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Atomistic Simulations of Heat Transport in Silicon Nanowires[1]

DAVIDE DONADIO, University of California Davis

Silicon is one of the best known materials of our age, cheap and readily available, being the basic constituent of semiconductor electronics. It would therefore be highly desirable to broaden its utilization for, e.g. renewable energy applications. Recently, it has been proposed that Silicon may be engineered to be an efficient thermoelectric material for use in solid state devices. Although a rather inefficient thermoelectric in its bulk form, at the nanoscale Si may become a poor heat conductor, while retaining good electronic conduction properties, and thus exhibit high efficiency in converting heat into electric current. However the fundamental reasons for the reported low heat conduction in Si nanowires (NW) are not yet understood, and different interpretations has so far appeared in the literature. Here we present atomistic simulations of heat conduction in Si NW of 1 to 3 nm diameter. Our results show that, depending on their surface structure, these wires may exhibit values of the thermal conductivity varying by two orders of magnitude, and as high as those of bulk Si. This clearly indicates that the increased surface to bulk ratio at the nanoscale may be only partially responsible for the decreased thermal conductivity observed experimentally. We also find that diffusive, yet extended, vibrational modes present in the case of wires with amorphous surfaces, are responsible for a dramatic decrease of a factor of 100 in the conductivity of purely crystalline NWs. Our findings suggest ways of engineering wires with even lower thermal conductivity, by increasing surface disorder, in particular by alloying Si with, e.g. Ge at the crystalline-amorphous interface.

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