PhD Proposal 2017

School: CentraleSupélec	
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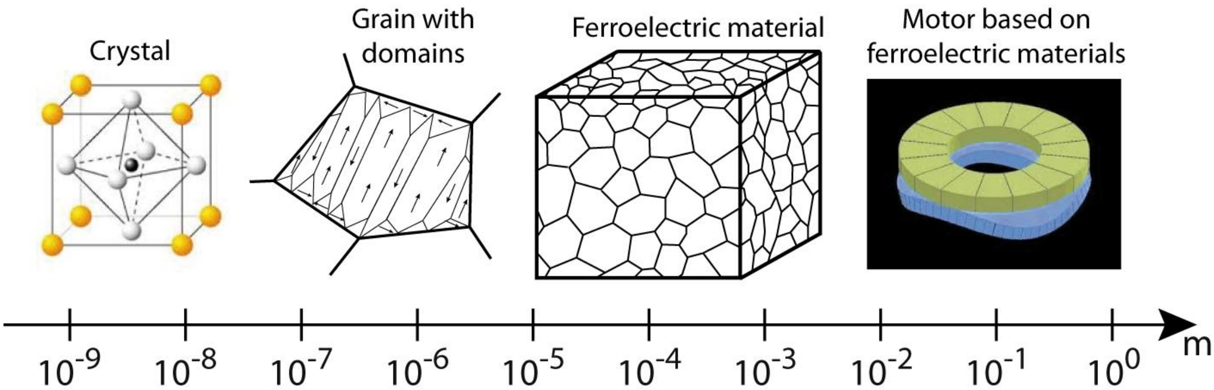
Title: Multi-Scale modelling of phase transition in ferroelectric materials
Scientific field: • **Engineering & Technology – Electrical, Electronic and Telecommunication Engineering** • **Natural & Life sciences - Material Sciences**
Key words: Piezoelectric materials, Multiscale approaches, Micromechanical models, Homogenization, Multi-physics, Phase transition, Domain switching, Nonlinear behavior, x-ray diffraction

<u>Details for the subject:</u>

Background, Context:

Ferroelectric ceramic materials are used extensively as dielectric and semi-conducting components, memory elements, and piezoelectric sensors, actuators and transducers. The coupling between electric and mechanical properties in ferroelectrics (notably the electric field induced strain) brings many opportunities for the design of innovative sensors and actuators. Automobile and aeronautic industry are exploring the replacement of some existing mechatronic devices by some "smart" devices based on ferroelectrics with the perspective to optimise weight and size.

In order to develop accurate design tools for these smart systems, considerable effort has been directed towards models that describe ferroelectric behaviour. They result in a wide range of modelling approaches to define the electromechanical response of a ferroelectric material submitted to an electromechanical loading. However, describing ferroelectric behaviour from the crystalline scale (smaller than nm) to the device scale (around cm or dm) is impossible to handle in classical numerical design tools such as Finite Element Models.



Multiscale models (also called micromechanical models) can be very useful to obtain the average behaviour of ferroelectrics based on the description of the physical mechanisms responsible for the macroscopic behaviour. These approaches can predict the macroscopic behaviour of heterogeneous materials based on a physical description of the behaviour at the crystal scale combined to statistical information about the microstructure. Scale transition rules are used to bridge the scales between the macroscopic and microscopic descriptions.

Research subject, work plan:

This thesis proposal is focused on Multi-Scale Modelling of ferroelectric materials. The work is based on an existing modelling tool to describe the constitutive behaviour of ferroelectric ceramics [1] combined with semi-analytical homogenization approaches to define the scale transition rules [2]. This tool is so far limited to the description of single phase materials, where most industrial materials are mixed phase.

A main objective of the project is to introduce phase heterogeneity in the existing model and to introduce a description of the mechanisms of phase transition under external loading. Indeed, the application of sufficient stress or electric field can induce a change in the relative proportions of existing phases [3]. This phase transition can be used to enhance the performance of the final device.

The modelling results will be compared to experimental data from lab macroscopic characterisation measurements but also from x-ray diffraction results obtained at Synchrotron facilities. Indeed, x-ray diffraction is a powerful tool to observe phase transitions and domain switching in ferroelectrics. It can provide a very strict validation approach to assess the performance of multiscale approaches. For that purpose, the prediction of x-ray diffraction patterns obtained on ferroelectric materials subjected to electro-mechanical behaviour will be included in the modelling output.

References:

[1] L. Daniel, D.A. Hall, P.J. Withers: A multiscale model for reversible ferroelectric behaviour of polycrystalline ceramics, Mechanics of Materials, 71:85-100 (2014).

[2] R. Corcolle, L. Daniel, F. Bouillault: Generic formalism for homogenization of coupled behavior: Application to magnetoelectroelastic behavior, Physical Review B, 78(21):214110 (2008).

[3] C. Chen *et al.*, Giant strain and electric-field-induced phase transition in lead-free $(Na_{0.5}Bi_{0.5})TiO_3$-$BaTiO_3$-$(K_{0.5}Na_{0.5})NbO_3$ single crystal, Applied Physics Letters, 108, 022903 (2016).