## Stage Master 2- 2024

## "Simulations of the influence of domain walls on the thermal conductivity in ferroelectric and ferroelastic materials"

Supervisors:
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**Deadline to apply: 15 November 2023**

Electronic switches and diodes, which can control electron flows, are key components in modern electronics. Their equivalents for heat flows are more challenging to obtain because phonons conducting heat are difficult to control. Yet, if efficient thermal switches and diodes were made, they would play a significant role in improving the energy efficiency of solid-state devices. Recently, domain walls in ferroelectric and ferroelastic materials have been proposed to tune the thermal conductivity in solid materials (Fig. 1). In general, **the atomic structure of interfaces (roughness, asperity, interphases etc) and its related interfacial thermal resistance controls the thermal conductivity in nanomaterials** [1,2] and in certain cases is the reason of the appearance of exotic properties, as thermal rectification [3], phonon ballisticity [4] or hydrodynamic regime [5].

Ferroelectric (respectively ferroelastic) materials spontaneously exhibit regions of uniform electric polarization (respectively strain), called domains. They are separated by planar defects known as domain walls [6]. The number of domains and their orientations can be controlled by applying an electric field (respectively a stress field) [7]. Experimentally, it has been shown that **domain walls can strongly reduce the thermal conductivity of materials** [8]. For instance, at room temperature, the thermal conductivity of thin films of $PbTiO_3$ can be divided by up to 3 when the number of domain walls is increased [9]. However, mechanisms governing the interaction between phonons and domain walls are still unclear.

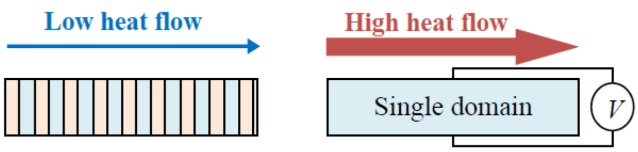


*Figure 1. Schematic of the influence of domain walls on the thermal conductivity.*

Calculations have been performed to clarify the behaviour of phonons near domain walls. First-principles calculations show variations in thermal conductivity when the density of domain walls is modified by applying an electric field [10,11]. In a ferroelastic material, nonequilibrium molecular dynamics simulations reveal that the thermal conductivity decreases linearly with the number of domain walls orthogonal to the direction of heat flow [12]. The thermal boundary resistance of 180° domain walls has also been assessed within the numerical formalisms of nonequilibrium molecular dynamics and nonequilibrium Green's functions [13].

Here, we propose to **investigate several parameters that could influence the thermal conductivity in prototypical ferroelectrics ($PbTiO_3$, $BaTiO_3$) and ferroelastics ($LaAlO_3$)**: number of domain walls, direction of the domain walls with respect to the heat flow, roughness and thickness of the domain walls, presence of dopants/defects at domain walls, influence of temperature.

This master thesis opens to nanotechnologies/nanosciences and to atomistic simulations.

**Purpose of the internship:** Learning the LAMMPS molecular dynamics code and a numerical code of wave propagation in a solid. This will involve understanding the physical mechanisms and comparing the results obtained with experimental results.
**Work to be done:** Understanding the concept of ferroelectric and ferroelastic materials and how to calculate their thermal properties; handling an already existing open-source code (LAMMPS) and final report.
**Internship gratification:** In accordance with the rules of INSA of Lyon
**Location:** CETHIL laboratory at INSA of Lyon, 9 Rue de la Physique, 69100 Villeurbanne
**Dates/duration:** Starting date the latest 1st of March, 5 to 6 months
**Contact:** konstantinos.termentzidis@insa-lyon.fr et guillaume.nataf@univ-tours.fr
**Framework:** OpenLabs INSA, Possibility of pursuing a thesis

**CETHIL**: CETHIL's research covers the fields of thermal energy and its application to various energy systems. This involves understanding the phenomena governing heat transfers as well as their couplings, at different length, time, or temperature scales and by all transfer modes (convection, conduction, radiation, phase change).

**GREMAN**: GREMAN is a laboratory specialized in materials, microelectronics, acoustics and nanotechnology, part of University of Tours, CNRS and INSA Centre-Val de Loire. The master project is complementary to the ERC Starting Grant DYNAMHEAT on “Ferroic Materials for Dynamic Heat Flow Control”.

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