Forces and vibration modes in a chain of single gold atoms

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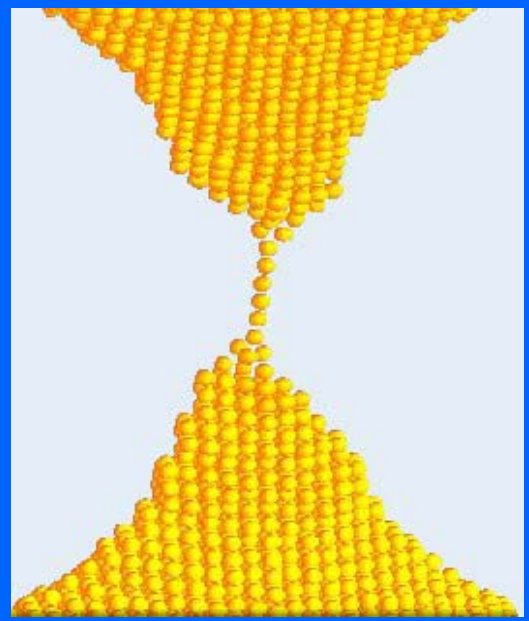
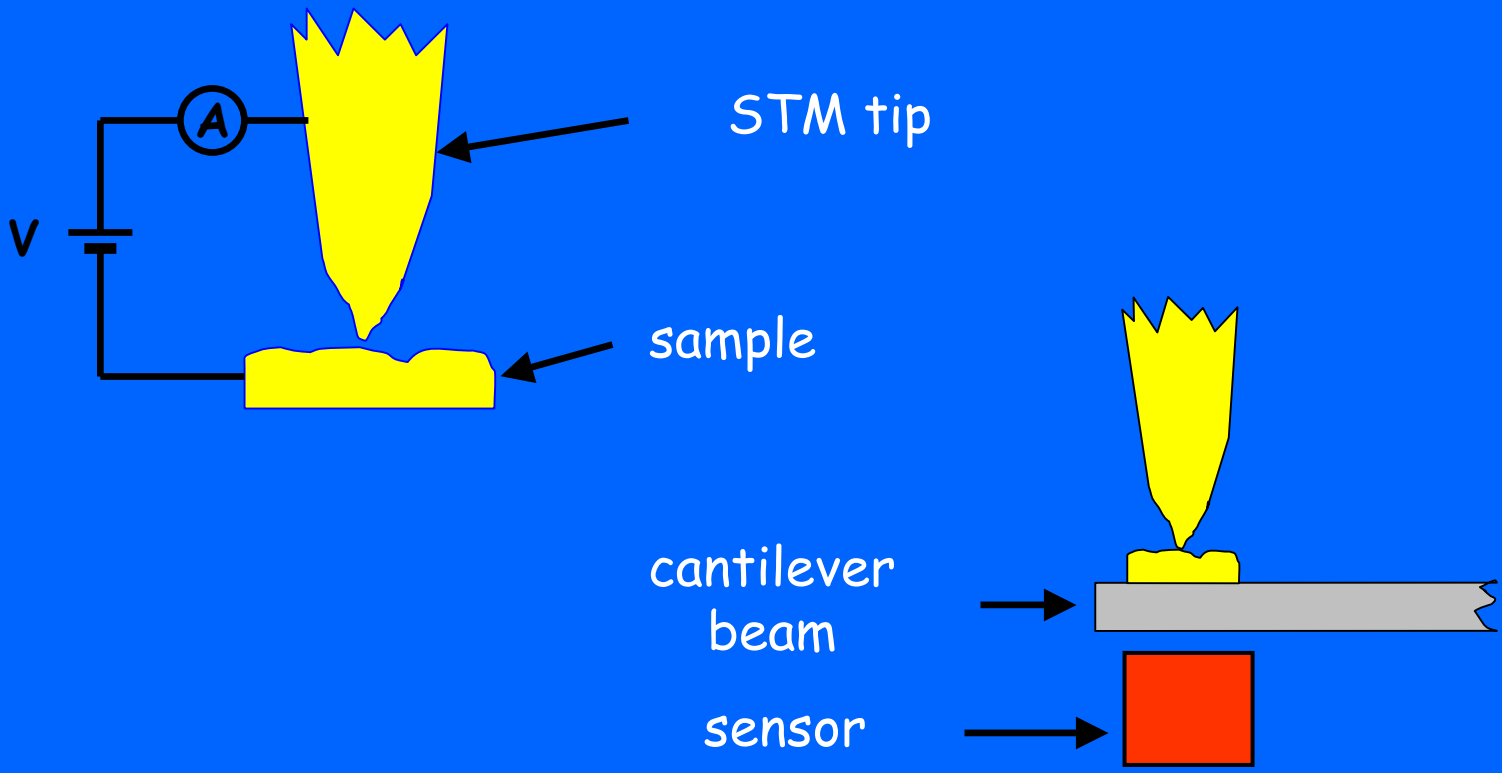
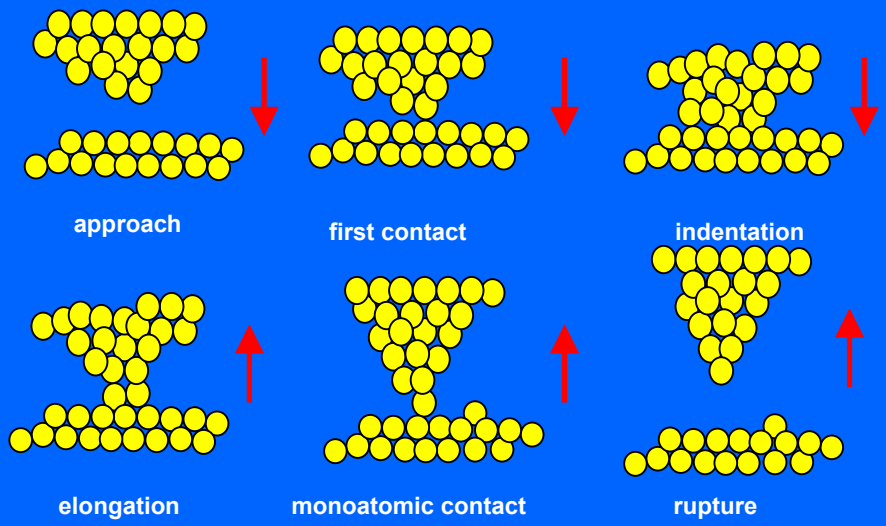


MD simulation by K. W. Jacobsen y M. R. Sørensen

scanning tunneling microscope (STM)
atomic force microscope (AFM)

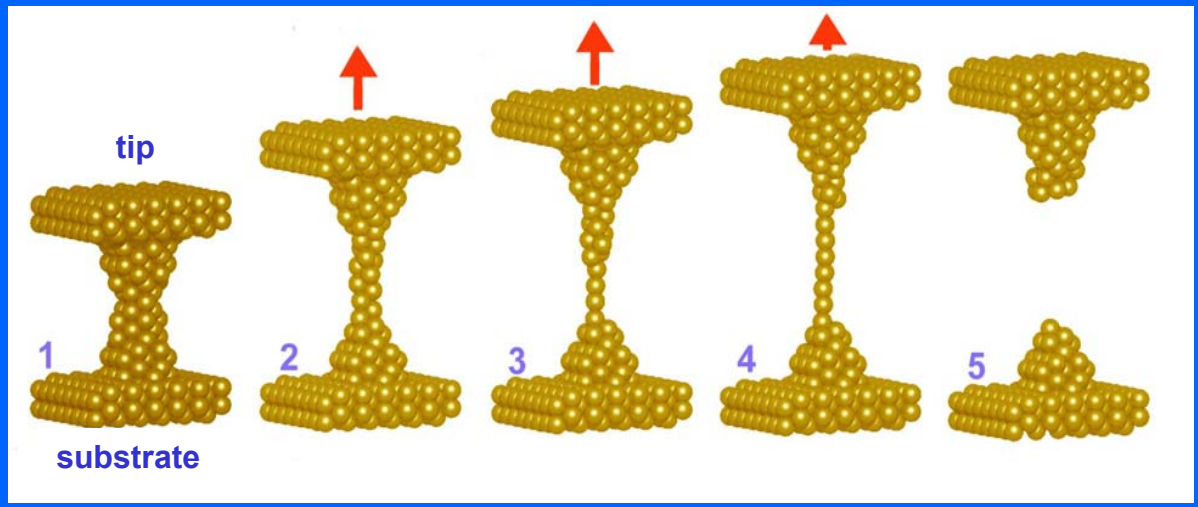


formation of an atomic chain



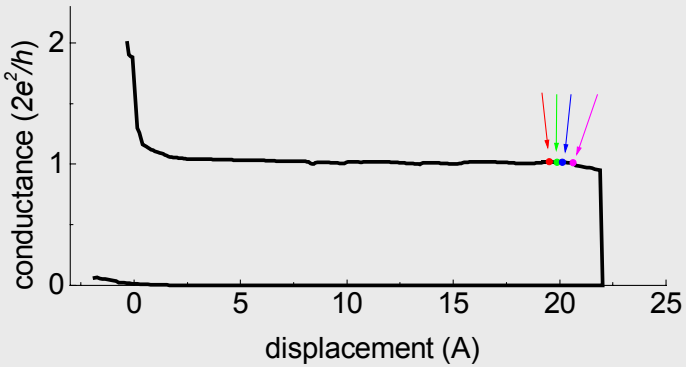
MD simulation by K. W. Jacobsen y M. R. Sørensen

