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Flexoelectricity-based Electromechanical Metamaterials

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Flexoelectricity-based electromechanical metamaterials

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It is well known that by deforming a special class of materials (piezoelectrics) electricity can be produced. This functionality makes piezoelectrics ubiquitous in sensors, actuators, and energy harvesting systems. What is a relatively new discovery is that by bending any dielectric at the nanoscale, significant electrical transduction can also be achieved. This is the so-called flexoelectric effect, a far less known and understood phenomenon by which electric polarization is coupled to strain gradients. Flexoelectricity is present in a much wider variety of materials, including non-polar dielectrics and polymers, but is only significant at small length-scales, where high strain-gradients develop. The key goal of this study is to identify through computational exploration design concepts for metamaterials or composites that constructively accumulate the flexoelectric effect of non-piezoelectric micro-structural elements, and make it available as an effective piezoelectric response at larger scales. If properly designed, an effective homogeneous deformation on the composite may create substantial strain gradients (and polarization) in its non-piezoelectric constituents.

In order to achieve this goal, we face several challenges, both computational and conceptual. Within the continuum phenomenological theory, the flexoelectric field equations are mathematically a coupled system of 4th order partial differential equations. The high-order nature of the PDE requires C1-continuous solutions, so the standard Finite Element Method (FEM) is not suitable, and advanced discretization methods are required such as meshfree methods [1,2] and mixed FEM [3]. Here, we will present a computational approach based on Immersed Boundary HB-spline approach. (Hierarchical) B-spline basis functions provide high-order continuity of the original unknowns and are efficiently evaluated and integrated. Since they are globally defined on a Cartesian parametric space, we consider a regular Cartesian mesh and make use of the Immersed Boundary concept to permit simulations on arbitrary domain shapes, which can be exactly represented. This high-order method is particularly attractive, since it can capture the exact geometry of the domain, can easily handle material inclusions and interfaces, considers spatial resolution adaptivity, can be easily extended to shape optimization and is amenable to parallel computation [4].

From fundamental symmetry arguments, only chiral (non-centrosymmetric) materials can exhibit properties characterized by odd-rank tensors such as piezoelectricity [5]. This is thus a key symmetry design restriction when using non-piezoelectric materials. In preliminary results, we have explored designs that exploit the small feature-size and chirality of the geometry and layout of constituents with different material properties (see Fig. 1). We consider in these examples a flexoelectric but not piezoelectric constituent and the sample is compressed. Design A shows that chiral geometry alone is not sufficient for effective piezoelectricity, i.e. there is no potential difference at the electrodes. The flexoelectric effect remains in the interior of the material and cannot be extracted. In Design B, the circles are inclusions made out of a stiff conductor. Interestingly, we now observe a progressive increase in electric potential as we move upwards in the composite. The maximum potential difference can be collected at the conductors in the second to last row. By selecting a soft conductor instead, in Design C, the potential difference increases towards the center of the sample, where it is significantly larger than in B. We have checked that the potential difference scales with the number of lattice repeats, suggesting scalability of the concept. These examples highlight the interplay between geometry and material properties required for performant flexoelectric composites.

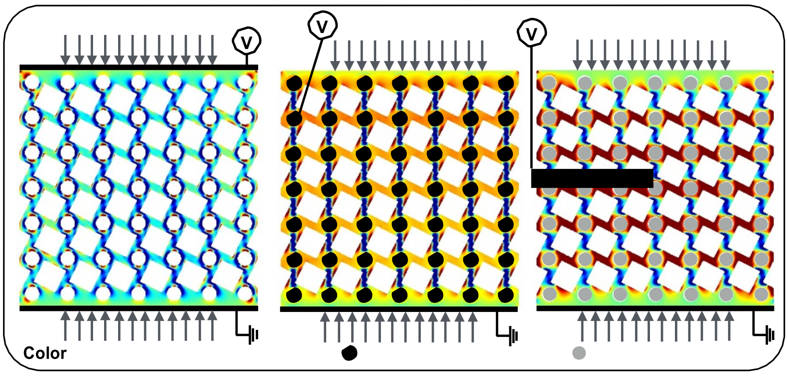

Figure 1: Three proof-of-concept designs for a flexoelectricity-based electromechanical transducer.

Besides bending, torsion also provides inhomogeneous deformation in 3D configurations. While torsion of bars is a standard technique to characterize strain-gradient elasticity, flexoelectricity has not been explored in rod geometries under torsion. We have developed a general formulation based on torsion mechanics to quantify the shear flexoelectric response in different crystal symmetry groups [6].

With these capabilities, we have explored 3D designs of flexoelectricity-based electromechanical transducers whose effective piezoelectric response is achieved through the bending and torsion of its non-piezoelectric micro-structural elements through the flexoelectric effect. Evidence suggests that this new effect may play a pivotal role in next- generation electromechanical sensors, actuators, and energy harvesters at sub-micron scales, significantly broadening the class of materials for electromechanical transduction and enabling new affordable, biocompatible and self-powered small- scale devices.

Acknowledgments

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References

[1] Abdollahi, Peco, C., A., Millán, D., Arroyo, M., and Arias, I., 2014. Computational evaluation of the flexoelectric effect in dielectric solids. *Journal of Applied Physics*, 116 (9), 93502.
[2] Abdollahi, A., Millán, D., Peco, C., Arroyo, M., and Arias, I., 2015. Revisiting pyramid compression to quantify flexoelectricity: A three-dimensional simulation study. *Physical Review B*, 91, 104103.
[3] Mao, S., Purohit, P. K., and Aravas, N., 2016. *Proceedings of the Royal Society of London A: Mathematical, Physical and Engineering Sciences*, 472(2190).
[4] Codony, D., Marco, O., Fernández-Méndez, S., and Arias, I., (2018), Immersed Boundary Hierarchical B-spline method for the Numerical Simulation of Nano-Scale Electromechanical Transduction, under review.
[5] Lakes, R., 2001. Elastic and viscoelastic behavior of chiral materials, *International Journal of Mechanical Sciences*, 43, pp.1579–1589.
[6] Mocci, A., Abdollahi, A., Arias, I., (2018), Quantification of shear flexoelectricity in ferroelectrics, under review.