Multiscale Modelling of Single Crystal PMN-PT Ferro-Electric Films as a Morphotropic Phase

Zian Wang*[1], Yujie Xie[2], Ligang Sun[2], Ling Chao[2], Li Dongfeng[2], Wei Jun[3], and Esteban Busso†[2]

[1]Center for Materials Modelling and Characterisation, Harbin Institute of Technology, Shenzhen – China

[2]Center for Materials Modelling and Characterisation, Harbin Institute of Technology, Shenzhen – China

[3]Shenzhen Key Laboratory of Flexible Printed Electronics Technology, School of Materials Science and Engineering, Harbin Institute of Technology, Shenzhen – China

Abstract

Recent advancements in wearable flexible hybrid electronic systems have driven the demands on their self-powered modules. Single crystal PMN-PT thin films near morphotropic phase boundary are well known for their exceptional piezoelectric properties, and are often chosen as the crucial functional material in these modules. However, the mechanisms behind their outstanding piezoelectric performance remain insufficiently understood due to the complex multiphase coexistence and multiscale hierarchical structure, necessitating a multiscale analysis strategy.

In this work, a phase-field modelling framework based on the Landau potential is employed to describe and predict the domain evolution as well as the mechanical and electrical responses of PMN-PT thin films used in flexible electronic devices. Due to the complicated microstructure of PMN-PT thin films, it is nearly impossible to extract the pure domain or domain wall material parameters from experimental data. Therefore, first-principles calculations at the electronic scale are utilised to calibrate the phase-field model parameters. The resulting phase-field model is numerically implemented into the finite element method to explore the electromechanical responses of PMN-PT thin films via the representative volume elements. The simulated behaviour, including macroscopic polarization–electric field hysteresis and piezoelectric response, is verified against experimental data obtained as part of this work. The proposed approach integrates electronic/atomic-scale properties into a continuum modeling framework to provide a comprehensive understanding of PMN-PT thin films performance. These simulations can offer valuable guidance to optimise their piezoelectric properties and performance stability, advancing the development of self-powered systems for the next-generation of flexible electronic devices.

*Speaker

†Corresponding author: epbusso@outlook.com