Current-induced forces
Electromigration

Indium atom transport over CNT

TEM image

CNT

In nanoparticle

Atomic steps on Ag(111)

Current induced cleaning of graphene

Basic concepts of electromigration

\[ \vec{F} = \left( eZ_d^* + eZ_w^* \right) \vec{E} \]

Effective valence. For metals typically \(-20 \ldots -50\)

Direct force: associated with Landauer dipole
Towards microscopic understanding of current induced forces

- Theory is mostly phenomenological
- Experiments probing forces on atomic scale are almost absent
Current induced single-atom switching

Current-induced single switching

Low tunnel current (molecule not rotating)

STM of molecules adsorbed to Cu(111)

Tierney et al., Nature Nanotechn. 6, 625 (2011)
See also: Perera et al., Nature Nanotechn. 8, 46 (2013)
Current-driven atomic waterwheels

Daniel Dundas*, Eunan J. McEniry and Tchavdar N. Todorov

A current induces forces on atoms inside the conductor that carries it\(^1\). It is now possible to compute these forces from scratch, and to perform dynamical simulations of the atomic motion under current\(2-6\). One reason for this interest is that current can be a destructive force—it can cause atoms to migrate, resulting in damage and in the eventual failure of the conductor. But one can also ask, can current be made to do useful work on atoms? In particular, can an atomic-scale motor be driven by electrical current\(^7-9\), as it can be by other mechanisms\(10-13\)? For this to be possible, the current-induced forces on a suitable rotor must be non-conservative, so that net work can be done per revolution. Here we show that current-induced forces in atomic wires are not conservative and that they can be used, in principle, to drive an atomic-scale waterwheel.

In this work we model a current-carrying atomic wire within the Ehrenfest approximation. This is a form of quantum-classical operator (see Methods). The curl of the force vanishes at equilibrium but, in general, it is nonzero when there is a current. Then the force itself is not the gradient of a potential and is not conservative. From the practical viewpoint, if an atom can be caught in a closed orbit, the non-conservative force can continually do work on it, creating a nanoscale waterwheel.

We assess this effect for the system in Fig. 1b: an atomic wire with a bend. The candidate for the waterwheel is the corner atom, labelled 0. We investigate its dynamics in the \(x-y\) plane using a nearest-neighbour single-orbital orthogonal tight-binding model. Here, \(H(<0)\) denotes the hopping integral in the chain, and \(H'(>0)\) its derivative with distance. We set the bend angle at \(\alpha = 90^\circ\) and give the corner atom an on-site energy shift \(E_0 = E_c\). All other on-site energies are set equal to zero. In this simple tight-binding model the onsite energy can be thought of as a way of varying the chemical identity of an atom. We can derive expressions for the current-induced force \(\Delta F = F(V, R) - F(0, R)\).
Atomic water wheel

The Berry force


\[ H = \sum_i \left( \frac{P_i^2}{2M_i} + V(R_i) \right) + H_c(R) \]

\[ \Psi = \psi(R)\phi(R) \]

The electron wavefunction \( \phi \) depends on the positions of the ions \( R \). Projecting out the electronic states,

\[ H_{\text{eff}} = \sum_i \frac{(P_i + A_i(R))^2}{2M_i} + W(R) \]

\[ A_i(R) = i\langle \phi(R) | \nabla_i \phi(R) \rangle \]

Leads to an effective “magnetic field”

\[ B_{ij} = \frac{\partial A_i}{\partial R_j} - \frac{\partial A_j}{\partial R_i} \]

Semi-classical Langevin equation for the motion of ion cores

\[ m\ddot{R} = -D\dot{R} - \eta \dot{R} + \mathcal{A}R + \mathcal{B}\dot{R} + F_f \]
Model system: two degrees of freedom


\[ m\ddot{R} = -DR - \eta \dot{R} + AR + B\dot{R} + F_f \]

\[
\begin{pmatrix}
\ddot{x} \\
\ddot{y}
\end{pmatrix}
= -
\begin{pmatrix}
\omega_1^2 & a \\
-a & \omega_2^2
\end{pmatrix}
\begin{pmatrix}
x \\
y
\end{pmatrix}
- 
\begin{pmatrix}
\eta & b \\
-b & \eta
\end{pmatrix}
\begin{pmatrix}
\dot{x} \\
\dot{y}
\end{pmatrix}
\]

\[
\Omega_{\pm} \approx \omega_1 + \frac{\Delta - i\eta}{2} \pm \frac{1}{2} \sqrt{\Delta^2 - \left(\frac{a}{\omega_1} + ib\right)^2}
\]

\[
\text{Im} \, \Omega_{\pm} \approx \frac{-\eta}{2} \pm \frac{ab}{2\omega_1\Delta}
\]
A model system: chain of Au atoms

