SCIENCES SORBONNE UNIVERSITÉ

2021-2022

Master thesis proposal

Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie

Campus Pierre et Marie Curie
Tower 23 - 4th floor -23-22
Director: A. Marco Saitta

Title: Phonons properties of the recently discovered allotrope of silicon Si_{24}

Keywords: Novel material, optoelectronics, photovoltaic, silicon, picosecond laser acoustics, Raman scattering, high pressure, diamond anvil cell.

Scientific description:

Si_{24}, a recently discovered allotrope of silicon, possesses a (quasi) direct band gap near 1.3 eV, say a high potential to transform silicon-based optoelectronics including solar energy conversion. Up to now, the lack of large, pure crystals has prevented the characterization of intrinsic properties and has delayed deposition-based metastable growth efforts. Very recently, our team report an optimized high pressure high temperature synthesis methodology for single-crystalline Si_{24} with crystals approaching the millimeter-size scale. Pure single-crystal of Si_{24} can be actually recovered from HP synthesis at room temperature using Na_4Si_{24} as precursor, where the sodium is completely removed from the structure by heating under vacuum. Contrary to diamond-structured silicon, this new Si_{24} allotrope has a porous, zeolite-like structure, with "channels" running through the entire structure. The two gaps, direct and indirect, of this silicon are very close ("quasi-direct" gap of about 1.35 eV), allowing the desired range for solar absorption which had never been achieved before. Si_{24} is also stable at room pressure up to 720 K, even in air. However, nothing is known about the elastic properties of this new orthorhombic silicon, neither about its structural stability or equation of state at HP and HT. The main goal of this internship will be to actively participate to a session of picosecond acoustics measurements, a quite new technics allowing the determination of the elastic constants of single-crystalline sample using a pump-probe optical (femtosecond laser) set-up. High pressure acoustics and Raman scattering experiments are also scheduled in order to check the stability of this new material under high strain.
This internship is conceived as the first part of a longer and more complete work on the quantitative description of the structural and dynamic properties of this new material with high technological potential. It is therefore particularly suitable for M2 students who wish to work in the field of experimental solid state physics with the project to continue in thesis.

Techniques/methods in use: Picosecond laser acoustics, diamond anvil cell, Raman.
Applicant skills: experimentalist
Industrial partnership: Not yet

Internship supervisor(s)
Frederic.decremps@sorbonne-universite..fr
yann.le_godec@sorbonne-universite.fr
oleksandr.kurakevych@sorbonne-universite.fr

Internship location: IMPMC (13/23, étage 3)
Possibility for a Doctoral thesis: Yes