formation of an atomic chain

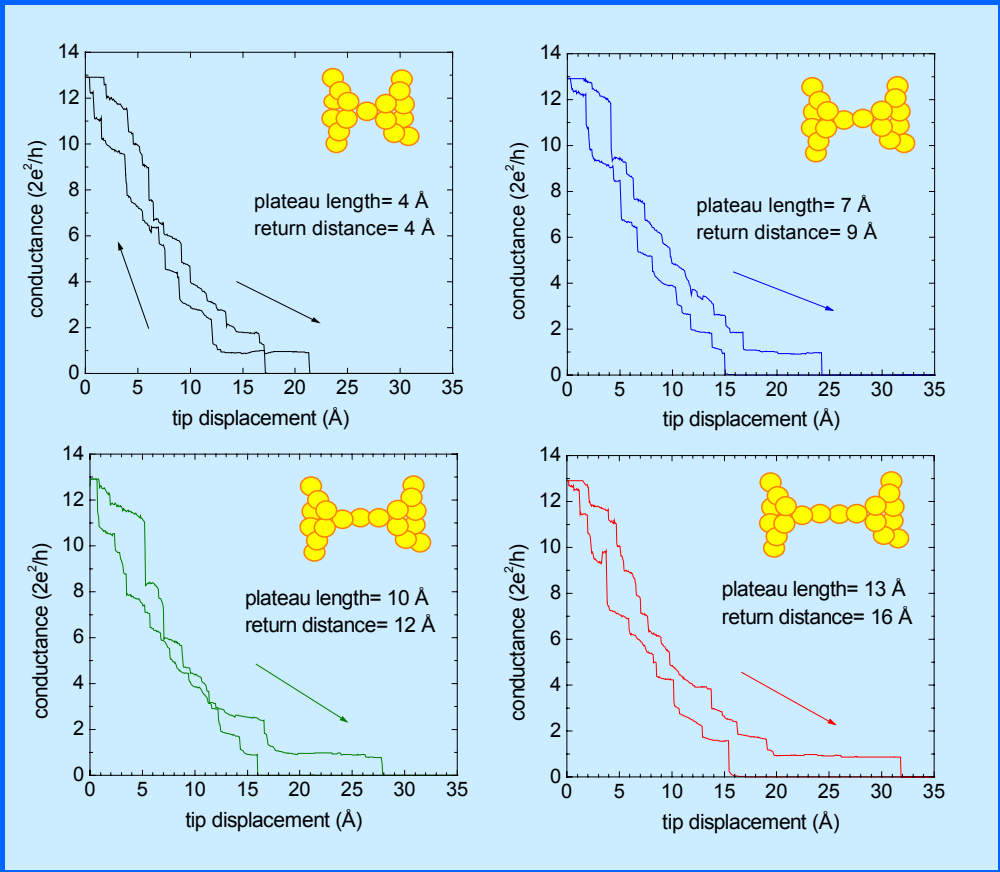


MD simulation by K. W. Jacobsen y M. R. Sørensen

- Conductance 1 quantum independent of **length** and **temperature**
- Very stable at low temperatures (hours)



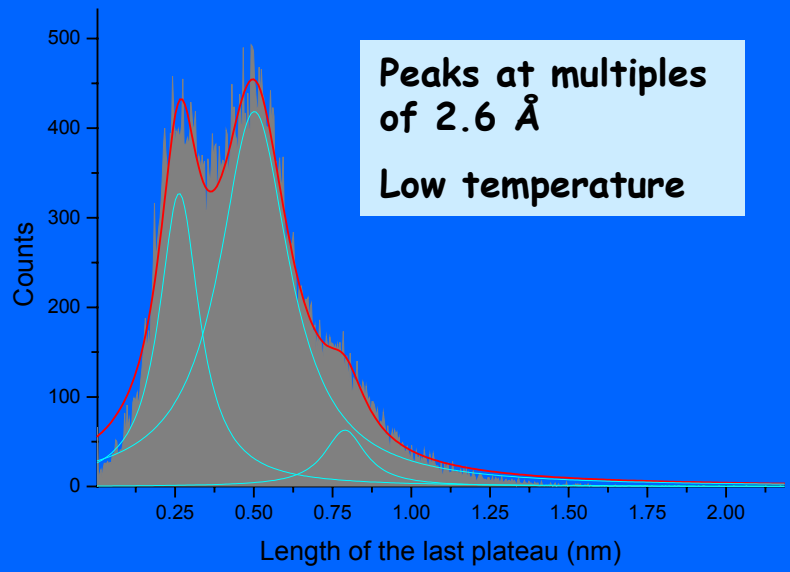
length of an atomic chain



Yanson, Rubio Bollinger, van den Brom,
Agraït, van Ruitenbeek, Nature **395**, 783 (1998)

Conductance 1 quantum independent of length

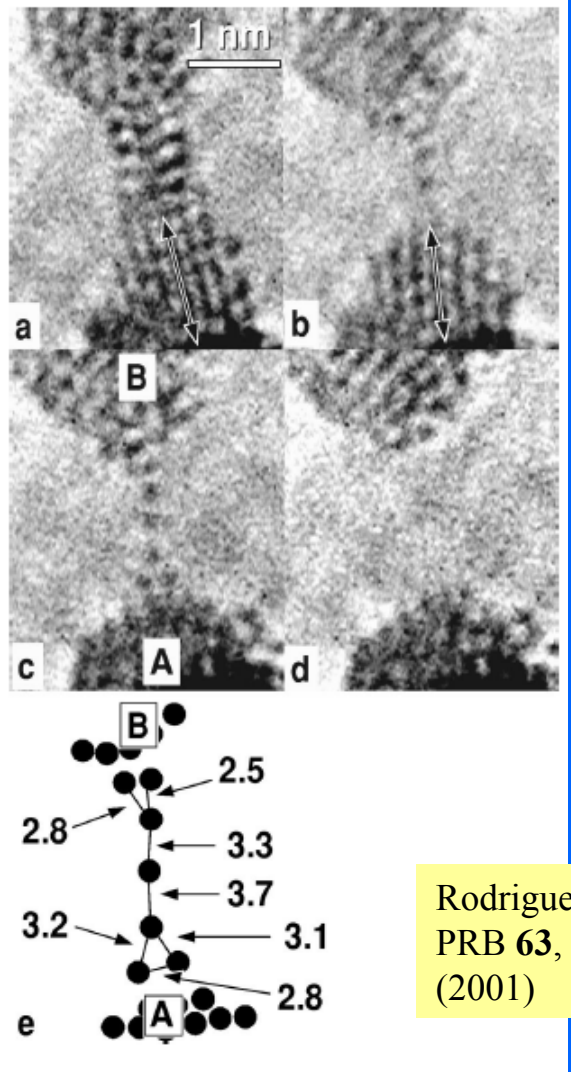
Low probability for long chains



Untiedt, Yanson, Grande, Rubio-Bollinger,
Agraït, Vieira, van Ruitenbeek,
PRB 2002