Experiments of current-induced breaking

- Rupture Trace
  - Point to stop trace and start to heat it increasing Vbias;
  - Burning point (Bp)

- Start point Plateau (Sp)
- Length plateau (L)

- Conductance $G_0$
  - Piezo displacement (V)

- Current $I$ (µA)
  - Voltage $V$ (V)

$V_{break}$
Experiments of current-induced breaking

Experiments of current-induced breaking

Experiments of current-induced breaking

Sabater, Untiedt, van Ruitenbeek, to be published
Experiments of current-induced breaking

Initial stability test at 10mV

Sabater, Untiedt, van Ruitenbeek, to be published
Pt chain: higher energy runaway mode
Pt chain: higher energy runaway mode
Can we do these experiments in a more controlled way?
Low-temperature STM

Au (111) atomic resolution

Electronic edge states

“The Beast”
Deposition of single atoms by low-T evaporation

Au ad-atoms over Au(111) surface
Lateral manipulation of atoms
Single atom manipulation: Au on Au(111)
Single atom manipulation: Au on Au(111)
Single atom manipulation: Au on Au(111)
Single atom manipulation: Au on Au(111)
Single atom manipulation: Au on Au(111)
Single atom manipulation: Au on Au(111)
Connected chain formation
Connected chain formation
Connected chain formation
Connected chain formation

Three atoms chain

😊😊😊
Single-molecule conductors

47 cycles

Courtesy: Wagner C. Fournier (Tautz) et al., PRB 84, 035435 (2011)
Single-molecule conductors

Fournier (Tautz) et al., PRB 84, 035435 (2011)
Building atomic conductors between tip and sample
3-dimensional STM control

feedback

Force field simulation
Force Field Simulation

Interatomic potential\(^1\):
Second-moment approximation (SMA) to the tight-binding Hamiltonian

1. R Cortes Huerto (Saul) et al., PRB 88, 235438 (2013)
Possible process suggested by simulation
STM control: The game

feedback
Can also do break junctions

feedback
The team

Christian Wagner
Sumit Tewari
Jacob Bakermans
Federica Galli
Roel Smit
Carlos Untiedt
Carlos Sabater
Tadashi Shiota
Raphael Muller
Marius Trouwborst
Sasha Vrbica
Irene Battisi
Elena Tartaglini
Jan Aarts

Support from

Sylvestre Bonnet
Tchavdar Todorov
Daniel Dundas
Mads Brandbyge
Stefan Tautz
Conclusions
CONFIRMED SPEAKERS

ADRIAN BACTOLD The Institute of Photonic Sciences
CLAUDE BOURBONNAIS University Sherbrooke
MADS BRANDTBYGE Technical University of Denmark
JUAN CARLOS CUEVAS Autonomous University of Madrid
MOHAMMED EL-NAGGAR University of Southern California
KARL-HEINZ ERNST University Zurich
FERDINAND EVERS Karlsruhe Institute of Technology
LEONHARD GRILL Fritz-Haber-Institut
RICHARD MCCREERY University Alberta
RON NAAMAN Weizman Institute of Science
JEAN-PIERRE SALVAGE Louis Pasteur University
STEFAN TAUTZ Forschungszentrum Jülich
TCHAVDAR Todorov Queen's University Belfast
SENSE JAN VAN DER MOLEN Leiden University
WILFRID VAN DER WIJL University of Twente
HERRE VAN DER ZANT Delft University of Technology
LATHA VENKATARAMAN Columbia University
FLORIAN VON WROCHEM SONY Germany
DOMINIQUE VUILLAUME University Lille
WULF WULFHEKEL Karlsruhe Institute of Technology

FIRST CIRCULAR

MOLECULAR MACHINES AND DEVICES

BEILSTEIN NANOTECHNOLOGY SYMPOSIUM 2014

BEILSTEIN-INSTITUT
TRAUERNHER STR. 7-9
60487 FRANKFURT AM MAIN
WWW.BEILSTEIN-INSTITUT.DE

16 - 18 SEPTEMBER, 2014
POTSDAM / GERMANY