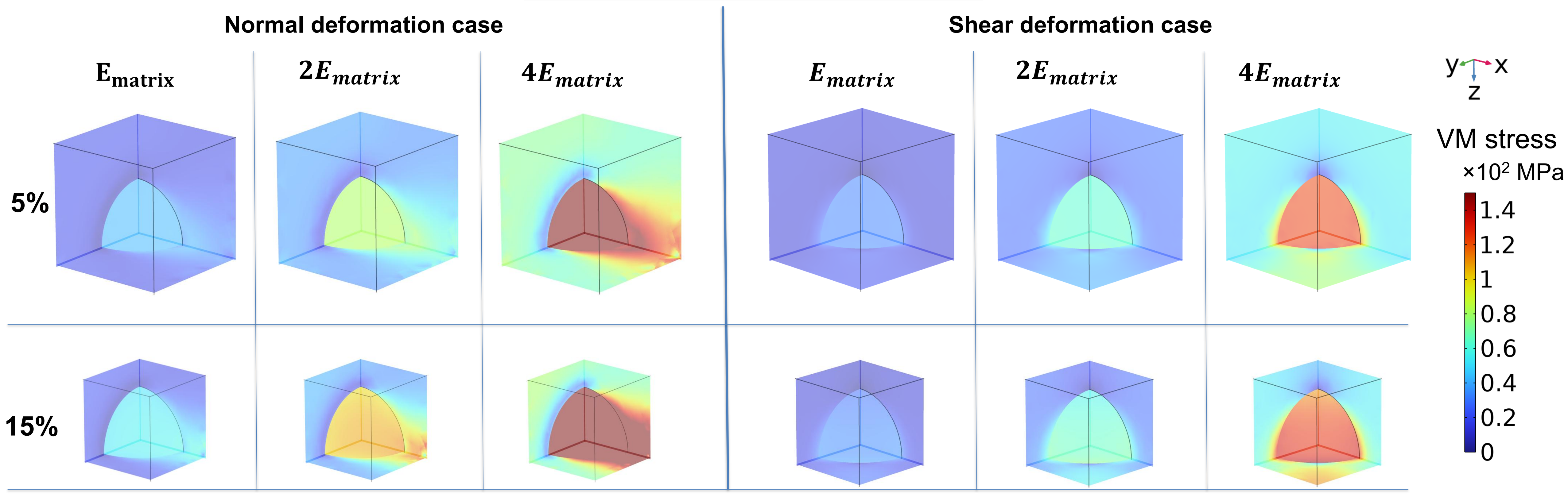


Effective dielectric permittivity of PLA/BaTiO3 composites



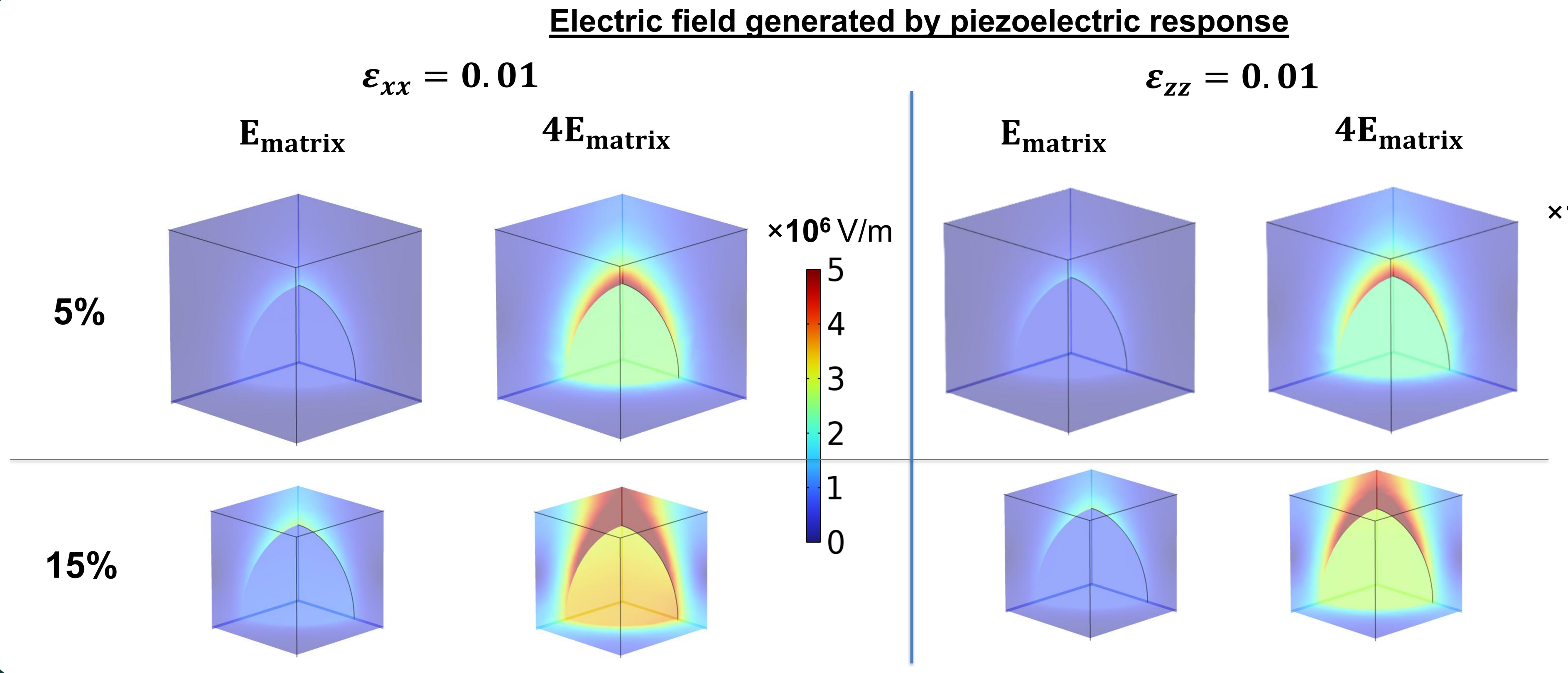
- matrix dominated response due to the isolated inclusions
- non-linear trend consistent with the Maxwell-Garnett model below percolation