HRTEM images of Au atomic

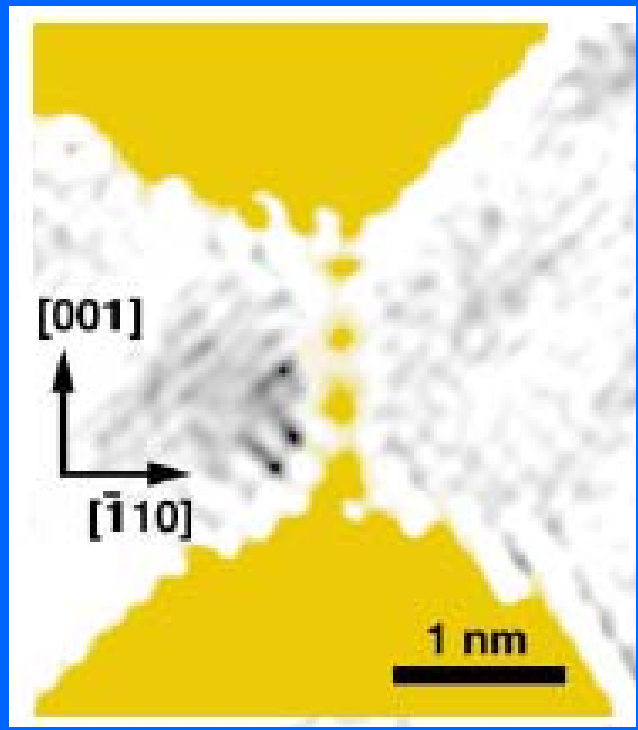
Room temperature



Rodrigues *et al.*, PRB **63**, 073405 (2001)

Stability ~ few seconds

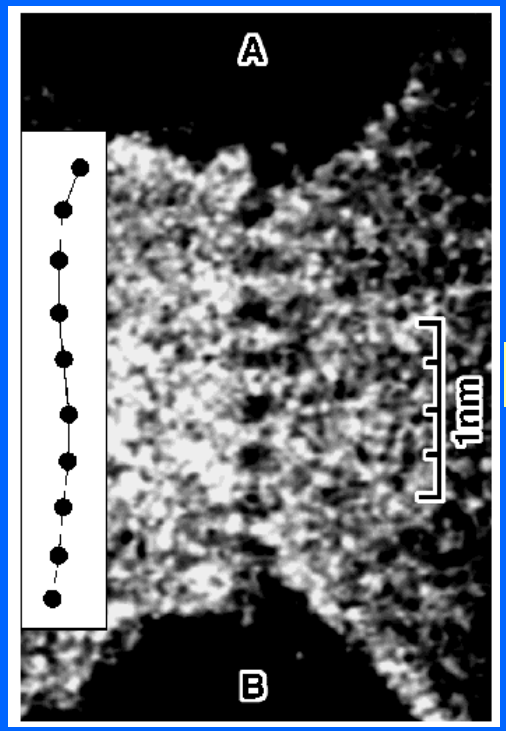
$G \sim 1\ G_0$



Ohnishi *et al.*, Nature **395**, 780 (1998)

HRTEM images of Au atomic

Room temperature



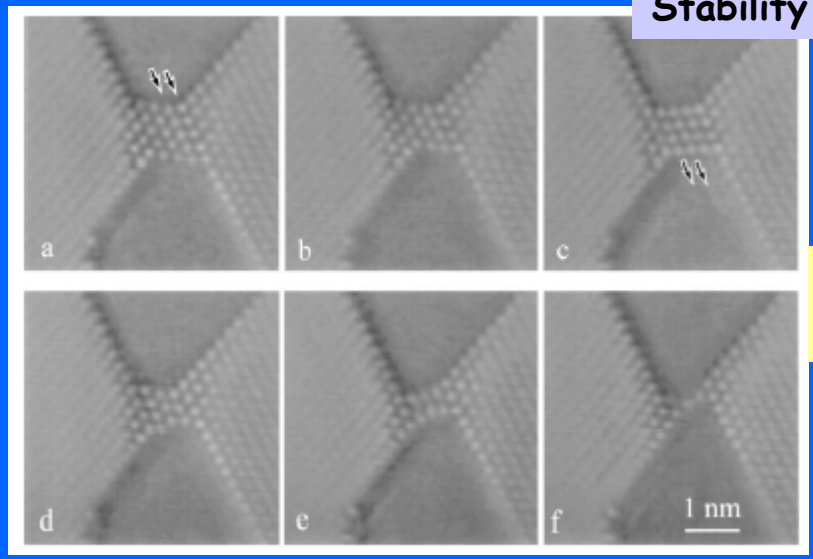
interatomic distance ~ 2.5 - 2.9 Å

Stability ~ 20 s

Non-conducting!

Kizuka *et al.*, JJAPL **40**, L71 (2001)

Stability ~ few seconds



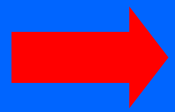
interatomic distance ~ 2.9 Å

Takai *et al.*, PRL **87**, 106105 (2001)

electronic transport in atomic chains

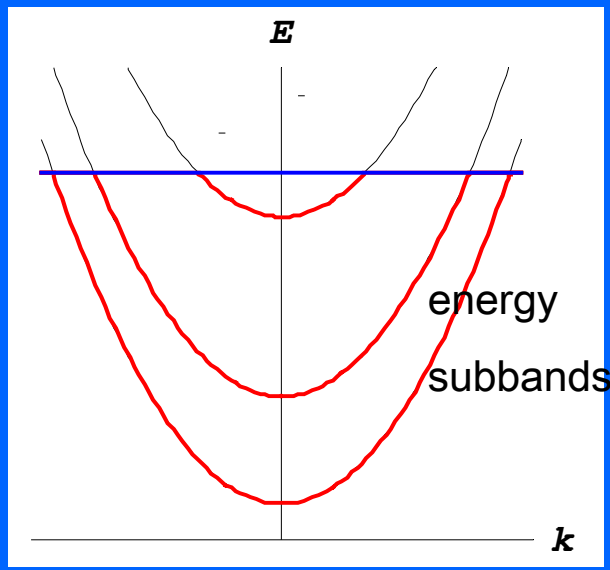
conductance $\not\propto 2e^2/h$

- independent of length
- independent of temperature



one (almost) completely open quantum channel

conductance: Landauer's approach



$$G = \frac{2e^2}{h} M$$

no scattering
M = number of modes

$$G = \frac{2e^2}{h} \sum_i T_i$$

scattering
T_i = transmission of each subband

mechanical properties of an atomic chain?

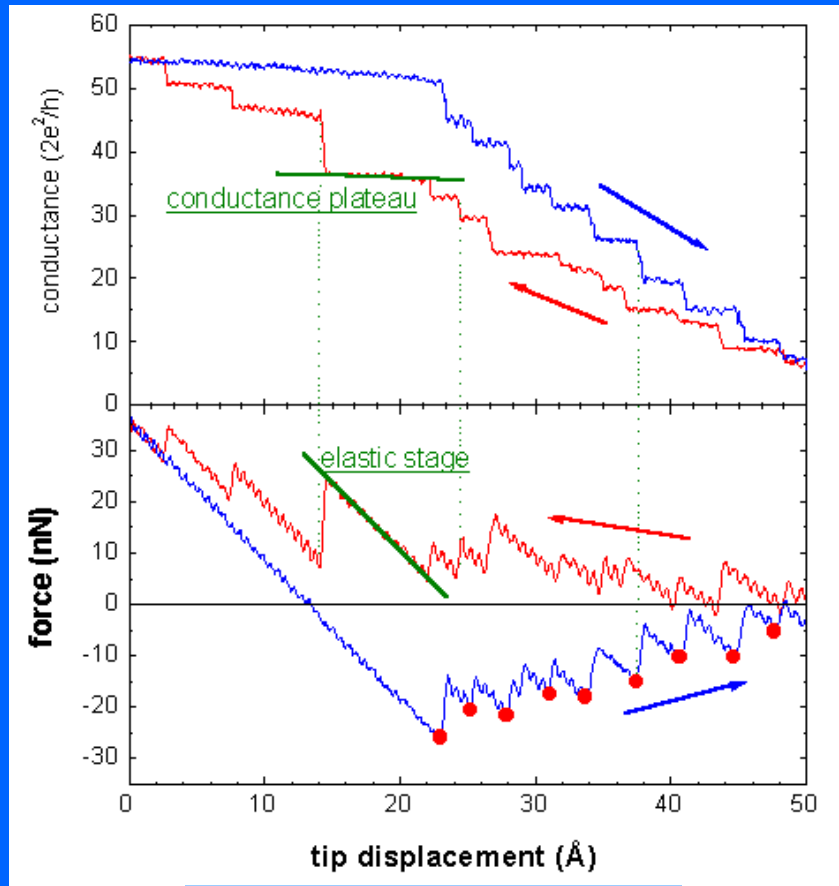
- force to break an atomic chain
- stiffness of the chain (related to bond stiffnes)
- vibration modes of an atomic chain

elastic and plastic deformation in nanoscopic metallic systems

- Correlation between conductance jumps and force relaxations
- Very strong: ideal strength (2-4 GPa)

