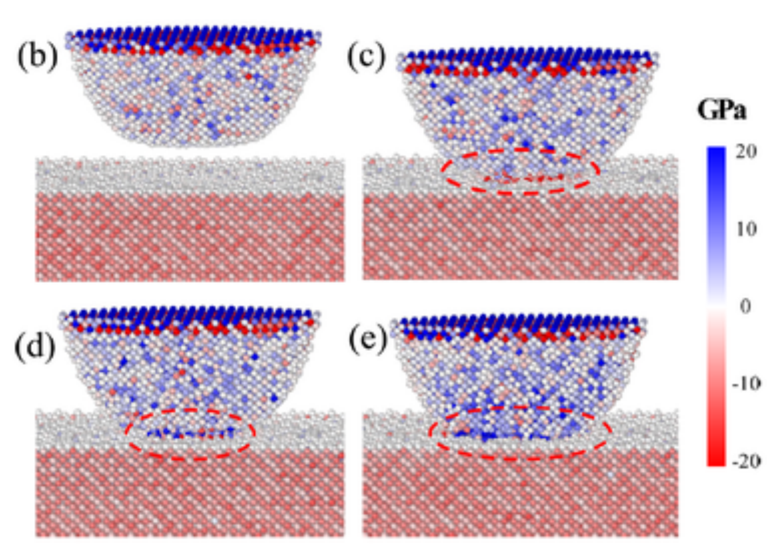
ATOMISTIC MODELLING INTERFACIAL PHONON TRANSPORT AT NANOCONTACTS

LABORATORY : Institut Lumière Matière

TEAM(S) : MMCI
ENERGIE

KEYWORD(S) : Atomistic Simulations / phonon dynamics / nanoscale thermal transport

SCIENTIFIC CONTEXT :



Atomistic simulations of the contact between a hot tip and a substrate.

Thermal transport at the nanoscale is vital for thermal management of modern electronic devices. At the nanometer length scales, heat dissipation is dominated by phonon transmission at interfaces. Interfaces at the nanoscale, are not perfect and characterized by asperities, roughness, etc. These imperfections even complicate the theoretical treatment of interfacial heat transport as their sizes may be smaller than phonon mean free path characterizing vibrations of the substrate atoms. The situation may be more complex when the substrate is amorphous, as phonons may coexist with localized excitations in amorphous materials [1]. Recent atomistic simulations performed in the group [1] showed that amorphizing an interface help enhance phonon transmission, but the exact mechanisms are still poorly understood and the transfer to nanocontacts has not yet been explored. Normal loading may also have an large effect on heat transfer

MISSIONS :

The student will investigate the thermal transport properties of nanocontacts between a metal and an amorphous substrate. Molecular dynamics (MD) and ab-initio DFT calculations will be employed to compute local heat flux and phonon transmission across these contacts [1,2]. The successful candidate should hold a Master degree in Physics, Physical Chemistry or Material Science. He/she should have knowledge and a taste for solid state physics (phonons), modeling and basic programming (fortran or C or python). Good communication skills and english writing are requested. The phD student will work at the Institute Lumière Matière (ILM) in Lyon, under the supervision of C. Adessi (UCBL prof.) and S. Merabia (CNRS) and in collaboration with K. Termentzids (CNRS, CETHIL Lyon). He/she will also interact with our experimentalist colleagues at INSA (S. Gomès) and at ILM (P. Vincent). Interest candidates should send an email along with a resume to Christophe Adessi (christophe.adessi@univ-lyon1.fr) and Samy Merabia (samy.merabia@univ-lyon1.fr).

OUTLOOKS :

Informal enquiries are welcome.

BIBLIOGRAPHY :

[1] J El Hajj, C Adessi, M de San Feliciano, G Ledoux, S Merabia, Enhanced thermal conductance at interfaces between gold and amorphous silicon and between gold and amorphous silica, Physical Review B 110 (2024), 115437

[2] P Mirchi, C Adessi, S Merabia, A Rajabpour, Lattice thermal conductivity and mechanical properties of the single-layer penta-NiN 2 explored by a deep-learning interatomic potential, Phys. Chem. Chem. Phys. 26 (2024), 14216-14227

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