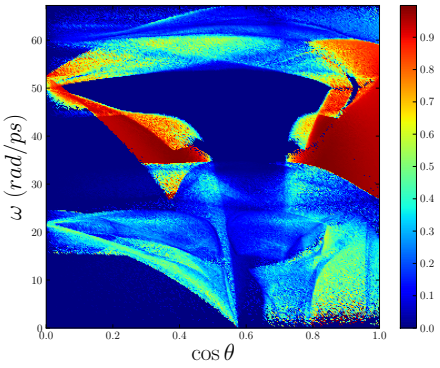
Thermal transmission at solid interfaces and across nanoscale vacuum gap : ab initio lattice dynamics calculation

A. Alkurdi[12] & S. Merabia[1]

[1] *Institut Lumière Matière, UMR5306 Université Claude Bernard Lyon 1-CNRS, Université de Lyon 69622 Villeurbanne Cedex, France*

[2] *Faculty of Sciences, Al-Baath University, P.B. 77, Homs, Syria*

Interfacial thermal conductance is of a great importance for many applications where thermal management at nanoscale is a vital issue [1]. In microelectronics for instance, there is a strong need to know how energy can be exchanged at separation distance of few nanometers where heat is primarily exchanged by acoustic waves for sub-nanometric gaps [2].



(Color inline) Phonon energy transmission at Si/heavy Si interface over all frequencies and transmission angle.

In this communication, we have performed lattice dynamics calculations on solid/solid interfaces using *ab initio* interatomic force constants [3] to predict interfacial phonon transmission as a function of both phonon frequency and wavevector. A spectral and angular analysis have been done to quantify the contribution of each phonon mode in a given scattering direction. The effect of bonding was studied at Si/Ge interface as well as the effect of the acoustic contrast at Si/heavy Si interface. Our results show that, in general, the transmitted thermal energy is not uniformly distributed over frequency and angle of transmission. In addition, we found that there is no critical angle but a spectral analysis of phonon transmission reveals a critical angle depending on the frequency. This can be used to devise high pass phonon filter via changing the orientation of the interface. In the case where the two solids separated by a nanometer scale gap, we also predict the influence of phonon tunneling mediated by evanescent waves.

1. D. G. Cahill *et al* *Appl. Phys. Rev.* **1** 011305, 2014
2. V. Chiloyan, J. Garg, K. Esfarjani and G. Chen *Nature Communications* **6** 6755 (2015)
3. M. Aouissi, I. Hamdi, N. Meskini and A. Qteish, *Phys. Rev.* B **74** 054302 (2006)