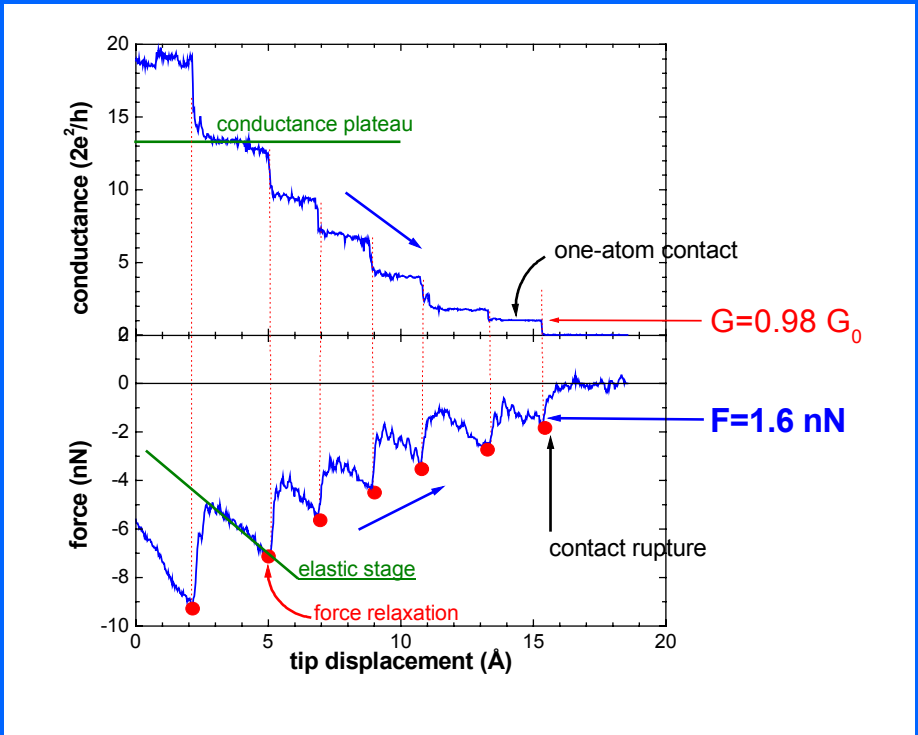
Elastic stages and sudden relaxations due to atomic rearrangements

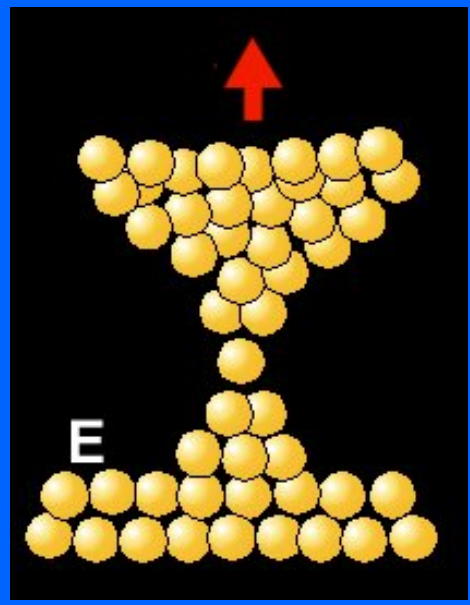
Plastic deformation by slip of atomic planes (absence of dislocations)



N. Agraït, G. Rubio, S.Vieira. *Phys. Rev. Lett.* **74** (1995).

breaking a one-atom contact



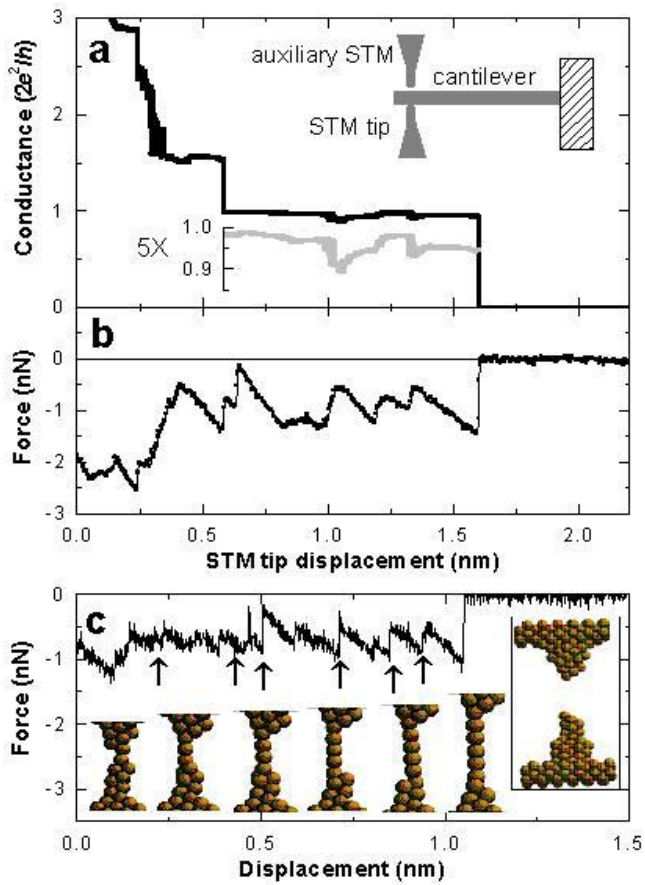


force to break the
one-atom contact = 1.6 nN

G. Rubio, N.Agraït,S.Vieira.
Phys. Rev. Lett. **76** (1996).

mechanical properties of atomic chains

G. Rubio-Bollinger, S.R. Bahn, N.Agraït, K.W. Jacobsen, S. Vieira.
Phys. Rev. Lett. **87** (2001).



elastic stages + atomic rearrangements during pullout of the chain

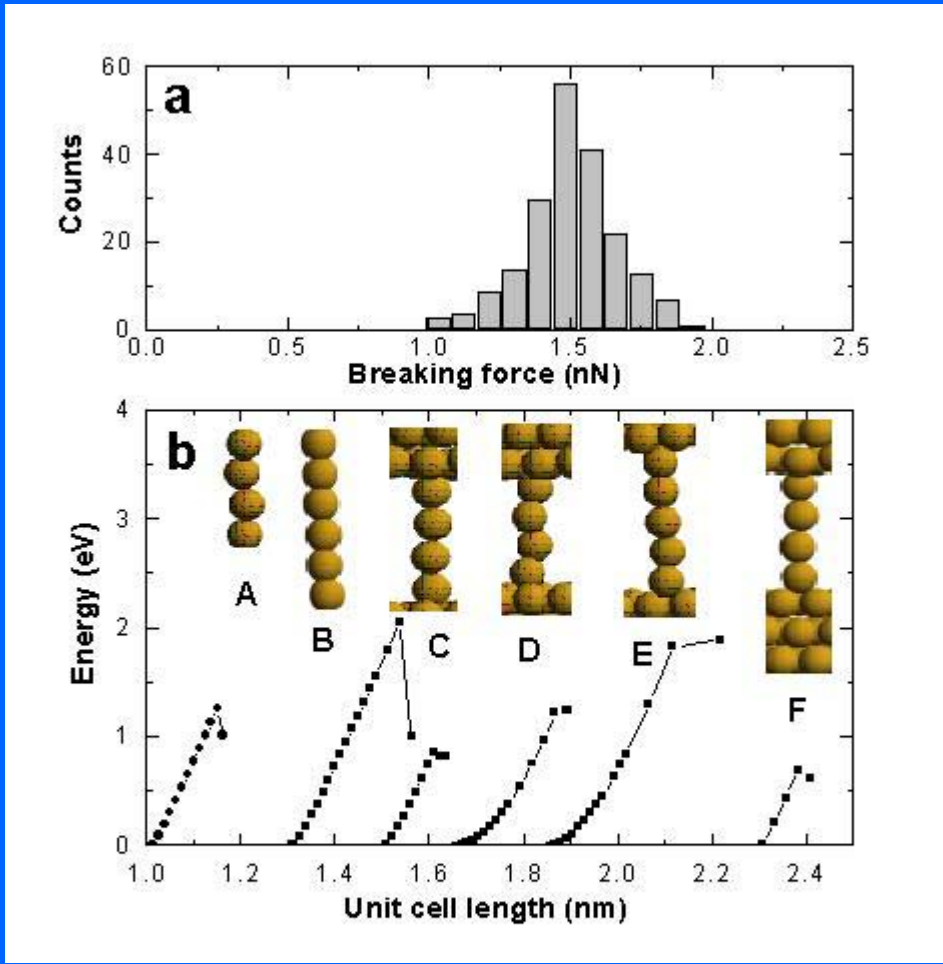
Experimental setup:
- low temperature
- very high mechanical stability ~ 1 pm
- sensor's spring constant ~ 400 N/m

