Unified Model for thermal transport in bulk, thin films and nanowires

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A general model able to explain the thermal conductivity for macro, micro and nanostructured systems is still an open challenge. Experimental measurements on these systems have shown a drastic size-dependent reduction of the thermal conductivity compared to bulk values. Much effort has been devoted to the development of models to provide an accurate understanding of this behavior[7,6,5,3]. At the moment, we can only confirm that when the size of the sample is reduced, classical boundary effects are expected, and below some nanometers in size, quantum confinement should also start to influence the thermal conductivity through the modification of the dispersion relations (folding phonons and aperture of gaps in the dispersion relations). However, it is still under debate which are the most important effects at the different length scales since most of the proposed models do not agree in the origin of the thermal conductivity reduction, if it is a classical or quantum effect, especially at the 10-100 nanometer scale. In order to obtain a thermal transport model valid at all ranges of sizes and temperatures, it is necessary to have some certainty about the limits of applicability of the classic and quantum approaches. As a consequence, it is essential to study in detail every contribution independently. We have explore the limits of validity of the approaches based on the classical Boltzmann transport equation (BTE). This should lead us to establish the classical to quantum thermal transport frontier when the thermal conductivity behavior in reduced size systems is addressed. Eventually, we obtain a thermal conductivity expression that provides results in good agreement with published data on bulk silicon, thin films and nanowires, with characteristic sizes above 30 nm and show that quantum confinement effects above these sizes are not needed to understand the thermal transport.

Our thermal conductivity expression is based on the Guyer-Krumhansl model[1], conversely to previous attempts, which are based on the more usual Callaway model[2]. The provided expression accounts for hydrodynamic effects in the thermal transport equations, and it is obtained after a more rigorous treatment of normal scattering processes than that described in the Callaway model. This allows to reproduce the predicted values of the thermal conductivity in the region where the Callaway model over-predicts them. In order to provide a general analytical expression valid for the different geometries (three dimensional, two dimensional and one dimensional materials), the form factor of the Guyer-Krumhansl model is replaced by an expression given by the Extended Irreversible Thermodynamics model[4]. The results fit very accurately to experimental values of bulk silicon, thin films at the micro and nanoscale and silicon nanowires.

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