Hierarchical nanostructured materials for phonon control and thermoelectric applications.

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Among the possible routes proposed to design materials with tailored phononic and thermal properties hierarchical nanostructuring displays a vast potential, especially for thermoelectric energy conversion, with unprecedented efficiency[1]. In fact, introducing different types of phonon scatterers , from the atomic scale to the nano- and meso-scale leads to an effective reduction of the thermal conductivity of materials.

Here we propose, by means of atomistic simulations, two different way to exploit the hierarchical nanostructuring, to improve the thermoelectric performance of bulk PbSe and of ultra-thin Silicon membranes. In the case of PbSe we propose an effective way of generating a broad distribution of grains (Fig.1) that scatter phonons over the whole frequency spectrum. For Si membranes, we elucidate the role of dimensionality reduction, alloying and surface nanopatterning [2] in tuning their phonon dispersion relations and thermal conductivity.

For both systems we provide a detailed mechanistic explanation of the effect of nanostructuring on phonon transport, proposing design rules and fabrication processes for enhanced thermoelectric performances.

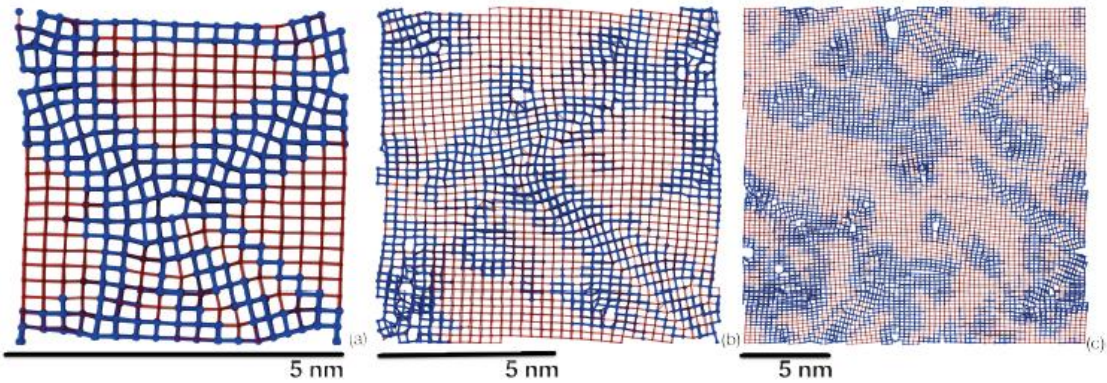

Fig 1 : Different scales of grain size distributions in PbSe

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(2) Davis, B. L.; Hussein, M. I. Nanophononic Metamaterial: Thermal Conductivity Reduction by Local Resonance. *Phys. Rev. Lett.* **2014**, *112*, 055505.