MD simulation using EMT

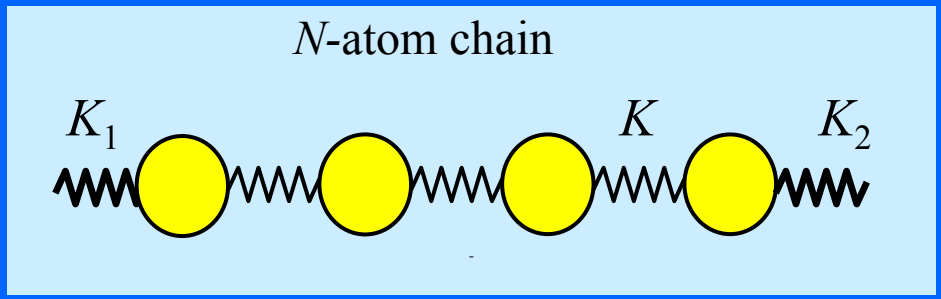
breaking an atomic chain

EXPERIMENT
- breaking force = 1.5 nN
- larger than during pullout
- independent of length

THEORY
- breaking force = 1.4 – 1.6 nN (depends on approximation for exchange-correlation)
- independent of connection to substrate
- bonds in the chain are stronger (x2) than in bulk due to low coordination enviroment



stiffness of an atomic chain

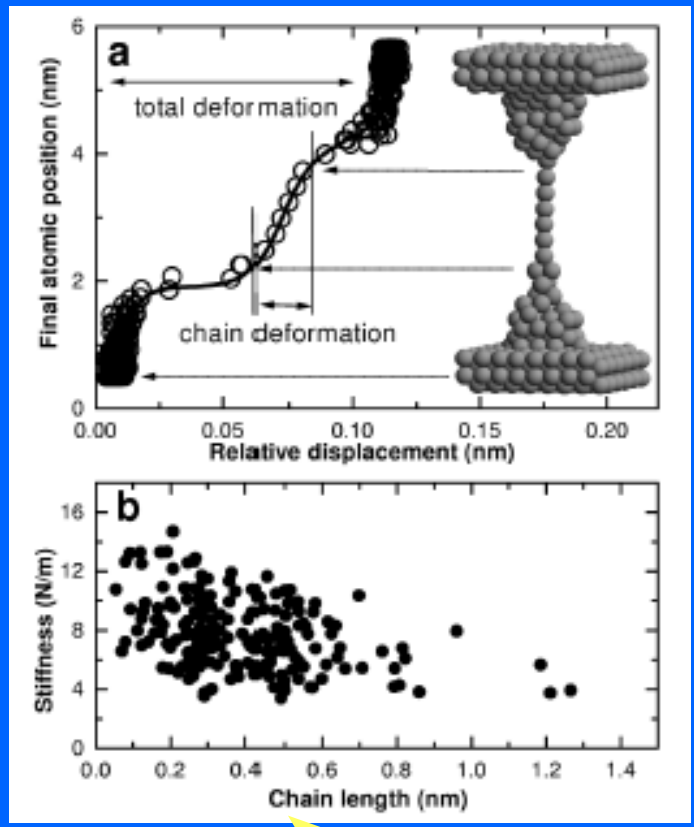


$$K_{tot} = \left(\frac{1}{K_1} + \frac{N}{K} + \frac{1}{K_2} \right)^{-1}$$

Chain can be much stiffer than electrodes:

- connections to electrodes can take most of the deformation

EMT MD simulation



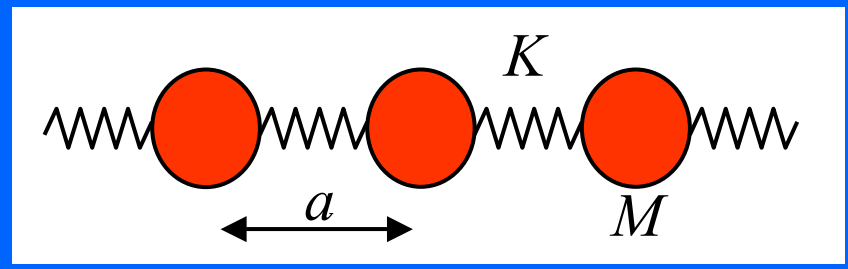
EXPERIMENT

vibration modes of an atomic chain

N = number of atoms

N longitudinal modes

2N transverse modes

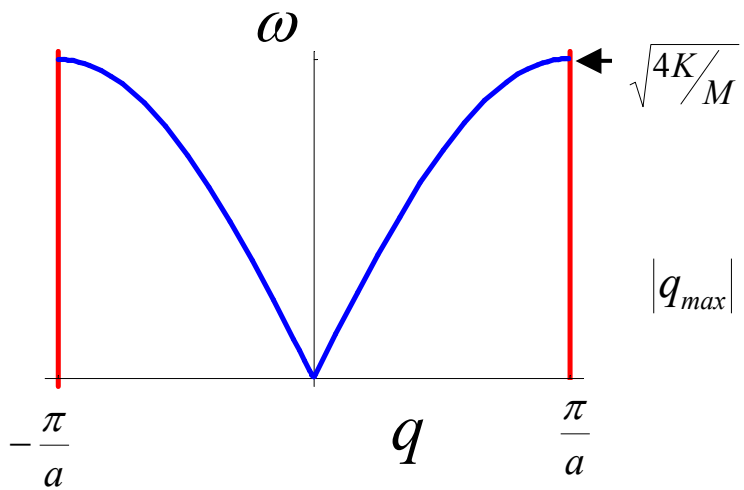


$$\omega^2 = 4\frac{K}{M}\sin^2\frac{qa}{2}$$

For a half filled band

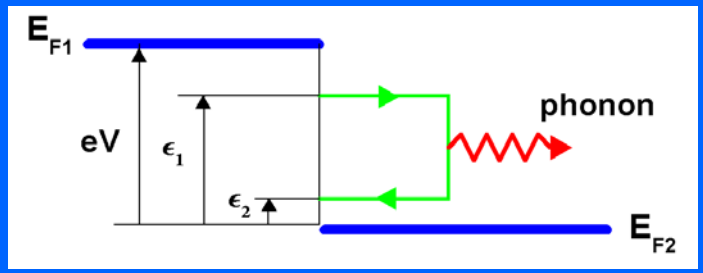
$k_F = \pi / 2a$

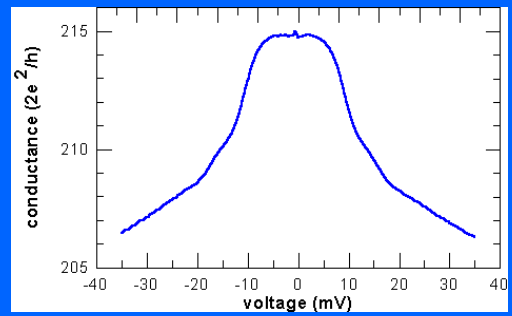
Longitudinal modes



$$|q_{max}| = \frac{\pi}{a} = 2k_F$$

Point-Contact Spectroscopy (PCS)



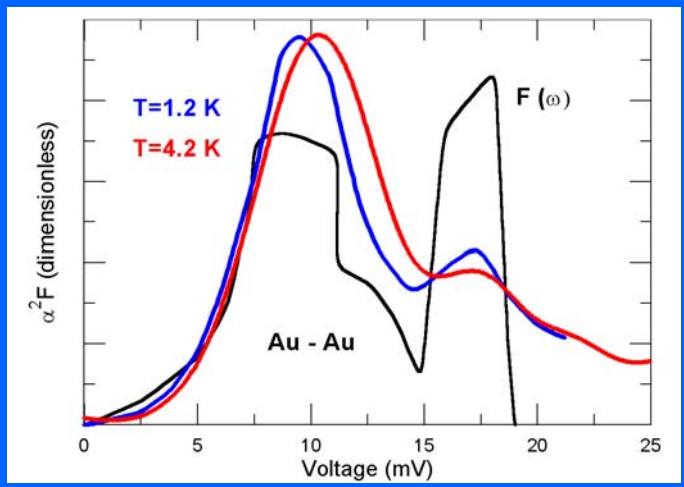


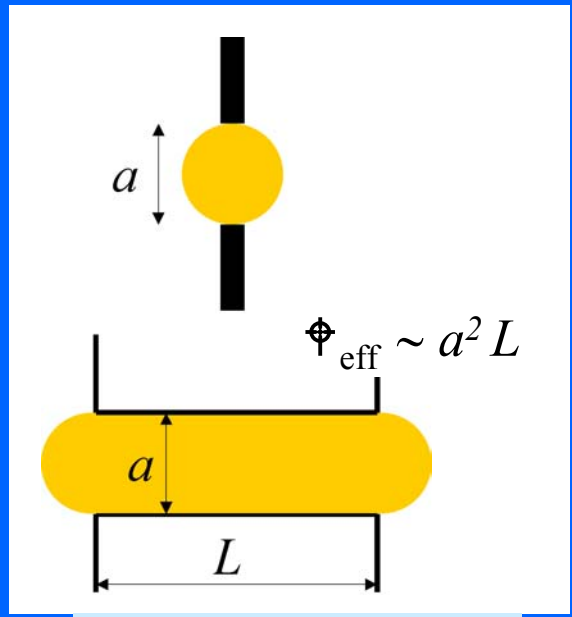
PCS probes local phonon DOS

$$\frac{d^2I}{dV^2} \propto \Omega_{\mathrm{eff}} N(0) \alpha^2 F_{\mathrm{ph}}(eV)$$

