Design of 3-D printable microstructured lead-free piezoelectric nanocomposites

Andres Saez[1], Federico C. Buroni[2], Luis Rodríguez-Tembleque[1,*], Anakkavoor K. Jagdish[4], Felipe García Sánchez[3], Roderick Melnik[4,1]

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

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

ABSTRACT

Piezoelectric materials and composites effectively harvest energy from mechanical stress and vibrations. Such stimuli are ubiquitous in the form of vibrations in the environment and also in the human body during physical activity. This gives rise to a range of applications ranging from wearable piezoelectric energy harvesters to larger structures in civil infrastructures. Piezoelectric nanocomposites consist of piezoelectric nanomaterials embedded in flexible matrices. Microstructures of such composites can be easily fabricated using additive processes such as 3D printing[1]. An important consideration here is to employ lead-free piezoelectric materials such as Barium Titanate and achieve performances comparable to lead-based composite materials[2]. Understanding the nanoscale electro-elastic interactions between the nano-material and the matrix is critical to tune the properties of these composites and enhance the performance. Further, it is also important to understand the effects of the microscale properties of crystal structure and composite geometry on piezoelectric performance. Here, we use coupled electro-elastic modelling to bring together the effects of nanoscale and microstructural considerations in the design of piezoelectric nanocomposites. We computationally investigate important aspects of piezoelectric composite design and performance. We first attempt to understand the nanoscale interactions between piezoelectric nano-particles and the matrix, specifically looking at interesting processes arising when these particles have physical contact hinting possible percolation effects. A second aspect of this design is to tune the stiffness of the composite using nanoscale substitution of mechanically stronger materials such as carbon nanotubes. This is critical for effectively coupling the applied mechanical stress to the embedded piezoelectric nano-particles, especially if the matrix is a relatively soft. We further explore also auxetic materials as possible matrix materials and their potential role in amplifying piezoelectric response. The third aspect of our investigation is related to the polycrystalline property of the piezoelectric material. When dealing with piezoelectric materials with sizes in the micrometer range at least in one dimension, the orientation of grains within a particle considerably affects the piezoelectric properties. This aspect has important implications for the performance of the nano-composite energy harvesting materials. Finally, we also consider the flexo-electric effect. At the nanoscale, non-local effects arise where strain gradients generate electrical flux leading to higher piezoelectric performances than predicted through linear piezoelectric theory. We build these aspects into a RVE and use finite element method to simulate the model. Further, we use the data from the nanoscale design to design complex microscale structures which can be fabricated by additive manufacturing processes. By tuning the effective electro-elastic coefficients of the composite, we will attempt to maximise the piezoelectric response while trying to retain the mechanical properties that will suit deployment scenarios such as in civil infrastructures and wearable components.

REFERENCES

[1] K. Kim, W. Zhu, X. Qu, C. Aaronson, W. R. McCall, S. Chen, *et al.*, "3D optical printing of piezoelectric nanoparticle–polymer composite materials," *ACS Nano,* vol. 8, pp. 9799-9806, 2014.

[2] D. Maurya, M. Peddigari, M.-G. Kang, L. D. Geng, N. Sharpes, V. Annapureddy, *et al.*, "Lead-free piezoelectric materials and composites for high power density energy harvesting," *Journal of Materials Research,* vol. 33, pp. 2235-2263, 2018.