INELASTIC SCATTERING AND LOCAL HEATING IN ATOMIC GOLD WIRES

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Atomic size conductors are ideally at the limit of miniaturization, and a big effort is devoted to them in the fields of electronics and more recently molecular electronics. Quantum effects become important leading to a physical behaviour of atomic-size conductors fundamentally different from macroscopic ones. Inelastic effects can take place in these junctions. Hence, studies concerning the ballistic regime need be revisited. Indeed, inelastic effects in tunnelling junctions have been used to identify the vibrational spectra of impurities or objects in the junction. This is the case of the inelastic electron tunnelling spectroscopy (IETS) both in metal-insulator-metal junctions [1] and in STM junctions (STM-IETS) [2]. Recently, similar vibrational signatures in the high-conductance regime have been revealed [3]. Agraït and co-workers have used and STM tip to create a free standing atomic gold wire between the tip and the substrate's surface. The STM has then been used to measure the conductance of the gold wire. By recording the conductance against the tip's displacement they have been able to determine the approximate sizes as well as the level of strain of the wire. The data show distinct drops of conductance at different tip-substrate voltages, leading to the conclusion that the conducting electrons were backscattered from the wire's vibrations. The onset of the drop coincides with the natural frequency of the wire at certain sizes and strains.

We present a detailed first-principles calculation of the inelastic scattering due to the phonons in atomic gold wires. We employ density functional theory (DFT) for the electronic structure combined with a non-equilibrium Green's function calculation of thecurrent and power flow within the self-consistent Born approximation (SCBA). We find that the scattering is due mainly to a single phonon mode (the alternating bond-length mode). We calculate the non-linear conductance vs. bias voltage for two limiting steady-state cases of power flow in the system: (i) Strong coupling to an external heat-sink -- all phonon energy flows to an external heat-bath, which fix the number of phonon quanta . (ii) No external heat-bath -- phonon energy can only flow back into the electronic degrees of freedom (electron-hole pair excitation). In this latter situation we get the phonon excitation at finite voltage using the assumption that the system is in a steady state. Our results which compares well with the experimental results suggest that significant phonon heating takes place in these experiments.

References:

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