東京大学グローバルCOEプログラム　機械システム・イノベーション国際拠点

東京大学 THE UNIVERSITY OF TOKYO

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Semi-Classical Langevin and NEGF Approach to Atomic Dynamics in Non-Equilibrium Nanosystems

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会場：東京大学工学部4号館　205号室

要旨

The influence of an electronic current on atomic dynamics is an important and intriguing problem in nanoelectronics. We have developed an approach based on the semi-classical Langevin equation(SCLE) to investigate the excitation of atomic dynamics in a nanoconductor in the presence of electrical current[1, 2, 3]. In the SCLE description the nonequilibrium electronic environment is described like an effective “bath” influencing the atomic dynamics causing fluctuations and dissipation. We will discuss how this formalism is related to the NEGF method, and compare results for e.g. vibrational heating based on the two approaches. The SCLE approach allows us to identify the forces acting on the atoms due to the electronic current. We show how the current can cause several types of instabilities in a nanoconductor which ultimately can lead to contact breakdown. These include run-away behavior due to excitation of "water-wheel" modes[4, 2, 3], and a laserlike amplification of the phonons for contacts with a n-p-junction character[5].

[1] M. Brandbyge and P. Hedegård. Phys. Rev. Lett., 72, 2919, 1994.
[2] Jing Tao Lü, M. Brandbyge, and P. Hedegård. Nano Lett., 10, 1657, 2010.
[3] Jing-Tao Lü, M. Brandbyge, P. Hedegård, T. N. Todorov, and D. Dundas. Phys. Rev.
B, 85, 245444, 2012.
[4] Daniel Dundas, Eunan J. McEniry, and Tchavdar N. Todorov. Current-driven atomic waterwheels. Nature Nanotech., 4(2):99–102, FEB 2009.
[5] Jing Tao Lü, P. Hedegård, and M. Brandbyge. Phys. Rev. Lett., 107, 046801, 2011.

主催：　東京大学グローバルCOEプログラム「機械システム・イノベーション国際拠点」
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