

Electron transport and phonons in atomic wires

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Abstract

A scanning tunnelling microscope (STM) at low temperatures is used to fabricate and measure the electronic transport properties of atomic wires up to 7 atoms in length. We observe that the conductance of these wires, which at zero bias voltage is $2e^2/h$, as corresponds to ballistic electron transport through a single conductance quantum channel, drops sharply at a well-defined voltage due to the inelastic scattering of electrons with phonons. This behaviour is characteristic of one-dimensional systems, where an electron can interact only with a phonon of a well-defined wavenumber. We find that the frequency of this phonon and the magnitude of the interaction depend strongly on the state of strain of the wire. We also explore the energy exchange mechanism between electrons and phonons in the wire itself which causes heating in these nanostructures. © 2002 Elsevier Science B.V. All rights reserved.

Freely suspended atomic wires of gold up to 7 atoms in length can be formed by drawing a one-atom contact using a scanning tunnelling microscope (STM) or related techniques (mechanically controlled break-junction, MCBJ) [1,2]. They have a zero bias conductance close to $G_0 = 2e^2/h$, independently of their length (see Fig. 1(a)). This is the expected behaviour for an atomic wire with a completely open single conductance quantum channel [3], and is consistent with the fact that a one-atom contact of gold has only one conductance quantum channel. The number of quantum

channels in a metallic atomic contact has been shown to depend on the chemical properties of the atoms [4].

We observe that at low temperature, the conductance of these atomic wires is voltage-dependent dropping suddenly by a few percent as voltage is increased beyond several millivolts (see Fig. 1(b)). A voltage-dependent conductance is also observed in ballistic point-contacts of much larger size, where it is associated to inelastic scattering of electrons with phonons and other elementary excitations [5] taking place in the bulk. These processes are voltage dependent because the electrons must be injected with enough energy to emit an excitation. In the case of phonons the derivative of the conductance shows peaks which correspond to peaks in the phonon density of states. The amplitude of the signal for contacts of different sizes is proportional to the volume

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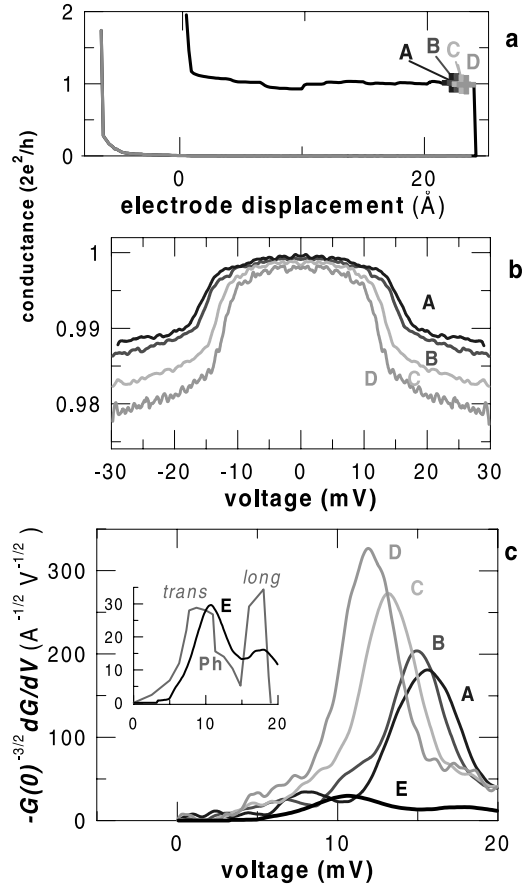


Fig. 1. (a) Conductance at fixed bias as the atomic wire is fabricated. Differential conductance (a) and its normalized derivative (b) vs voltage of an atomic wire of about 20 nm in length. The increase in the separation between the electrodes for each of the successive curves A, B, C, D, is 0.5 \AA . The conductance is measured using a lock-in technique with a modulation of 0.5 mV, and the derivative is computed numerically. In panel (c) a typical curve corresponding to a point-contact is also shown (curve E), for comparison. The inset shows again curve E and the phonon spectrum (Ph) of the bulk for Au. The derivative of the conductance is normalized to $G(0)^{3/2}$. The peaks at about 10 and 18 meV correspond to the peaks in the phonon density of states for transverse and longitudinal phonons, respectively. The measurements were performed at a temperature of 2 K.

around the contact, and consequently, to $G(0)^{3/2}$, where $G(0)$ is the zero bias conductance, since the conductance of a ballistic point-contact is proportional to the contact area. This reflects the fact that only those electrons scattered in the

immediate vicinity of the contact have a significant probability of coming back through the contact.

