RESEARCH SUBJECT TITLE: “Simulations of thermal properties of novel 1-2-3D nanomaterials based on graphene allotropes”

Name of the laboratory: CETHIL UMR5008, Website: https://cethil.insa-lyon.fr/

Name of the research team: MiNT (Micro et NanoThermique)

Name of the supervisor: Konstantinos TERMENTZIDIS
University / Institution: INSA of Lyon, CNRS Research Director
E-mail adresse: konstantinos.termentzidis@insa-lyon.fr
Doctoral School: MEGA (ED 162) - Mécanique, énergétique, génie civil, acoustique
Lab Language: English or French
Minimum language level required:

- English: reading/writing/speaking C1
- French: speaking B2
- Other:

Abstract:

The thermal conductivity in nanostructures and nanosctructured materials is not any more an extrinsic property of the material but depends strongly on size and the presence of interfaces, defects, doping, native oxides, amorphisation etc. The subject has attracted the scientific interest the two last decades [1-2] and continues to intrigate the scientific community specially with the appearence of new phenomena beyond the diffusive Fourier law; the latter fails to predict the thermal properties of nanomaterials. Parallel to that, the rapid evolution of the elaboration and fonctionalisation methods to produce a variety of graphene allotropes give us now the opportunity to go beyond the "graphene era": we can now propose new 1D; 2D and even 3D nanoarchitectured materials based on graphene and its allotropes with tuned physical properties.

The aim of the current PhD thesis is to study by the use of atomistic simulations (molecular dynamics simulations and wave packet propagation) the thermal properties of mechanical stressed or relaxed nanostructured materials based on graphene [3,4], biphenylene [5], amorphous graphene, diamene or 2D diamond [6,7] or a plethora of other 2D graphene allotropes as seen in figure-1. These allotropes will be studied seperately or combined in one nanostructure with purpose to examine and design materials with tailored physical properties.

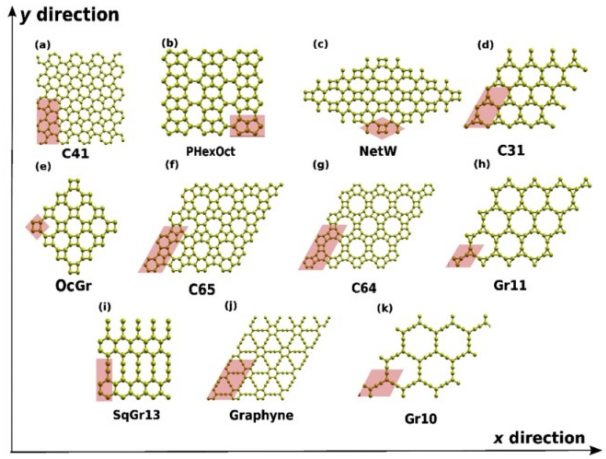

Figure-1 : *Atomic topologies of several graphene allotropes. The periodic unit cells are highlighted in pink. (a) to (h) contain only sp2 bond, while (i) to (k) contain both sp and sp 2 bonds. Figure taken by Carbon 110, 443 (2016)[8]*

The interest of this PhD subject is both fundamental : appearence of collective phonon modes, hydro-thermodynamics regime of heat transport [9] and thermal interference (see figure-2) [10] or rectification [11,12] as well applicative interest : heat dissipation and thermal management in next generation electronic circuits or the developement of novel phononic

devices. The goal is to understand the lateral and vertical phonon transfer in these 2D pristine graphene allotropes, but also combine them to obtain a 3D nanoarchitectured structures by calculating their thermal transport properties in order to proposed materials with thermal properties by design. The wave propagation (exemple in fig.2) will be also used to examine the spectral and polarisation decomposition impact on the heat dissipation.

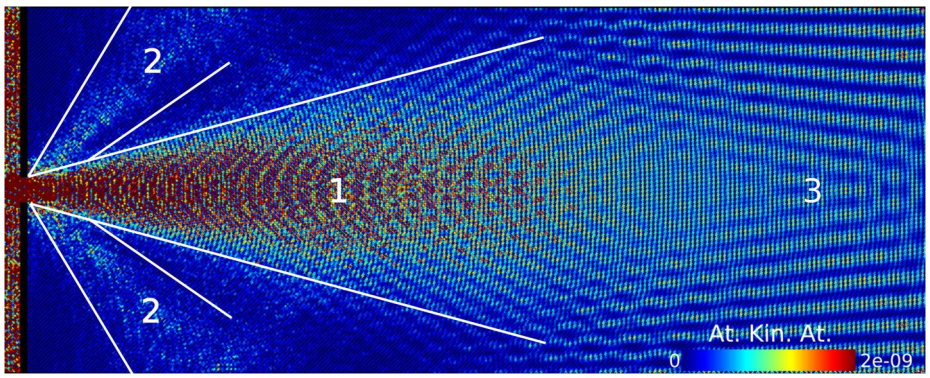

Figure-2 : *Visualization of diffraction of a 6 THz continuous longitudinal plane wave by an aperture of a width of 3 nm using a void barrier. The color scale represents the kinetic energy per atom in eV (taken from ref[10]).*

The PhD candidate will be fully incorporated into the MiNT group, offering a unique opportunity to interact with French national, European and International teams working on Micro and Nano thermal transport as well Energy and Nanomaterials.
Applicants need to have a solid base in Engineering, Physics, Nanotechnology or Material Science and good programming skills. The knowledge of Molecular Dynamics Simulations is not mandatory, nevertheless priority will be given to candidates with backround in atomistic simulations.

Expected duration of the thesis: 42 months

References:
[1] D. Cahill, J. Applied Physics **93**, 793, 2003
[2] D. Cahill et al, Applied Physics Reviews **1** ,011305, 2014
[3] A. Balandin, Nature Materials **10**, 569, 2011
[4] Y. Han et al, RSC Adv., 12, 22581-22589 (2022)
[5] X. Zhang et al, J. Phys. Chem. C 128, 13, 5632–5643 (2024)
[6] Y. Gao, et al, Nature Nanotech 13, 133 (2018)
[7] P. Sorokin and B. Yakobson, Nano Lett. 21, 5475 (2021)
[8] H. Sun et al, Carbon 110, 443 (2016)
[9] P. Desmarchelier et al, Intern. J. Heat and Mass Transfer 194, 123003 (2022)
[10] P. Desmarchelier et al, J. Applied Physics 135(1), 015103 (2024)
[11] H. Wang et al, Nature Communications **8**, 15843, 2017
[12] P. Desmarchelier, A. Tanguy and K. Termentzidis, Phys. Rev. B 103, 014202 (2021)