Crystalline silicon that conducts heat like a glass

Silicon nanowires as efficient thermoelectric materials, Nature 451, 1680 (2008)

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Enhanced thermoelectric performance of rough silicon nanowires, Nature 451, 1680 (2008)

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Thermoelectric materials can generate electricity from waste heat or be used as solid-state Peltier coolers. Large scale applications in both these promising areas are, to date, inhibited by too small material efficiencies. A good thermoelectric has high thermopower S, high electrical conductivity σ, but low thermal conductivity κ, – a challenging requirement since the three quantities are generally interdependent. However, in recent years, the field is undergoing a renaissance with the discovery of new ways to decouple the three quantities.

A beautiful example of such decoupled property tuning are the two above studies on silicon nanowires. Bulk silicon is a poor thermoelectric, its largest drawback being the very high thermal conductivity (which short circuits any temperature gradient across the material). Both above groups have shown how to suppress it without adveresely affecting the other two properties: instead of bulk silicon they used silicon nanowires. If the nanowire diameter is small enough (10 to 20 nm reached in Boukai et al., 50 nm in Hochbaum et al.)

the thermal conductivity is dramatically (up to 200-fold at 200 K) suppressed, close to the value for amorphous silicon. With much less effect on the electrical conductivity and on thermopower a thermoelectric figure of merit of $ZT = S^2 T\sigma/\kappa \approx 1$ at 200 K (Boukai et al.) and $ZT \approx 0.6$ at 300 K (Hochbaum et al.) is reached. It is not these ZT values which make the work so important but the very clear proof of principle that "phonon engineering" can work very efficiently.

Silicon nanowires cannot compete with the Bi_2Te_3/Sb_2Te_3 superlattice reported by Venkatasubramanian an coworkers in 2001 [Nature 413 (2001) 587]. 10 Å/50 Å thick p-type structures were reported to have a room temperature ZT of 2.4. This is about double the value of the best room temperature thermoelectric known till then, the p-type alloy $(Bi_2Te_3)_{0.25}(Sb_2Te_3)_{0.72}(Sb_2Se_3)_{0.03}$. Venkatasubramanian an coworkers argued that in high quality thin film superstructures the alloy scattering is weaker, leading to higher charge carrier mobilities. The mechanism for the reduced thermal conductivity in the superstructure remained unclear.

The new results on silicon shed much light on this situation. Both groups have shown experimentally that the reduction of the lateral dimension

- most dramatically affects the lattice thermal conductivity (suppresses it)
- is most efficient if the typical phonon mean free path is longer but the electron mean free path is shorter than this dimension

Of course more theoretical work is needed to better understand the underlying microscopic mechanisms.

Whether technical problems to use nanowires (or superlattice thin films) in real commercial devices can be overcome remains to be found out. In any case, "phonon engineering" appears as a highly promising route to bring materials of high power factor $S^2\sigma$, but too high thermal conductivity such as, e.g., Kondo insulating compounds, on the thermoelectric stage, – whether in nanoscopic or “internally structured” bulk form.