At low temperatures atomic chains are very stable, once formed experiments can be performed on them during hours. We have measured the conductance of atomic chains as a function of voltage for many different atomic chains. Fig. 1(c) shows that the normalized derivative of the conductance has a large peak whose amplitude is much larger than that corresponding to a point-contact. As the chain is submitted to elastic strain the peak changes markedly in amplitude and shifts in voltage, while the background as well as the zero bias conductance remains mostly unchanged. This behaviour strongly suggests that the background features correspond to backscattering processes in the bulk while the peak is related to backscattering processes in the chain itself.

In a one-dimensional wire at zero temperature, where only phonon emission is possible, electrons will not interact with phonons below a threshold voltage $\hbar\omega_{2k_F}/e$ (see Figs. 2 and 3). A sudden decrease in conductance (a peak in its derivative)

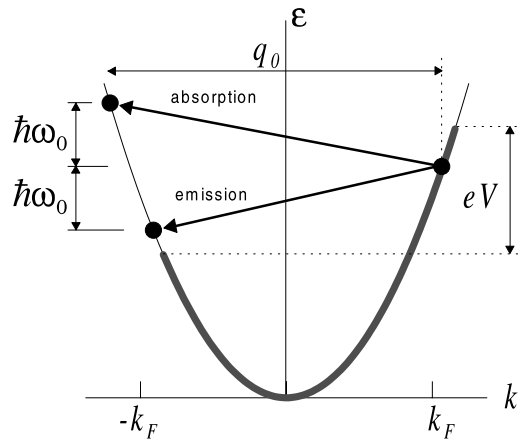


Fig. 2. Allowed inelastic transitions in a one-dimensional band. The only allowed transitions are from a state with wavenumber $\sim k_F$ to a state with wavenumber $\sim -k_F$, that is electrons can only interact with one phonon whose wavenumber is $q_0 \approx 2k_F$. For an atomic wire with a single conduction electron per atom, $k_F = \pi/2a$, where a is the interatomic distance, and consequently $q_0 = \pi/a$, which corresponds to the phonon of wavelength $2a$. Note that the figure is not drawn to scale: phonon energies are about 2 orders of magnitude smaller than electron energies.

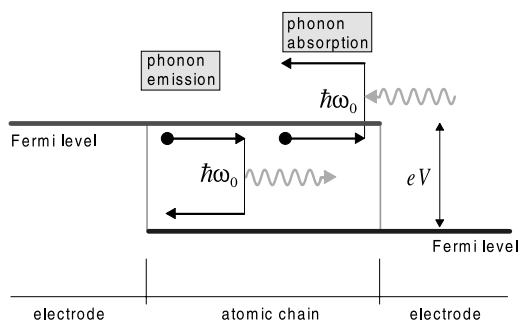


Fig. 3. Schematic representation of phonon emission and absorption processes in a one-dimensional ballistic wire. In the wire there are two Fermi levels which define the occupation of electronic states: for the right-going electron states up to the Fermi level of the left electrode are occupied, while for the left-going electrons the occupation of states is up to the Fermi level of the right electrode [6]. The separation of these Fermi levels is eV , where V is the voltage difference applied to the electrodes. Electronic transitions are possible when the final electronic state is unoccupied, consequently, phonon emission is possible only for voltages $eV > \hbar\omega_{2k_F}$. On the other hand there is no threshold for phonon absorption.

signals the onset of the phonon emission process. The position of the drop gives the energy $\hbar\omega_{2k_F}$ of the interacting phonon, that is the $2k_F$ phonon. Thus a single peak in the derivative is a signature of one-dimensionality. Note that in a one-dimensional wire all electron–phonon interaction processes result in backscattering (see Fig. 2) and consequently in a decrease in conductance. In the experimental conductance curves the drop in conductance is somewhat rounded due to the nonzero temperature and also because of the uncertainty in the momentum of the electron due to the finite length of the chain.

To gain some insight into the interplay between ions and electrons in the atomic wire, we can model the atomic chain as a portion of length L of an infinite one-dimensional wire. The conductance of the wire at a given voltage is proportional to the backscattering probability for an electron injected at this voltage. Thus at the threshold the conductance drop can be written as $\Delta G/G_0 = -L/\ell$, where ℓ is the inelastic mean free path for an infinite one-dimensional wire. ℓ is given by the probability per unit time w that an electron in a state higher above the Fermi level than $\hbar\omega_{2k_F}$ emits a phonon. At zero temperature,

we can write using time-dependent perturbation theory [7]

$$\frac{1}{\ell} = \frac{w}{v_F} = \frac{L}{2\pi} \frac{2\pi}{\hbar} \frac{1}{2k_F} |M_{2k_F}|^2 = \frac{2am^2}{m_i\hbar^3} \frac{V_{ei}^2}{\omega_{2k_F}}, \quad (1)$$

where M_{2k_F} is the matrix element for the electron–phonon interaction at wavenumber $2k_F$; a is the interatomic distance; m_i is the mass of the ion; V_{ei} is the Fourier component of the electron–ion interaction potential; and m is the mass of the electron. Thus from the conductance curves we can obtain in addition to the frequency of the $2k_F$ phonon, the magnitude of the corresponding electron–phonon matrix element.

