Research Internship for 2020-21

Laboratory:
Centre de Nanosciences et Nanotechnologie (C2N),
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Monte Carlo Simulation of static and dynamic thermal properties of nanostructures

Scientific Context

Nanostructures and in particular nanowires have acquired in the last years a prominent role in several cutting-edge researches and could be used in particular as a material for **renewable energy** [1].
As the Fourier heat equation does not rigorously describe the thermal transport at the nanoscale due to the occurrence of out of equilibrium phenomena, we have developed a unique **home-made Monte Carlo simulator** based on the Boltzmann's transport equation for phonons. Our advanced simulator specifically developed to the nanoscale includes a Full-band description of the material properties (dispersion cf. Fig. 2 and scattering rates) that are parametrized by using ab-initio calculations [3] [4].
An internship position is available in the **COMputationnal electronICS group** which aims to **investigate the nanoscale heat transfer** by using our ab-initio Monte Carlo Simulator.

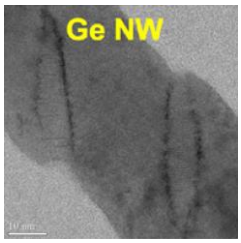

Fig. 1. Ge polytype nanowire designed at C2N [2] including many interfaces

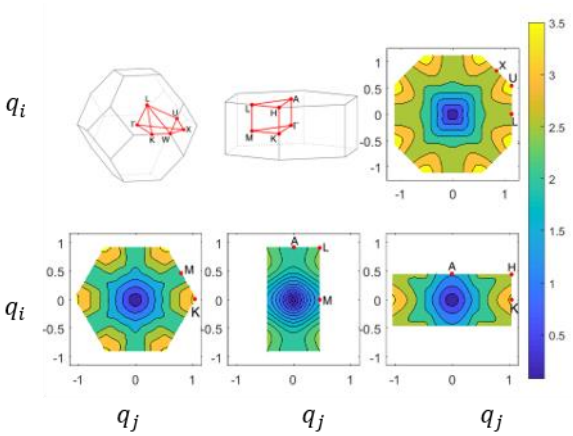

Fig. 2. Cartography of the angular frequency ω in the BZ. Wave vectors qi,j are in [10^10 2π/m]. Schema of the BZ in (a) Si3C, (b) Si2H. Isoenergies in (c)the (110) plane of Si3C, (d),(e),(f) in planes of Si2H

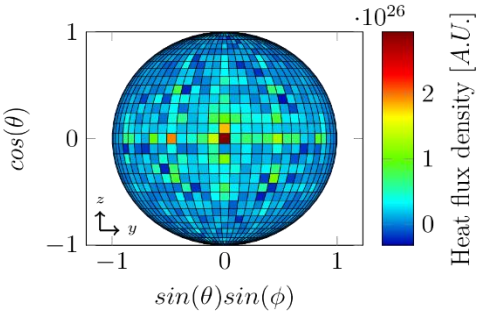

Fig. 3. Angular phonon distribution of heat flux in hexagonal Si

Methodology and objectives

The internship has 3 objectives:

- **(i)** Using the available code to study the thermal transport across single interfaces [5] between different materials/phase,
- **(ii)** Computing the static and transient thermal properties of polytype nanowires (cf. fig 1) with a realistic geometry,
- **(iii)** Making comparison between theoretical and experimental results.

Skills learned during the thesis

The student will acquire a broad range of skills: in solid state physics (phonon transport, band structure, phonon spectrum, electron-phonon interaction and phonon-phonon interaction), technology devices, and scientific programming (Fortran and/or C/C++, Matlab).

Besides, the results that would be obtained during this internship could be easily published in scientific journals. This internship could be a relevant preliminary work for pursuing a Phd thesis in our group.

Candidate's Profile

Candidates must be at least in the first year of the Master program in Physics, Electronics, Materials Science or related disciplines. We are seeking creative and highly motivated individuals well trained and skilled in scientific research. Programming experience is also desirable, but not mandatory.

Please join a CV, a list of courses that you have followed and results of exams in the framework of your master program, and any other information that you judge useful.

References:

[1] Vineis, C. J., Shakouri, A. , Majumdar, A. and Kanatzidis, M. G. (2010), Nanostructured Thermoelectrics: Big Efficiency Gains from Small Features. Adv. Mater., 22: 3970-3980. doi:10.1002/adma.201000839

[2] L. Vincent, et al., Novel Heterostructured Ge Nanowires Based on Polytype Transformation, Nano Lett., 14 (8), pp 4828–4836 (2014)

[3] Davier, B., Larroque, J., Dollfus, P., Chaput, L., Volz, S., Lacroix, D., & Saint-Martin, J. Heat transfer in rough nanofilms and nanowires using Full Band Ab Initio Monte Carlo simulation. Journal of Physics: Condensed Matter, 30(49), 495902 (2018)

[4] Chaput, L., Larroque, J., Dollfus, P., Saint-Martin, J., & Lacroix, D. (2018). Ab initio based calculations of the thermal conductivity at the micron scale. Applied Physics Letters, 112(3), 033104.

[5] Larroque, J., Dollfus, P., & Saint-Martin, J. (2018). Phonon transmission at Si/Ge and polytypic Ge interfaces using full-band mismatch based models. Journal of Applied Physics, 123(2), 025702.