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msm

BSc Project

Design of efficient nano-thermal rectifier using MD simulations

Thermal rectification of heat at the nano/micro-scale would enable novel ways of thermal management with key applications in electronic cooling, heat logic and/or energy harvesting. A thermal rectifier is the heat analogous to an electrical diode, meaning that it conducts heat in one direction better than in the other. However, the design of these rectifiers is hindered by the complex physics of heat conduction, and current available thermal diodes roughly reach rectification ratios that are suitable for application.

The design of new structures is key to obtain a breakthrough in reliable thermal rectification. Since the experimental investigation of novel structures is time consuming and the transport phenomena at nanoscale is difficult to predict in advance, we propose to use Molecular dynamics (MD) simulations to understand the phenomenon of thermal rectification and to virtually design devices with maximum rectification ratio.

Goal: Identify the optimal geometry of **graphene-based nanostructures** in terms of thermal rectification efficiency using MD simulations.

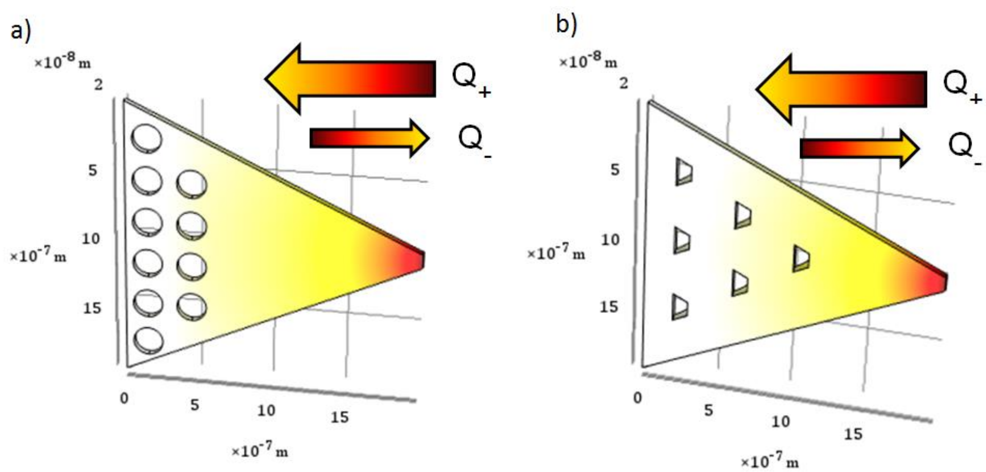

Figure 1. Sketches of possible defected triangular shaped graphene sheets with expected thermal rectification. a) symmetrical pore region at one end, b) asymmetrical pores along the structure.

Method: Because of its unique thermal and structural features, graphene, a one-atom-thick carbon-based membrane, presents high promises in achieving high thermal rectification efficiency. Non-equilibrium MD simulations will be used to study the thermal conduction of triangular-shaped graphene structures of different geometries with the presence of a broad spectrum of defects at different positions and with different sizes (**Figure 1**). Thermal rectification will be correlated to the geometrical properties of the graphene structure, allowing to identify the best design that ensures the highest rectification factor. The developed model can subsequently be used as a base for similar simulations in the future.

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