“Phase Field Modelling near the Morphotropic Phase Boundary in Lead-Free Ferroelectrics”

Oscar Torres, PhD Candidate

Lead-free ferroelectric (FE) materials are currently of great interest for replacing ubiquitous Lead Zirconate Titanate (PZT) in electromechanical applications, with maximal dielectric and piezoelectric properties observed near the Morphotropic Phase Boundary (MPB) region. However, existing theoretical descriptions cannot describe the MPB directly or shed light on the structural state near this region, while other models combine the response of the adjoining FE phases in a contrived way. In this project, a novel phase-field model is proposed for MPB FEs. The approach integrates the thermodynamics of each FE phase independently. The formulation accounts for coupling to different fields, such as electrostatic or electromechanical coupling, and it can be extended to model polycrystalline FEs in 3-D, allowing study of the structural state and origin of the enhanced properties near the MPB of lead-free FEs.

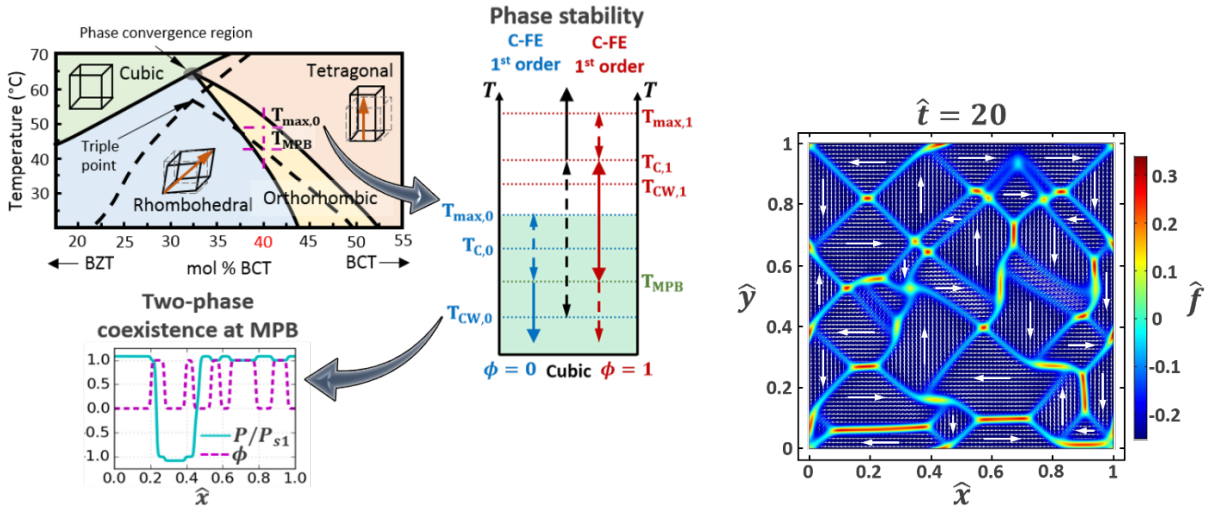

Figure 1. (left) Phase diagram, phase-stability analysis and 1-D domain configuration of BZT-BCT showing coexistence of tetragonal and rhombohedral FE phases near MPB, and (right) formation of FE domains in 2-D of a single-crystal material with tetragonal symmetry, with polarization vector superimposed on free energy distribution.

Biography

Oscar joined the group in 2015 as a PhD student after obtaining his MSc in Mechanical Engineering with a specialisation in Computational Thermo-sciences from La Universidad del Zulia (Venezuela). His master’s thesis was titled “Predicting Performance Curves of a Progressive Cavity Pump with Metallic Stator using Computational Simulation”. From 2007 to 2014, he worked as a Project Engineer for two engineering consultancy companies developing major projects in the petrochemical, power and oil & gas sectors in Venezuela. He moved to New Zealand to keep improving his professional and academic career in a prosperous, safe and family-friendly environment.

Email: oscar.torresmatheus@pg.canterbury.ac.nz