$$\Delta G \propto G^{3/2}$$

$$\Delta G / G \propto a$$



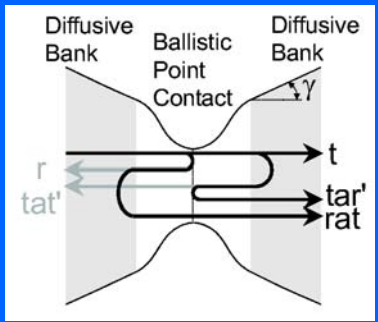


Effective volume for inelastic scattering

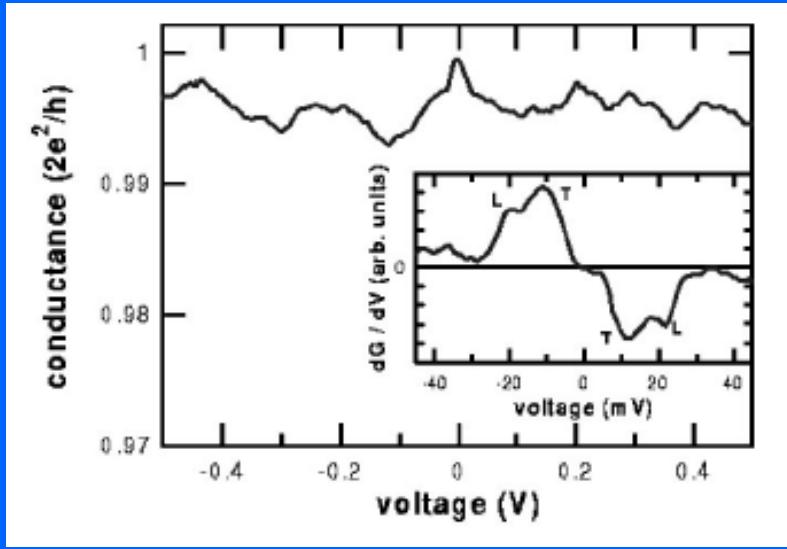
Point-Contact Spectroscopy (PCS) in one-atom contacts

Conductance fluctuations due to elastic scattering near the contact

Ludolph *et al.*, PRL **82**, 1530 (1999)



PCS of a one-atom contact



For one channel

$\Delta G \sim T(1-T)^{1/2}$

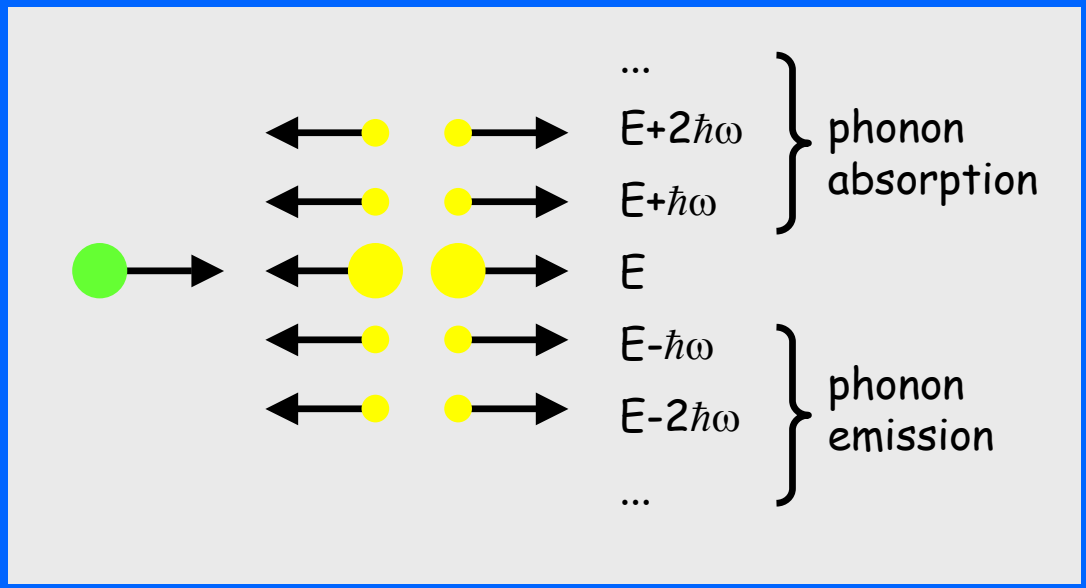
Untiedt *et al.*, PRB **62**, 9962 (2000)

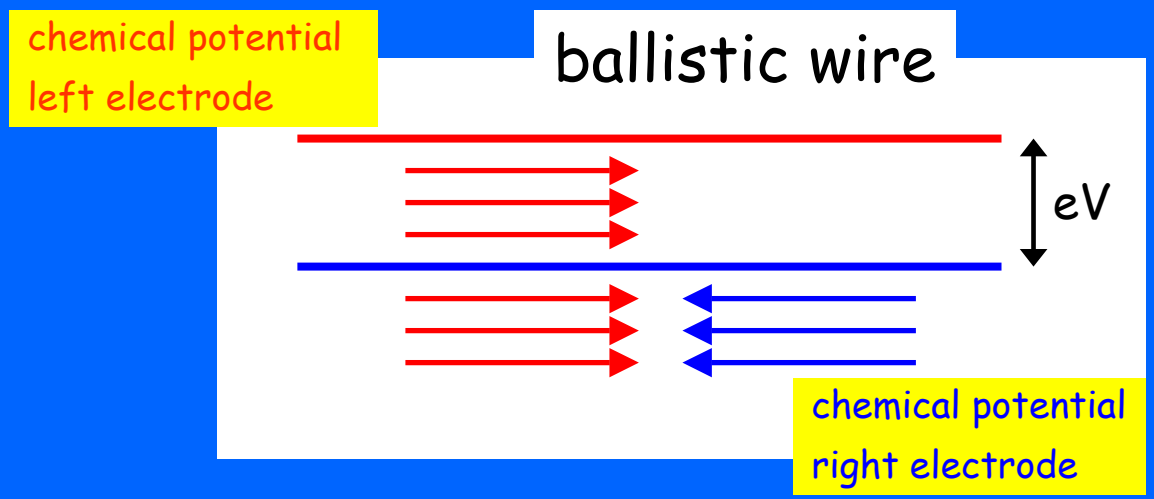
Conductance drop due to phonons:

$\Delta G \propto G^{3/2}$

$\Delta G / G \approx 0.15\ \%$

e-ph interaction in 1d (infinite atomic chain)





only longitudinal modes interact

at low T:

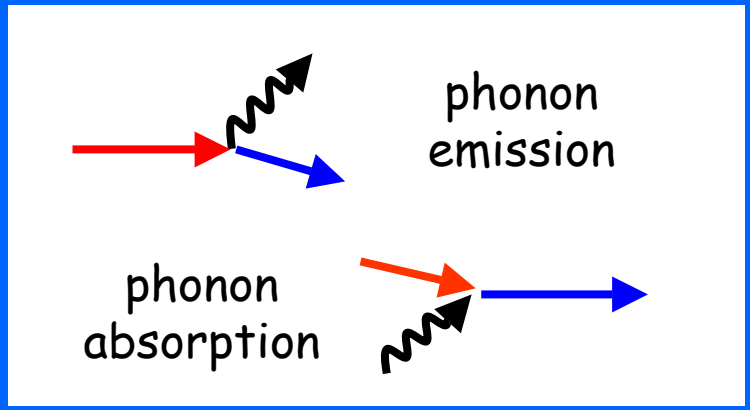
- phonon absorption is always possible
- phonon emission for $eV > \hbar\omega$

e-ph interaction in 1d (infinite atomic chain)

energy conservation

$E_{el} \sim 1\ \text{eV}$
$E_{ph} \sim 1\ \text{meV}$

$E'_{el} \approx E_{el} \Rightarrow |\mathbf{k}'| \approx |\mathbf{k}| \approx k_F$



momentum conservation

emission: $\mathbf{k} = \mathbf{k}' + \mathbf{q} \Rightarrow q = 0$ or $q = 2k_F$

absorption: $\mathbf{k} + \mathbf{q} = \mathbf{k}' \Rightarrow q = 0$ or $q = -2k_F$

