Theoretical Studies of the Non-Linear Transport Properties of Molecular Wires

Massimiliano Di Ventra, UC San Diego, DMR-0133075

Local heating occurs when electrons diffusing in a conductor release energy to the ions via scattering with phonons. The amount of heat generated in a given portion of the conductor depends on several factors: the strength of the electron-phonon interaction, the current density, the background temperature, and the inelastic electron mean free path. In a nanoscale junction, the inelastic electron mean free path is large compared to the dimensions of the junction. As a consequence, each electron releases only a small fraction of its energy during the time it spends in the junction. However, there can still be substantial local heating due to the large current density in nanoscale junctions. We have shown (see Fig. 1) that local heating increases dramatically with increasing bias, mainly due to excitation of longitudinal modes, but it is also considerably suppressed by thermal dissipation into the electrodes, provided good thermal contacts exist between the nanostructure and the bulk electrodes. When inefficient heat dissipation into the electrodes occurs very high local temperatures can be generated at very low biases, which can lead to structural instabilities of the nanojunction.

This work has been done in collaboration with

Mike Zwolak (masters student)
Y.C. Chen (post-doc)

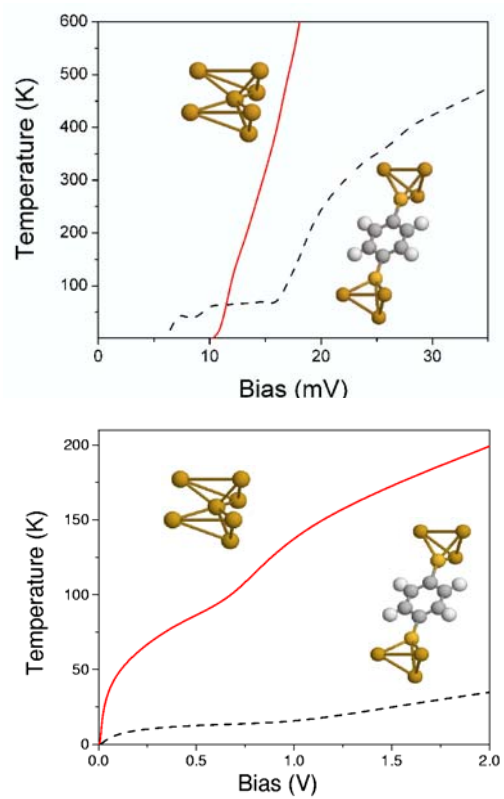

Figure 1. *Top* - Local temperature as a function of bias for a molecular junction (dashed line) and a gold point contact (solid line). No heat dissipation into the electrodes is taken into account. *Bottom* – Local temperature when dissipation into the electrodes is taken into account.

Y.C. Chen, M. Zwolak, M. Di Ventra, *Nano Lett.* **3**, 1691 (2003)

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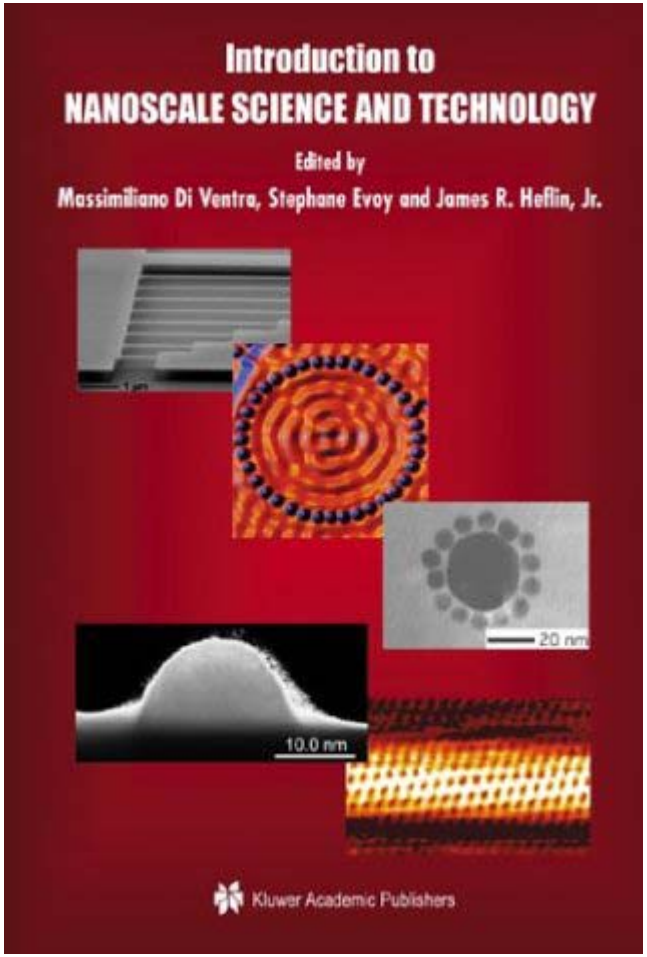
Education:

1 undergraduate,
3 grad students,
4 post-docs.

One undergraduate student has received an NSF Graduate Fellowship for 2003-06. A post-doc has become Associate Professor at Fudan University.

Undergraduate Textbook:

Nanoscale science and technology is a young, promising field that encompasses a wide range of disciplines including physics, chemistry, biology, electrical engineering, chemical engineering, and materials science. With rapid advances in areas such as molecular electronics, synthetic biomolecular motors, DNA-based self-assembly, and manipulation of individual atoms, nanotechnology has captured the attention and imagination of researchers and the general public. The PI has co-edited a comprehensive textbook which provides a broad and thorough introduction to the field. The book has been published by Kluwer in July 2004 and is aimed specifically at undergraduate seniors and early graduate students in all of the disciplines enumerated above. The book consists of twenty-three chapters arranged in seven sections. All chapters have been written by experts from each respective field. Exercises and general references are provided at the end of each chapter to encourage students to expand on the topics discussed in the book. A CD-ROM containing color copies of all figures accompanies the book, allowing rapid preparation of lecture materials by faculty.