Reduced Joule heating in nanowires

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The temperature distribution in nanowires due to Joule heating is studied analytically using a continuum model and a Green’s function approach. We show that the temperatures reached in nanowires can be much lower than that predicted by bulk models of Joule heating, due to heat loss at the nanowire surface that is important at nanoscopic dimensions, even when the thermal conductivity of the environment is relatively low. In addition, we find that the maximum temperature in the nanowire scales weakly with length, in contrast to the bulk system. A simple criterion is presented to assess the importance of these effects. The results have implications for the experimental measurements of nanowire thermal properties, for thermoelectric applications, and for controlling thermal effects in nanowire electronic devices.

The thermal properties of nanostructures such as nanowires, nanotubes, graphene, and nanometric devices have attracted much attention recently because of the unexplored physics of thermal transport at nanoscale dimensions. In particular, the thermal properties of nanowires (NWs) have been studied both for possible applications and for basic science, and an important question is that of the thermal properties during current flow. Indeed, Joule heating leads to reduced performance and breakdown of nanowire electronic devices. It is also utilized to probe NW electronic transport properties, and to controllably functionalize nanowires. Joule heating is also relevant to applications in thermoelectrics, to current-heated magnetic nanowires, and is important in assessing the reliability of field-emission devices based on NWs. In all of these cases, the temperature distribution along the NW due to Joule heating plays an important role, and so far analytical expressions for the full nanowire geometry in contact with a thermal environment have not been presented.

Here we provide such expressions and show that the nanometer size plays a crucial role in determining the temperature distribution in Joule-heated nanowires, due to heat flow from the surface that cannot be neglected due to the high surface to volume ratio, even when the thermal conductivity of the environment is relatively low. As a consequence, the temperatures reached inside the nanowire are significantly lower than predicted by bulk models, which are often used to model temperature distributions in NWs. The maximum temperature also scales differently with the length of the NW, increasing much more weakly with length. A criterion is proposed to assess the importance of these effects, which can be used, for example, when evaluating the need for more involved three-dimensional temperature simulation tools, or when designing thermal measurement systems.

To be specific, we consider the system shown in Fig. 1a. There, a nanowire of radius $R$ and length $L$ is thermally and electrically contacted by two infinite planar contacts at $z = \pm L/2$ and held at temperature $T = 0$. A uniform electronic current $I$ flows through the NW, causing Joule heating. In the steady-state, the temperature distribution between the two contacts is given by

$$\frac{\partial^2 T(r, z)}{\partial r^2} + \frac{1}{r} \frac{\partial T(r, z)}{\partial r} + \frac{\partial^2 T(r, z)}{\partial z^2} = -\rho \theta (r-R)$$

where $\rho = I^2 \rho/(\pi R^2)^2 \kappa_{NW}$ with $\rho$ the NW electrical resistivity and $\kappa_{NW}$ the NW thermal conductivity. The key physics is found in the presence of the theta function on the right hand side of this equation, and in the boundary conditions at the surface of the NW. These boundary conditions can take different forms depending on the thermal relation between the nanowire and its environment. Here we focus on the case of intimate contacts, but we expect the results to be relevant to a broad range of situations. In addition, the case of intimate contacts has the advantage of not requiring unknown interface parameters, and is relevant to core/shell NWs with minor modifications to account for the shell thickness.

For intimate thermal contacts, the temperature is continuous at the interface $T_{NW} (r, z) |_{r=R} = T_{env} (r, z) |_{r=R}$, and because the environment surrounding the NW has in general a different thermal conductivity $\kappa_{env}$ the flux continuity at the surface gives a boundary condition

$$\kappa_{NW} \frac{\partial T_{NW} (r, z)}{\partial r} \bigg|_{r=R} = \kappa_{env} \frac{\partial T_{env} (r, z)}{\partial r} \bigg|_{r=R}.$$  

When $\kappa_{env} = 0$, the temperature gradients are entirely in the axial direction and the problem reduces to the steady-state temperature distribution in a bulk material

$$\frac{d^2 T_{bulk}(z)}{dz^2} = -\rho.$$  

This equation is often referred to as that for “one-dimensional” heat transport, and is often used to analyze the thermal properties of NWs. The solution of the bulk equation for a NW between $z = -L/2$ and $z = L/2$ is

$$T_{bulk} (z) = \frac{P}{2} \left( \frac{L^2}{4} - z^2 \right),$$

with the maximum temperature

$$T_{bulk}^{max} = \frac{pL^2}{8}.$$
FIG. 1: Panel (a) shows the system under consideration: a nanowire of length \( L \) and radius \( R \) between two plates held at \( T = 0 \). The nanowire and environment have thermal conductivities \( \kappa_{NW} \) and \( \kappa_{env} \). The color map shows a typical temperature profile with blue corresponding to zero temperature and red to the largest temperature. Panel (b) shows the temperature distribution along the length of a 10 nm radius nanowire, plotted for three values of the ratio of thermal conductivities between the environment and the nanowire. Panel (c) is the radial temperature distribution normalized to the temperature at the origin, for the same nanowire as in (b).