1 electron/atom $\Rightarrow$ $k_F = q = \pi / 2a$
$q = \pm \pi / a$

Brillouin zone mode

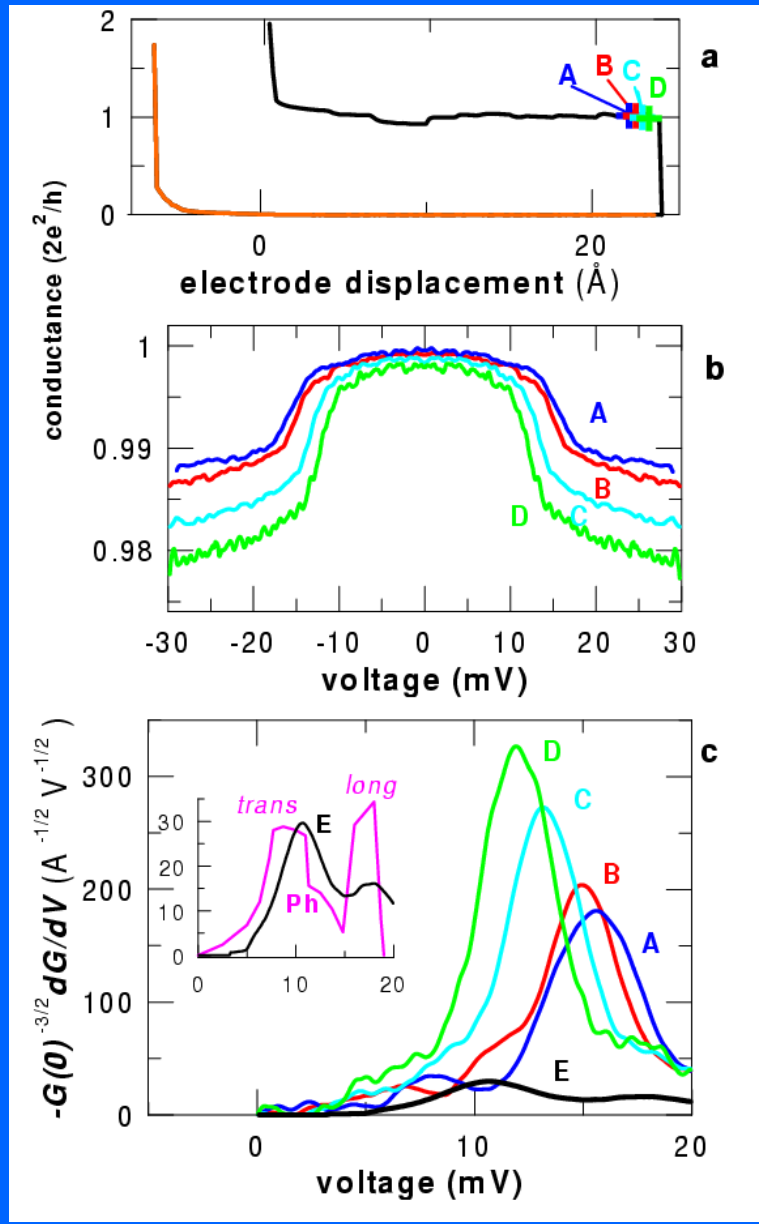
- electrons only interact with Brillouin-zone phonons
- electrons are always backscattered

electron-phonon interaction in an atomic chain

threshold for e-ph interaction:

no inelastic scattering below threshold

- dependence on strain



Phys. Rev. Lett. **88** (2002).

Conductance of a finite wire of length L

- Probability per that an electron in state *k* will emit a phonon in the chain

$$P_k^{em} = \frac{L}{\ell}(n_{q_{\max}} + 1) \qquad \text{for} \quad \varepsilon_k - \varepsilon_F > \hbar\omega_{q_{max}}$$

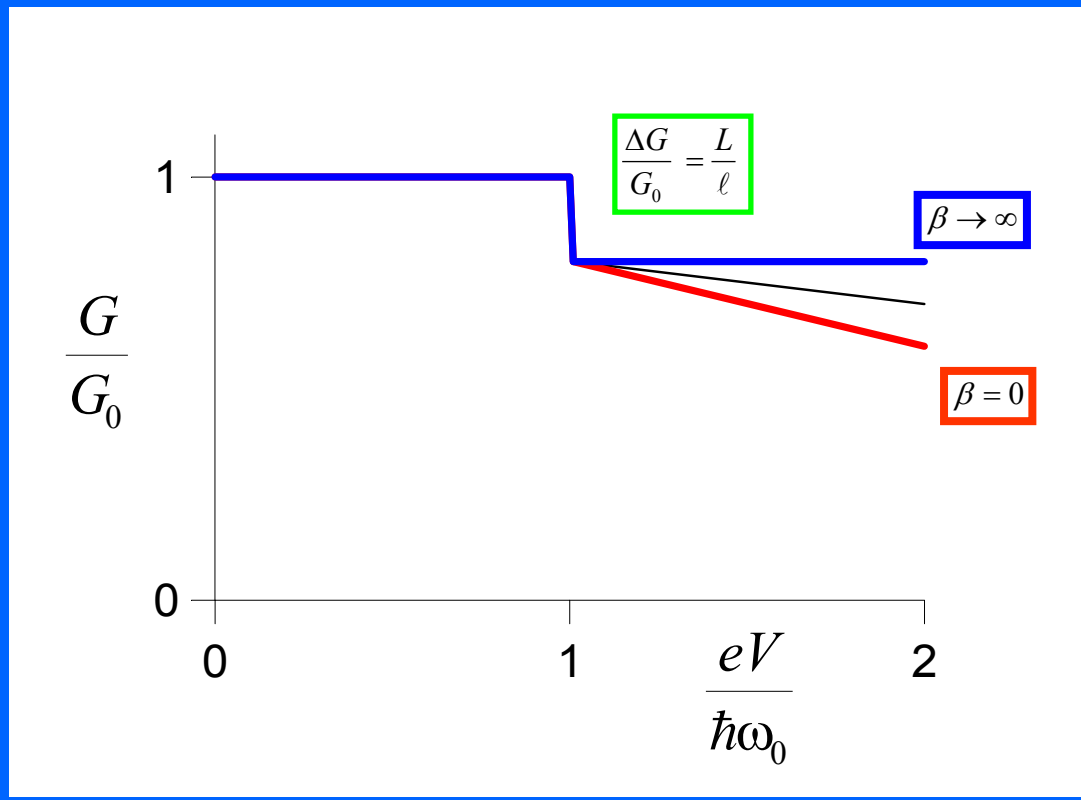
- Probability per that an electron in state *k* will absorb a phonon in the chain

$$P_k^{ab} = \frac{L}{\ell} n_{q_{\max}} \qquad \text{for} \quad \varepsilon_k - \varepsilon_F > 0$$

At $T = 0$, the phonon population n_q is zero and only emission is possible

The conductance of the chain is

$$\frac{G}{G_0} = 1 - \left(P_k^{em} + P_k^{ab}\right)$$



e-ph interaction in atomic chains of different lengths

increasing length:

- peak height increases (linearly)
- frequency is unaffected

stretch:

