Atomic Chains: Wires Formed From Metal Atoms

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It has recently been discovered that during the fracture of nanocontacts, using STM-related techniques, gold spontaneously forms freely suspended chains of single atoms [1,2], and this was independently verified by transmission electron microscopy [3]. At low temperatures (liquid helium) these chains are surprisingly stable. They form metallic wires with a conductance of $2e^2/h$, indicating that they have a single completely open quantum channel. They can sustain very large current densities of up to $8x10^{14}$ A/m² showing that the electron transport is ballistic, and that most of the power is dissipated in the electrodes far away from the contact.





Using a scanning tunneling microscope supplemented with a force sensor, we have studied the mechanical properties of chains of atoms. We find that the bond strength of

this nanowire is about twice that of a bulk metallic bond. We perform ab initio calculations of the force at chain fracture and compare quantitatively with experimental measurements. The observed mechanical failure and nanoelastic processes involved during atomic wire fabrication are investigated using molecular dvnamics simulations, and we find that the total effective stiffness of the nanostructure is strongly affected by the detailed local atomic arrangement at the chain bases.

Fig.2. Simultaneous conductance (top) and force (middle) measurements during chain fabrication and breaking. The conductance on the last plateau is shown on anexpanded scale to illustrate small variations in the conductance. The inset shows a schematic drawing of the experimental setup. Bottom: Calculated force evolution obtained from molecular dynamics simulations. The arrows indicate the points at which a new atom pops into the chain and snapshots of the structure at these positions are shown [4].



The voltage dependence of the conductance of metallic atomic wires at low temperatures shows that inelastic scattering of electrons sets in at a finite voltage due to the excitation of the vibrations of the ions of the atomic chain. This well-defined threshold for dissipation is characteristic of the electron-phonon interaction in one-dimensional systems. We observe that the mechanical tensioning of the atomic chain results in bond softening, which is reflected in a decrease of the phonon frequency and a dramatic enhancement of the electron-phonon interaction.



Fig. 3. (a) Short and long atomic wire, ~ 0.4 and ~2.2 nm, respectively. Panels (b-d) show the differential conductance and its derivative at points S, M, and L, respectively. The various curves in (b-d) were acquired at intervals of 0.03, 0.03 and 0.05 nm, respectively. The wire in (d) has a length of about 7 atoms[5].

REFERENCES

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