Introduction

Responsable : Samy Merabia

Laboratoire : Institut Lumière Matière, CNRS et Université Lyon I

E-mail : samy.merabia@univ-lyon1,fr

Durée du module : 1h30

Objectifs

Provide some theoretical elements to understand phonon dynamics in nanostructured materials- Illustrate the versatility of molecular dynamics simulations to address interfacial energy transport.

Contenu – programme

Minimizing the lattice thermal conductivity is a bona-fide challenge for the design of thermoelectric materials. This goal may be achieved either through the consideration of complex materials including clatrates ; alternately, nanostructuring the materials may help in a substantial reduction of the lattice conductivity, as superlattices for instance. In all cases, the mechanisms at the origin of the reduction of the conductivity remain partly understood. The aim of this short course is to illustrate how molecular dynamics simulations may help in a fundamental understanding of the relevant mechanisms, which in turn may help in conceiving materials displaying low conductivity.

To start with, we will provide some theoretical elements concerning lattice thermal conductivity. We will first review the analysis of thermal conductivity in crystals by Maradudin, and present the phenomenological models describing phonon-phonon scattering (Callaway and Holland models).

This general presentation will serve to introduce the molecular dynamics simulation technique, that will be illustrated first in the determination of the lattice thermal conductivity of bulk materials. The advantages of the different methods-non-equilibrium and equilibrium will be briefly addressed. We will also illustrate the possibility to perform phonon spectroscopy on relatively simple systems.

In the last part of this course, we will put emphasis on the description of interfacial energy transport : phonons are partially reflected or transmitted by an interface, which provides a finite thermal boundary resistance, which can lead to a reduction of the overall thermal conductivity. Despite decades of research, the origin of this resistance is still unknown. We will discuss how molecular dynamics simulations may give clue to a microscopic description of phonon interfacial transmission. We will conclude by outlining some open problems.