Ultra-thin silicon membranes and silicon nanowires as nanophononic and thermoelectric devices

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Engineering silicon at the nanoscale paves the way to new applications of this cheap, abundant, and technologically and environmentally friendly material. Transistors in nanoelectronics have reached the 10 nm size limit, implying very high density but also critical issues regarding heat dissipation. The fabrication of crystalline silicon nanowires and ultra-thin silicon membranes with characteristic size of the order of 10 nm or less gives rise to thermal and electronic properties that enable the use of silicon as a low-temperature thermoelectric material for sensing and energy harvesting. At the same time, nanowires, thin films and membranes can be potentially employed as the basic platform to develop nano-resonators, phononic crystals or metamaterials, with a variety of applications. It follows that an efficient exploitation of nanoscale silicon stems from a better understanding of its electronic, phononic and thermal properties, and especially on the impact of confinement and surfaces.

In this work we unravel the effect of dimensionality reduction and the prominent role of surface structure and surface resonances in tuning the phonon dispersion relations and the thermal conductivity of silicon nanostructures, including ultrathin membranes [1], [2] and silicon nanowires [3], [4]. In particular we show how surface roughness and surface oxidation affect phonon transport in silicon nanostructures, reducing dramatically their thermal conductivity 1. We also compute the electronic properties of silicon membranes as a function of thickness and the concentration of dopants, identifying the conditions that maximize the thermoelectric figure of merit, both for periodic extended materials and for open systems in device configuration.

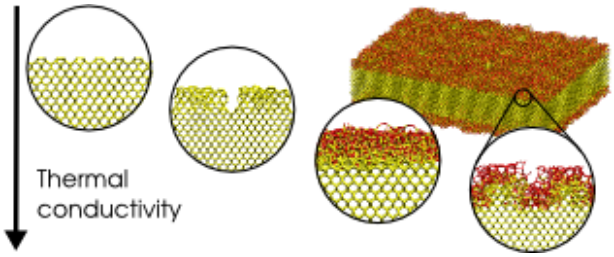

Fig. 1. Atomistic models of crystalline, rough and surface oxidized silicon membranes, for which we have compute phonon dispersion relations, thermal conductivity and phonon mean free paths.

A combination of large scale molecular dynamics, lattice dynamics and electronic structure calculations provide parameter–free recipes to optimize materials for thermoelectric, nanoelectronic and phononic applications. Indeed from these calculations we envisage strategies to finely tune silicon membranes to further improve their thermoelectric performances.

Acknowledgment

This work has been supported by the European Commission FP7-ENERGY-FET project MERGING, contract number 309150.

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ISBN 978-0-692-50554-0