Our experimental results (see Fig. 4) show that as the atomic chain is stretched the frequency of the $2k_F$ phonon decreases, that is, the atomic chain softens, as it is to be expected for an increase in the interatomic distance for an atomic chain [9]. The inelastic mean free path ℓ is also observed to decrease, which from Eq. (1) implies an enhancement of the electron–phonon interaction matrix element. This enhancement is about 25% larger than that expected from the frequency and chain length dependence of M_{2k_F} . However, exact agreement is not to be expected due to the simplicity of the model. A more detailed comparison would require accurate modelling of transport in the nanowire.

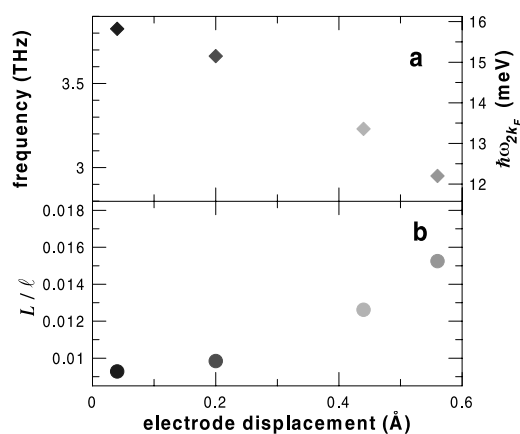


Fig. 4. The effect of elastic deformation of the atomic chain (a) and (b) show the frequency of the $2k_F$ phonon and the ratio of the length of the chain L to the inelastic mean free path ℓ , respectively, for the chain in Fig. 1 as the chain is stretched.

A one-dimensional metal is predicted to be unstable due to electron–phonon interactions: a transition to a semiconducting or insulating state would eventually take place at low temperature – the so-called Peierls transition [8]. At present we are pursuing evidence of this mechanism with experiments at lower temperature: a softening of the $2k_F$ mode should take place as the temperature is lowered, due to the divergence of the electronic polarizability.

Another aspect that we have investigated in our experiments with atomic chains is the mechanism for energy exchange between the electrons and phonons, that is, how the electrons exchange energy with the ions of the chain. If the chain is initially at zero temperature, which implies that there are no phonons present, the electrons will traverse it without interacting with the ions, that is, without dissipation, as long as the bias voltage is below the threshold. Above the threshold, phonons are emitted giving rise to a nonequilibrium phonon population in the chain. The average number of phonons at any given voltage results from the balance between phonon emission, phonon absorption, and the rate of phonon escape to the leads, which depends on the acoustic matching to the electrodes, that is, on the mechanical coupling of the atomic chain to the electrodes.

Heating of the atomic chain by the hot electrons traversing it is manifested in the slope of the conductance after the threshold, from which we can estimate the average number of phonons in the chain $\langle n_{2k_F} \rangle$ and their dwell time τ_{ph} , which is the inverse of the rate of phonon escape. For the chain in Fig. 1, we obtain that $\langle n_{2k_F} \rangle$ grows linearly with voltage, being zero for $eV = \hbar\omega_{2k_F}$, and about 0.2 for $eV = 2\hbar\omega_{2k_F}$, while $\tau_{\text{ph}} \sim 10^{-12}$ s, which implies that phonons are only weakly localized in the chain. The energy transferred to the chain by the electrons is $\langle n_{2k_F} \rangle \hbar\omega_{2k_F}$. Note that only phonons with wavenumber $2k_F$ can be emitted or absorbed and the resulting phonon population is completely out of equilibrium and the temperature of the chain is not defined.

We must remark the double role played by electrons: they both *heat* and *cool* the atomic chain. As a consequence even in the limiting case in which phonons were localized in the chain, there would be finite average phonon population, resulting from the balance between heating and cooling. Cooling by phonon absorption will also act if the chain is at nonzero temperature and the bias voltage is below the threshold. In this case the hot electrons will deplete the $2k_F$ -phonon mode, cooling the chain.

We have reported new results on an extremely simple system: a one-dimensional metal formed by a few gold atoms with one conductance quantum channel. Detailed transport measurements give qualitative information about the ion–ion and electron–ion interactions, and of the energy exchange mechanisms between the electrons and the atoms forming the chain. This characterization of transport is an essential step towards the development of atomic size electronics, where dissipation is of the utmost importance.

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