Thermal transport in thermoelectric materials: ab initio modelling of Time Domain Thermo Reflectance measurements

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Owing to limitations of energy resources and environmental issues, the necessity to use global energy sources more efficiently becomes critical. A promising way to convert waste heat directly into energy is using thermoelectric devices. A limitation to improve the performance of thermoelectric systems using bulk materials is due to the fact that it is difficult to obtain materials with high thermoelectric power factor and low thermal conductivity simultaneously. Nanostructured semiconductor materials can overcome this obstacle by increasing phonon scattering in a controlled way. Presently, nanoscale thermal characterization is a critical issue to analyse these nanomaterials.

An important problem is to theoretically interpret the measurements obtained by Time Domain Thermo Reflectance (TDTR). As pointed out by Koh and Cahill [1], frequency modulation of the laser pump may change the value of the measured thermal conductivity. This has been qualitatively interpreted in terms of a simplified two fluid model, but a quantitative model is still missing. In this talk I will present ab initio calculations aimed at providing a more detailed account of the physics behind frequency modulated TDTR measurements of SiGe thin films.

This work is developed at CEA-Liten energy harvesting laboratory. CEA-Liten gathers a multidisciplinary team investigating fundamental (theoretical modelling of nanomaterials) and applied (material and thermo generator manufacturing; heat exchanger design, power management) challenges towards competitive thermal energy harvesting industrial products.

[1] Y.K. Koh and D. Cahill, PRB **76**, 075207 (2007)