#### **PROCEEDINGS**

# **Mixed Finite Element Approach for Semiconductor Structures**

Qiufeng Yang<sup>1</sup>, Xudong Li<sup>2</sup>, Zhaowei Liu<sup>3</sup>, Feng Jin<sup>1,\*</sup> and Yilin Qu<sup>1,\*</sup>

<sup>1</sup>State Key Laboratory for Strength and Vibration of Mechanical Structures, Xi'an Jiaotong University, Xi'an, 710049, China <sup>2</sup>Ningbo Institute of Materials Technology and Engineering, Chinese Academy of Sciences, Ningbo, 315201, China <sup>3</sup>College of Mechanics and Materials, Hohai University, Nanjing, 211100, China

\*Corresponding Authors: Feng Jin, Yilin Qu. Email: jinfengzhao@263.net, quyilin\_95@126.com

## ABSTRACT

Compared to piezoelectric effects restricted to noncentrosymmetric crystalline structures, flexoelectric effects exist universally in all crystalline structures [1,2]. Meanwhile, some crystals, say silicon, are also semiconductive, which raises interest in studying the interactions between mechanical fields and mobile charges in semiconductors with consideration of piezoelectricity or flexoelectricity [3,4]. In order to explain these coupling effects, macroscopic theories on elastic semiconductors considering piezoelectricity or flexoelectricity were proposed by Yang and co-authors [5,6]. For piezoelectric semiconductors, the formulation of finite elements is relatively straightforward since the governing partial derivative equation (PDE) is twice-order. As for elastic semiconductors with consideration of flexoelectricity, it is more challenging to formulate its finite element due to the strain gradients in the constitutive relations making the governing PDE fourth-order. For the fourth-order PDE,  $C^1$  continuity is required for the displacement tensor when we use traditional finite elements (FEs) for the numerical solution, which brings difficulties in the FE implementation [7,8]. In the present work, instead of using  $C^1$  elements, we develop an alternative mixed finite element with  $C^0$  continuity for solving the problem. The convergency and accuracy of the developed element are verified, respectively. The validated mixed FE method is then used to study the problem of an infinite-length tube with an axisymmetric cross section. Our FE methods provide a tool for exploring the coupling effects in elastic semiconductors.

## **KEYWORDS**

Piezoelectricity; flexoelectricity; semiconductors; mixed finite elements

**Funding Statement:** This work was supported by the National Natural Science Foundation of China (NNSFC; No. 11672223) and 111 Project version 2.0.

**Conflicts of Interest:** The authors declare that they have no conflicts of interest to report regarding the present study.

### References

- 1. Maranganti, R., Sharma, N. D., Sharma, P. (2006). Electromechanical coupling in nonpiezoelectric materials due to nanoscale nonlocal size effects: Green's function solutions and embedded inclusions. *Physical Review B*, 74(1), 014110.
- 2. Sharma, N. D., Maranganti, R., Sharma, P. (2007). On the possibility of piezoelectric nanocomposites without using piezoelectric materials. *Journal of the Mechanics and Physics of Solids*, *55(11)*, 2328-2350.



This work is licensed under a Creative Commons Attribution 4.0 International License, which permits unrestricted use, distribution, and reproduction in any medium, provided the original work is properly cited.

- 3. Yang, M. M., Kim, D. J., Alexe, M. (2018). Flexo-photovoltaic effect. Science, 360(6391), 904-907.
- 4. Zou, H., Zhang, C., Xue, H., Wu, Z., Wang, Z. L. (2019). Boosting the solar cell efficiency by flexo-photovoltaic effect? *ACS nano*, *13(11)*, 12259-12267.
- 5. Qu, Y., Jin, F., Yang, J. (2020). Effects of mechanical fields on mobile charges in a composite beam of flexoelectric dielectrics and semiconductors. *Journal of Applied Physics*, 127(19), 194502.
- 6. Qu, Y., Jin, F., Yang, J. (2021). Torsion of a flexoelectric semiconductor rod with a rectangular cross section. *Archive of Applied Mechanics*, *91(5)*, 2027-2038.
- 7. Amanatidou, E., Aravas, N. (2002). Mixed finite element formulations of strain-gradient elasticity problems. *Computer Methods in Applied Mechanics and Engineering*, *191(15-16)*, 1723-1751.
- 8. Soh, A. K., Wanji, C. (2004). Finite element formulations of strain gradient theory for microstructures and the  $C^{0-1}$  patch test. *International Journal for Numerical Methods in Engineering*, 61(3), 433-454.