Stage Master 2 - 2025

Molecular dynamics simulations of the influence of domain walls on the thermal conductivity in barium titanate

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Deadline to apply: 1st December 2024

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 [1]. 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 ferroelectrics 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** [2,3] and in certain cases is the reason of the appearance of exotic properties, such as thermal rectification [4], phonon ballisticity [5] or hydrodynamic regime [6].

Ferroelectric materials spontaneously exhibit regions of uniform electric polarization, called domains. They are separated by planar defects known as domain walls [7]. The number of domains and their orientations can be controlled by applying an electric field [8]. Experimentally, it has been shown that **domain walls can strongly reduce the thermal conductivity of materials** [9]. However, mechanisms governing the interaction between phonons and domain walls are still unclear.

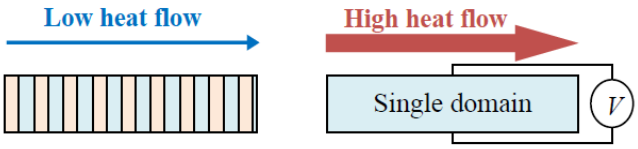

Figure 1. Schematic of the influence of domain walls on the thermal conductivity.

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]. Nonequilibrium molecular dynamics simulations reveal that the thermal conductivity decreases linearly with the number of domain walls orthogonal to the direction of heat flow [11]. 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 [12].

Here, we propose to **investigate several parameters that could influence the thermal conductivity in the prototypical ferroelectric $BaTiO_3$**: 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. The topic **is a continuation of a previous successful internship where preliminary calculations were performed.**

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 materials and how to calculate their thermal properties; handling an already existing open-source code (LAMMPS) and final report.
Internship gratification: 4.35€/hour (around 600€ per month).
Location: University of Tours, Parc Grandmont, 31 Av. Monge, 37200 Tours
Dates/duration: Starting in February-March 2025, 5 to 6 months
Framework: OpenLabs INSA

How to apply?

Prospective candidates should send their CV and a cover letter by email **before the 1st of December to**: guillaume.nataf@univ-tours.fr, konstantinos.termentzidis@insa-lyon.fr, yves.lansac@univ-tours.fr, yhjang@dgist.ac.kr

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