

Nanoscale heat transfer

The classical theory of heat transport is based on Fourier's law, which states that the flow of heat is proportional to the temperature gradient. This assumption leads to the classical form of the heat equation, which has been successfully used to model the temperature in materials for over 200 years. However, as technology advances, situations arise where the standard heat equation is no longer accurate and certain accepted properties turn out to be invalid.

Experimental data and simulations have demonstrated that at the nanoscale heat does not necessarily flow in the classical manner. For example, experiments of laser heating of ultrathin layers or simulations of heat transport in solids using molecular dynamics show dramatic discrepancies with respect to classical laws. The unpredictable behaviour makes the design stage of future nanoscale devices very difficult. Understanding heat transport at this scale and proposing modified versions of the classical equations (that prove to be valid) is a key point in order to ease the design of these future devices.

Various attempts have been made to develop an accurate mathematical model for heat flow, perhaps two of the most well-known are the Maxwell-Cattaneo and the Guyer-Krumhansl equations. The first introduces a relaxation time into the heat flow expression that has the effect of changing the governing equation to a form of wave equation, which then exhibits significantly different behaviour to the standard heat equation. The second introduces nonlocal effects that incorporate interesting new phenomena such as heat viscosity.

In this project we intend to examine these novel forms of heat equation, and study their validity at the nanoscale. We will investigate:

1. The effect of factors such as the relaxation time, nonlocalities, size dependent material properties (which results in a higher order equation).
2. How the new forms of heat equation affect the heat flow and at what length-scales they are valid, i.e. when is the classical heat equation sufficiently accurate?
3. The effect of boundary and initial conditions: indeed what are appropriate conditions at the nano-scale?

The results of the mathematical study will be linked to experimental observations. Do the results confirm experimental findings? Is any new behaviour predicted by the work and can this be used to guide future nano-scale experiments or the design of nano-devices?

For further reading see:

Wikipedia, Relativistic heat conduction.

F.X. Álvarez, D. Jou. Boundary Conditions and Evolution of Ballistic Heat Transport. *J. Heat Transfer* 132(1), 2010, doi:10.1115/1.3156785

A. Sellitto, F.X. Álvarez, D. Jou. Second law of thermodynamics and phonon-boundary conditions in nanowires. *J. Appl. Phys* 107(6), 2010, doi: 10.1063/1.3309477

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