Huge reduction of heat conduction observed in flat silicon channels

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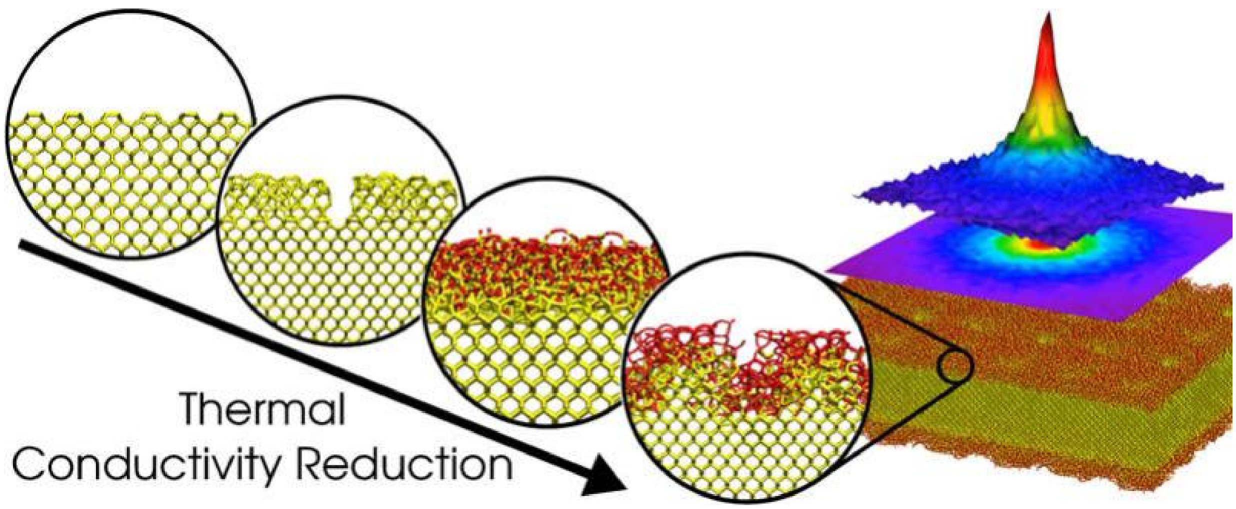

The different circles represent the studied surfaces of the Si membranes: crystalline, rough, flat with native SiO_2, and rough with native SiO_2. The right image shows a representative thermal map on the membranes upon a localized thermal excitation used to measure the thermal conductivity.

Combining state-of-the-art realistic atomistic modelling and experiments, a new paper describes how thermal conductivity of an ultrathin silicon membrane is controlled to a large extent by the structure and the chemical composition of the surface. A detailed understanding of the connections of fabrication and processing to structural and thermal properties of low-dimensional nanostructures is essential to design materials and devices for phononics, nanoscale thermal management, and thermoelectric applications.

The ability of materials to conduct heat is a concept that we are all familiar with from everyday life. The modern story of thermal transport dates back to 1822 when the brilliant French physicist Jean-Baptiste Joseph Fourier published his book "Théorie analytique de la chaleur" ("The Analytic Theory of Heat"), which became a corner stone of heat transport. He pointed out that the thermal conductivity, i.e., ratio of the heat flux to the temperature gradient, is an intrinsic property of the material itself.

The advent of nanotechnology, where the rules of classical physics gradually fail as the dimensions shrink, is challenging Fourier's theory of heat in several ways. A paper published in *ACS Nano* and led by researchers from the Max Planck Institute for Polymer Research (Germany), the Catalan Institute of Nanoscience and Nanotechnology (ICN2) at the campus of the Universitat Autònoma de Barcelona (UAB) (Spain) and the VTT Technical Research Centre of Finland (Finland) describes how the nanometre-scale topology and the chemical composition of the surface control the thermal conductivity of ultrathin silicon membranes. The work was funded by the European Project Membrane-based phonon engineering for energy harvesting (MERGING).

The results show that the thermal conductivity of silicon membranes thinner than 10 nm is 25 times lower than that of bulk crystalline silicon and is controlled to a large extent by the structure and the chemical composition of their surface. Combining state-of-the-art realistic atomistic modelling, sophisticated fabrication techniques, new measurement approaches and state-of-the-art parameter-free modelling, researchers unravelled the role of surface oxidation in determining the scattering of quantized lattice vibrations (phonons), which are the main heat carriers in silicon.

Both experiments and modelling showed that removing the native oxide improves the thermal conductivity of silicon nanostructures by almost a factor of two, while successive partial re-oxidation lowers it again. Large-scale molecular dynamics simulations with up to 1,000,000 atoms allowed the researchers to quantify the relative contributions to the reduction of the thermal conductivity arising from the presence of native SiO_2 and from the dimensionality reduction evaluated for a model with perfectly specular surfaces.

Silicon is the material of choice for almost all electronic-related applications, where characteristic dimensions below 10 nm have been reached, e.g. in FinFET transistors, and heat dissipation control becomes essential for their optimum performance. While the lowering of thermal conductivity induced by oxide layers is detrimental to heat spread in nanoelectronic devices, it will turn useful for thermoelectric energy harvesting, where efficiency relies on avoiding heat exchange across the active part of the device.

The chemical nature of surfaces, therefore, emerges as a new key parameter for improving the performance of Si-based electronic and thermoelectric nanodevices, as well as of that of nanomechanical resonators (NEMS). This work opens new possibilities for novel thermal experiments and designs directed to manipulate heat at such scales.

More information: "Tuning Thermal Transport in Ultrathin Silicon Membranes by Surface Nanoscale Engineering." *ACS Nano*. DOI: 10.1021/nn506792d

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