To obtain the solution for the NW, we first calculated the Green’s function for the differential equation in Eq. (1) with the boundary condition in (2), and integrated over the source term \( p \theta (r - R) \). The solution is readily obtained as

\[
T(r, z) = \frac{4p}{L} \sum_{n=1,3,5,...} \sin \left( \frac{n\pi(z + L/2)}{L} \right) \left( \frac{L}{n\pi} \right)^3 \times \left[ 1 - \frac{\beta I_0 \left( \frac{n\pi R}{L} \right) K_1 \left( \frac{n\pi R}{L} \right)}{I_1 \left( \frac{n\pi R}{L} \right) K_0 \left( \frac{n\pi R}{L} \right) + \beta I_0 \left( \frac{n\pi R}{L} \right) K_1 \left( \frac{n\pi R}{L} \right)} \right]
\]

where \( \beta = \kappa_{env}/\kappa_{NW} \), and \( I_\nu \) and \( K_\nu \) are modified Bessel functions of order \( \nu \). In the limit \( \beta = 0 \) the solution can be shown to reduce to that of the bulk case, Eq. (4).

Figure 1a shows the calculated temperature in the whole system for a general case, showing the heat loss to the environment, while Fig. 1b shows the temperature profile along the axis of a 10 nm radius NW of length 1 \( \mu \)m for three values of the ratio of thermal conductivities \( \beta \). While for small values of \( \beta \) the profile approaches that of the bulk solution, for larger values of \( \beta \) the maximum temperature reached in the nanowire can be orders of magnitude lower. (This arises despite the fact that the radial temperature gradients in the nanowire are still fairly small, as shown in Fig. 1c.) Figure 2 shows the temperature reduction more clearly by plotting the maximum temperature as a function of \( \beta \) for NWs of length 1 \( \mu \)m and of radii 1, 10, and 100 nm. The deviation from the bulk solution depends strongly on the NW diameter, with the maximum temperature dropping rapidly as \( \kappa_{env}/\kappa_{NW} \) increases beyond a value that is strongly diameter dependent.

As an example, for a 10 nm radius NW with the thermal conductivity of bulk SiGe (10 W/mK) in air with thermal conductivity 0.045 W/mK, we have \( \beta = 0.0045 \) and the maximum temperature is almost a factor of five smaller than the bulk solution would predict. The same NW surrounded by SiO\(_2\) would have \( \beta \approx 0.1 \) and the effect is even more striking. (While the actual thermal boundary conditions for these systems might be different than that given by Eq. (2), the same behavior is anticipated with \( \beta \) replaced by the equivalent parameter describing the thermal properties of the interfaces).

As expected, these effects become even more important for longer nanowires, with a further reduction of the nanowire maximum temperature. However, in addition to this qualitative expectation, there is also a change in the scaling of the maximum temperature with length. Indeed, as Fig. 3 shows, the bulk solution predicts a maximum temperature that scales with the length squared; in contrast, for a nanowire with larger \( \beta \), the scaling is much different, and depends much more weakly on length.

To provide a simple expression describing these effects we consider the first mode in the above expansion, normalized by the first mode of the bulk expression:

\[
T(r, z) = 1 - \frac{\beta I_0 \left( \frac{n\pi R}{L} \right) K_1 \left( \frac{n\pi R}{L} \right)}{I_1 \left( \frac{n\pi R}{L} \right) K_0 \left( \frac{n\pi R}{L} \right) + \beta I_0 \left( \frac{n\pi R}{L} \right) K_1 \left( \frac{n\pi R}{L} \right)}.
\]

(7)
Thus the nanoscale dimensions. For a 10 nm radius NW of length 1 \( \mu m \), deviations arise even when \( \kappa_{env} \) is only 0.1\% of \( \kappa_{NW} \).

In summary, we presented a simple analytical expression for the temperature distribution in Joule-heated nanowires. We find that the temperature reached in nanowires during Joule heating can be significantly less than that obtained from standard bulk models. This originates from heat loss at the nanowire surface that cannot be ignored due to the high surface to volume ratio, even when the thermal conductivity of the environment is relatively low. The work presented here is straightforward, but given the ubiquitous presence of Joule heating in nanostructures, it should be relevant to many areas of nanoscale thermal transport, including thermoelectric devices based on nanowire arrays, nanoscale transistors, and electrically driven light-emitting nanodevices.

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