

Environmentally-friendly Auxetic Piezoelectric Composites for Additive Manufacturing: Nonlocal and Nonlinear Effects

Anakkavoor K. Jagdish¹, Federico C. Buroni², Felipe Garcia-Sanchez³,
Roderick Melnik^{1,4,*}, Luis Rodriguez-Tembleque⁴, Andres Saez⁴

¹ MS2Discovery Interdisciplinary Research Institute, Wilfrid Laurier University
Waterloo, Ontario, Canada, N2L 3C5

² Department of Mechanical Engineering and Manufacturing, University of Seville,
Camino de los Descubrimientos s/n, Seville E-41092, Spain

³ Department of Civil Engineering, Materials, and Manufacturing, University of Malaga
Av. de Cervantes, 2, 29016 Málaga, Spain

⁴ Department of Continuum Mechanics and Structural Analysis, University of Seville,
Camino de los Descubrimientos s/n, Seville E-41092, Spain

ABSTRACT

Our main focus in this contribution is on the design and modelling issues of lead-free piezoelectric composites, amenable to 3D printing, in order to achieve their higher performance. Although the developed modelling framework is quite general and can be applied to other materials, as an example, our results are discussed in the context of barium titanate oxide piezoelectric inclusions embedded into a polymeric matrix.

We start with an auxetic matrix, that is a material having a negative Poisson ratio [1]. Such a matrix assists in the redistribution of the external stress acting on the piezocomposite in order to produce the maximum piezoelectric response. Our model is based on a fully coupled system of electro-mechanical interactions, accounting for nonlinear effects and flexoelectricity. Nonlinearities are coming from the application of size-dependent higher order piezoelectricity theory. The size-dependent properties, including electromechanical, are pronounced at smaller scales, e.g., due to the nonlocal coupling effect between strain gradient and polarization (flexoelectricity). Although such effects might often be negligible at the macroscopic level, they can influence the overall design principles of composite materials, created on the basis of hierarchically architected microstructures, for 3D printing and subsequent applications. Moreover, possible defects and agglomerations of added nanoparticles in such composite materials under certain conditions may create an environment for flexoelectricity to play a more pronounced role. We provide a detailed and systematic analysis of the contribution of these effects to the overall response of the structure.

In applications, stress and/or thermal gradients, among other factors, can force changes in the properties of microstructures, detectable at the macroscopic level. Next we note that softening of Young's modulus and negative Poisson ratio can also be achieved in the BaTi-based materials where phase transformations could play a critical role (e.g., [2] and references therein). We simulate such transformations and corresponding microstructure evolution based on the Landau-Ginzburg theory, and use the resulting input for our developed multiscale modelling framework.

Finally, we compare the performance of such multifunctional composite smart materials with more traditional designs based on the PVDF embedded matrix and the same type of barium titanate inclusions [3].

REFERENCES

- [1] J. Dagdelen, J. Montoya, M. de Jong, K. Persson, "Computational prediction of new auxetic materials", *Nat. Commun.*, 18, Art. 323, 2018.
- [2] R.S. Lakes, "Negative-Poisson's-Ratio materials: Auxetic solids", *Annu. Rev. Mater. Res.*, 47, 1.1-1.19, 2017.
- [3] N. Phatharapeetranun, B. Ksapabutr, D. Marani, J. R. Bowen, V. Esposito, "3D-printed barium titanate/poly-(vinylidene fluoride) nano-hybrids with anisotropic dielectric properties", *J. Mater. Chem. C*, 5, 12430-12440, 2017.