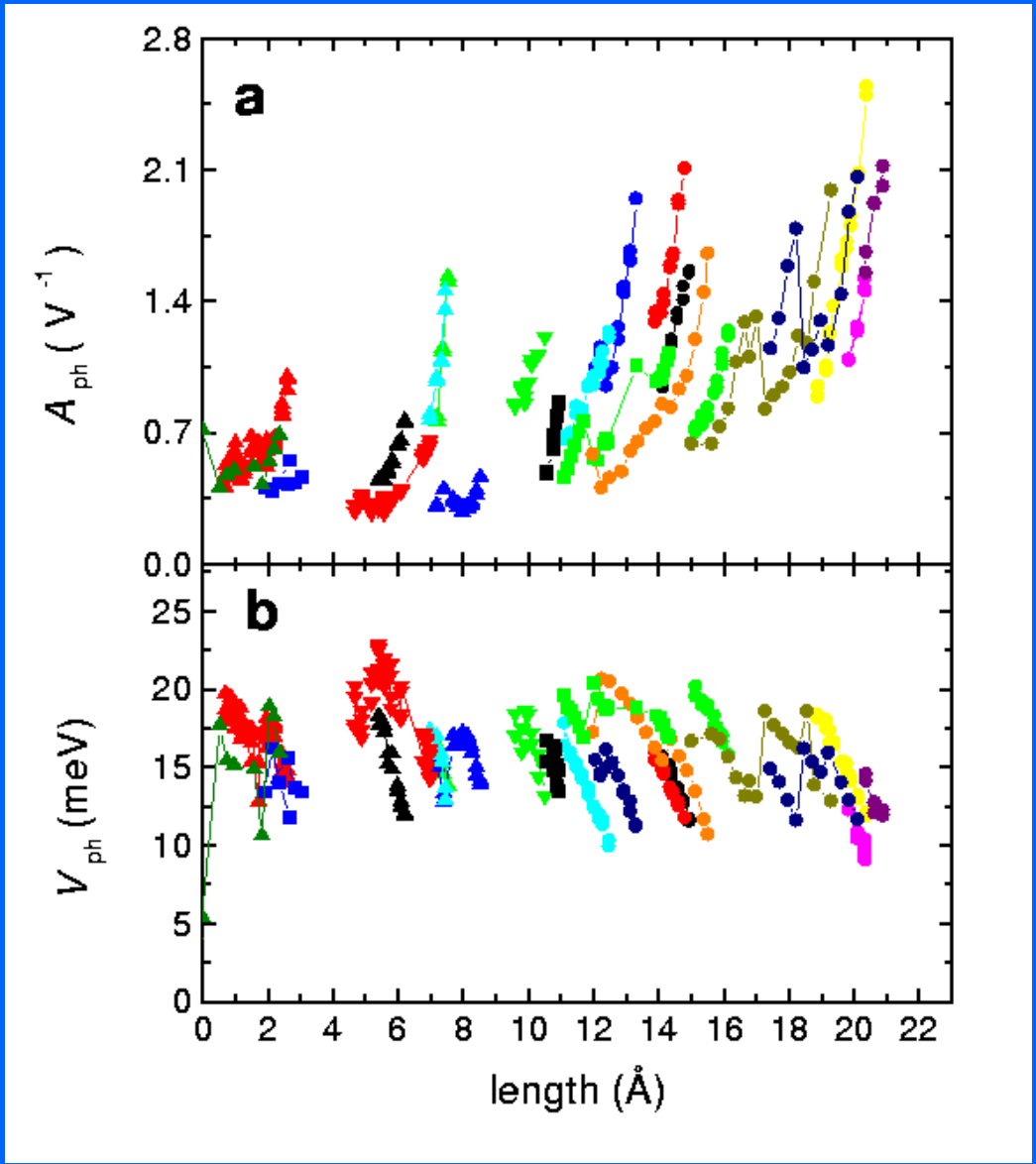
- peak height increases
- frequency decreases

Observed frequencies

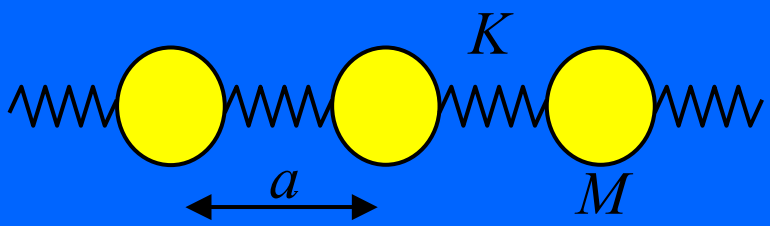
10 - 22 meV (2.3 - 5.3 THz, 80 - 180 cm^{-1})

Interatomic bond elastic constant

$4K = m\omega^2 = 90 - 18$ N/m



dependence on length and frequency



$2k_F$ – mode

$$u_j = A\cos j\pi \;\; \cos\omega t$$

$$E_{kin} = \frac{1}{2} M\omega^2 A^2 N$$

quantization

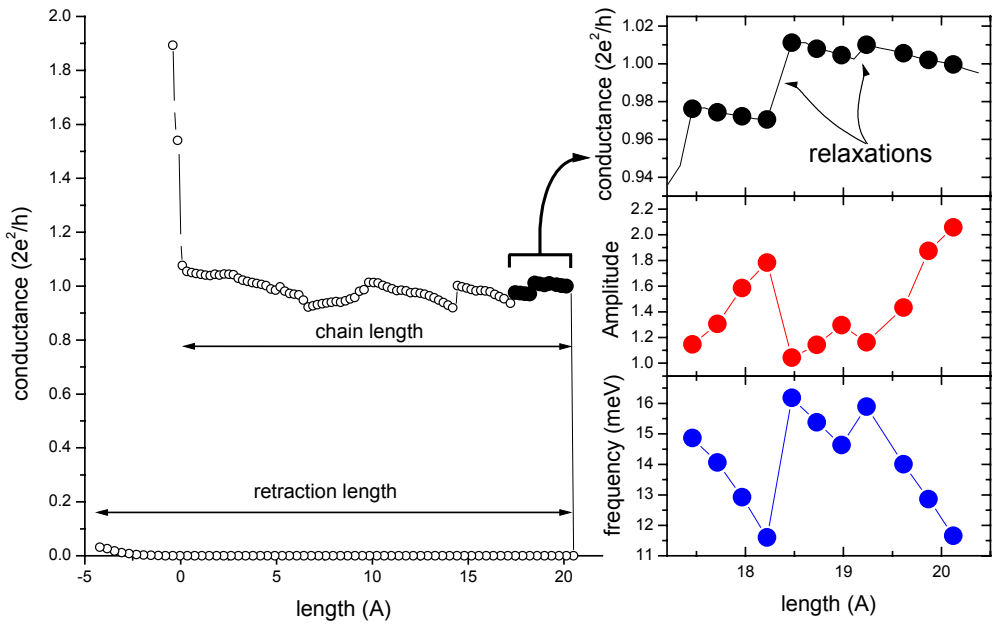
$$E_{kin} = \hbar\omega$$

$$A = \sqrt{\frac{2\hbar}{M\omega N}}$$

scattered wave ~ AL

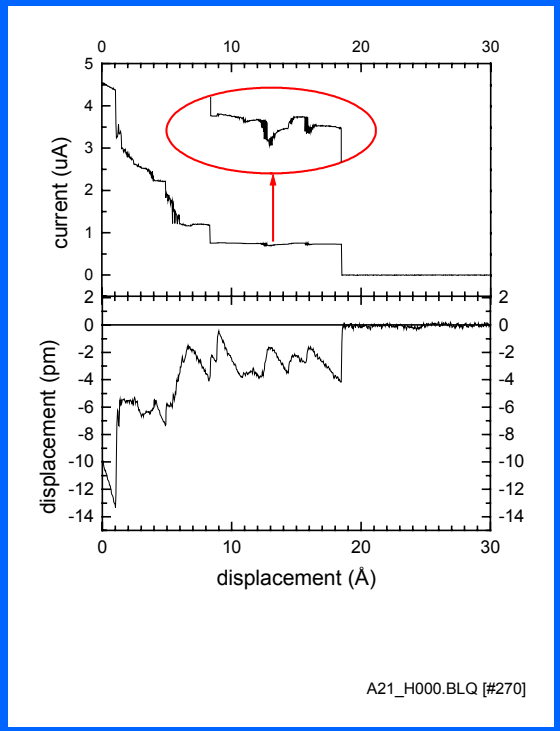
scattered current ~ $A^2L^2 = \frac{2\hbar a}{M}\frac{L}{\omega}$

mechanical relaxations and phonons



elastic stages (linear)

+ atomic rearrangements (relaxation)



force relaxation ⇒ amplitude and frequency relaxations

Au atomic chains

- Very stable at low temperature
- One quantum channel (Au)
- Enormous current densities
- Strength interatomic bonds: stronger than bulk
- Stiffness of interatomic bonds
- Vibrational modes
- Electron-phonon interaction

Future work

- Formation mechanisms
- Equilibrium structure
- Dissipation and heat conduction at the nanoscale
- Coupling of mechanical and electrical properties
- Influence of adsorbates on transport
- Stability against Peierls distortions
- Hybrid chains