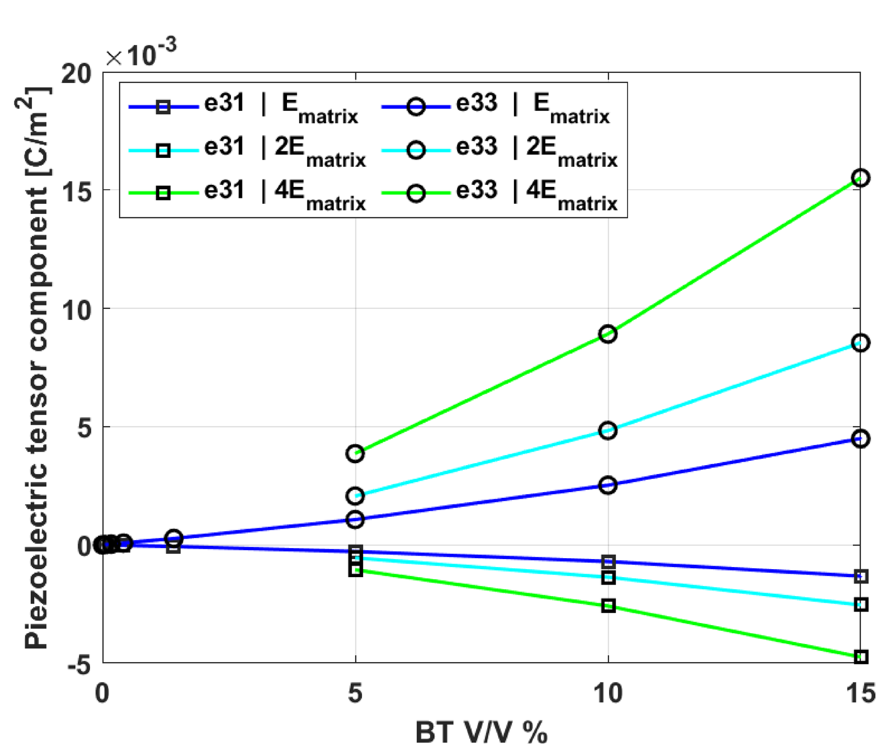
Stress distribution in PLA/BT composites



- Increased particle loading with increasing matrix stiffness and $BaTiO_3$ volume fraction.
- Stress concentration is mainly amplified along the imposed deformation direction.

Electric field generated by piezoelectric response





- Piezoelectric tensor components not linear with V/V%
- Interaction between stress field around particles at higher concentrations
- Matrix-particle mechanical contrast play an important role in dictating particle sollecitation, hence homogenized piezoelectric properties

CONCLUSIONS

- A FEM-based RVE homogenization framework was developed to **predict the effective electromechanical response of PLA/BT composites**.
- **BT volume fraction moderately increased the effective dielectric permittivity**, consistently with isolated high-permittivity inclusions in a low-permittivity PLA matrix.
- Local electric field maps showed **field amplification in the surrounding polymer**.
- Mechanical simulations indicated. **increased particle stress with both matrix stiffness and filler volume fraction**
- The framework supports the **rational design of electrically active polymer–ceramic composites for bone graft applications**.

FUTURE WORK/ REFERENCES/ACKNOWLEDGMENT

Future work

- Extend the model to **random particle distributions** and **non-ideal particle–matrix interfaces**.
- Couple the **homogenized composite properties with scaffold-scale geometries**.
- Validate the numerical predictions through experimental mechanical and piezoelectric characterization and finally **assess cell response under mechanically induced electrical stimulation**.

References

[1] D'Alessandro et al., *Biomolecules*, 2021, 11, 1731.
[2] Kemppi et al., *Colloids Surf. B Biointerfaces*, 2021, 199, 111530.
[3] Padurariu et al., *ACS Appl. Mater. Interfaces*, 2023, 15, 13535–13544.

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