Isogeometric Analysis of Flexoelectricity in Functionally Graded Structures

A Thesis

Submitted by

SAURAV SHARMA

(D17052)

For the award of the degree of

DOCTOR OF PHILOSOPHY

SCHOOL OF ENGINEERING

INDIAN INSTITUTE OF TECHNOLOGY MANDI

Mandi, Himachal Pradesh -175075

July 2021

DECLARATION

I hereby declare that the Thesis titled "**Flexoelectricity in Functionally Graded Structures**" submitted by me, to the Indian Institute of Technology Mandi for the award of the degree of **Doctor of Philosophy (PhD)**, is a bona fide record of the research work carried out by me in the **School of Engineering**, Indian Institute of Technology Mandi, under the supervision **of Dr. Rajeev Kumar and Dr. Mohammad Talha.** The contents of this thesis, in full or in parts, have not been submitted to any other Institute or University for the award of any degree or diploma. In keeping with the general practice, due acknowledgements have been made wherever the work described is based on findings of other investigators.

IIT Mandi (H.P.)

Date: 20 May, 2021

Saurav Sharma

THESIS CERTIFICATE

This is to certify that the Thesis titled "**Flexoelectricity in Functionally Graded Structures**" submitted by **Saurav Sharma** to the Indian Institute of Technology Mandi for the award of the degree of **Doctor of Philosophy (Ph.D.)**, is a bona fide record of the research work done by him under our supervision in the School of Engineering, Indian Institute of Technology Mandi. The contents of this thesis, in full or in parts, have not been submitted to any other Institute or University for the award of any degree or diploma.

Dr. Rajeev Kumar
Associate Professor
School of Engineering
IIT Mandi

Date:

Dr. Mohammad Talha
Associate Professor
School of Engineering
IIT Mandi

Date:

ACKNOWLEDGEMENT

My thanks go out to all the people who have been instrumental in making this work possible. First of all, I would like to offer my sincerest gratitude to my thesis advisors, Dr. Rajeev Kumar and Dr. Mohammad Talha, for their innovative inputs to my research project and for giving me guidance and encouragement throughout this work.

I am extremely thankful to Dr. Rajeev Kumar for his support and the direction that he has provided to this work from the beginning. He has not only provided me the utmost support and guidance from the beginning of my research work but also provided me freedom and motivation to work on the research problems of my choice. In addition to being my thesis supervisor, he has always been a great teacher to me, imparting the basic concepts required for my work.

I convey my deepest appreciation and thanks to Dr. Rahul Vaish for his inestimable help and support in my research work. I cannot go without expressing my admiration for his genuine ideas and physical intuitions that make him a successful researcher. He has always provided me his invaluable mentorship and advice in every possible aspect of my academic experience at IIT Mandi. I am extremely thankful for all the encouragement and motivation he has provided to me.

I also wish to acknowledge the members of the doctoral committee, Dr. Vishal Singh Chauhan, Dr. Rajesh Ghosh, and Dr. Manoj Thakur, for their careful examination of the work and their invaluable comments and insights, which made a deep impact on my research.

The work of this thesis would not have been possible without the direct or indirect contributions from my friends and colleagues at IIT Mandi. I sincerely thank my research colleagues, Dr. Anuruddh Kumar, Raj Kiran, Diwakar Singh, and Kamalpreet Singh, for all their help and support in my research work. The rich technical discussions with them have helped me a lot in overcoming the obstacles faced during my research work. I also wish to acknowledge the amazing support and advice by Satish Kumar, Abhishek Banagunde, Tarun Kumar, Jitendra Adhikari, Prakash Poudel, and all the other members of the Smart Materials and Structures lab. I also owe a huge thanks to Dr. Khyati for all her help, especially in manuscript preparation, during the initial phase of my research work.

Most importantly, I submit my gratitude to my parents and my brother for always encouraging me to achieve my academic goals and being the source of all the positivity and optimism in my life.

PREAMBLE

Smart materials that respond to electromechanical coupling have become essential components of modern engineering structures as well as advanced micro/nano electromechanical systems. The most popular class of materials for this purpose is piezoelectric materials. However, piezoelectricity only exists in a certain type of materials (non-centrosymmetric), which are often brittle in nature and toxic due to their lead content. A new phenomenon, known as "Flexoelectricity", has recently emerged in this direction, which enables the piezoelectric-like response in virtually all the dielectric materials. Flexoelectric effect increases with the decreasing size, and thus, the flexoelectric output at micro and nano scales becomes very high.

Flexoelectricity requires a non-uniform strain/electric field in a dielectric material to exhibit an electromechanical response. This requirement is generally met by having non-uniform or varying geometry of the structures. Through this work, we propose the use of Functionally Graded Material (FGM) to have a gradient of electrical and mechanical field variables. The graded composition is found to have an enriching effect on the flexoelectricity, both qualitatively and quantitatively. Qualitatively, the graded composition provides the geometry independent electromechanical response and provides the freedom of choosing any shape. On the other hand, for the quantitative aspect, the magnitude of flexoelectric response in FGM composition is found to be many folds higher than that achieved through non-uniform geometry. The direct effect (sensing) and the converse effect (actuation), both are examined under mechanical and thermal loads in an FGM structure of regular shape. Further, a novel strategy is developed to trigger a universal converse flexoelectric response in homogeneous structures, through varying electric field direction inside the structure. Three different configurations with different electrical boundary conditions are proposed for this purpose. It is found that these configurations can be utilized to achieve actuation in two perpendicular directions. Later, these configurations are compared with the other two methods to generate converse flexoelectricity, i.e., trapezoid shape and FGM. Different combinations of these three methods were also examined and compared. While the FGM was found to outperform the other individual configurations, the varying electric field direction strategy was successful in developing the converse flexoelectricity independent of geometry and material composition.

Based on the large magnitude of flexoelectric response in FGM, the possibility of harnessing flexoelectric coupling for novel applications was realized. In this sequence, two novel applications of this unique universal phenomenon, namely, flexocaloric effect and polarization switching, are investigated in FGMs. In polarization switching study, poling of ferroelectric materials achieved through purely mechanical means by virtue of flexoelectric polarization induced due to mechanical loading is studied. The result of such poling is the coexistence of both flexoelectric and piezoelectric phenomena in the same sample. Later, the effective electromechanical coupling due to the interplay of these two coexisting phenomena is analyzed. It was found that while the two couplings act destructively in direct effect, the converse effect can be enhanced by up to 90% of pure flexoelectric coupling. On the other hand, in flexocaloric effect, the entropy change, due to flexoelectricity generated electric field, triggers a temperature change in the material. This can be used for solid-state cooling in a cyclic manner. Finally, a basic research gap in the field of flexoelectricity, i.e., defining the parameters for the quantification of energy conversion in flexoelectricity, is addressed. Towards a better understanding of this phenomenon, we have defined performance indexes to quantify the energy conversion efficiency of flexoelectricity in different modes of operations and investigated its interplay with piezoelectricity. The values of these indexes were examined in three different materials, namely, barium titanate ($BaTiO_3$), Er-doped BST ceramic ($Ba_{1-x}Ti_{0.96}Sn_{0.04}O_3$ + x mol. % Er), and polyvinylidene difluoride (PVDF).

CONTENTS