Modelling emergent effects in low coordination geometries during metallic nanojunction formation

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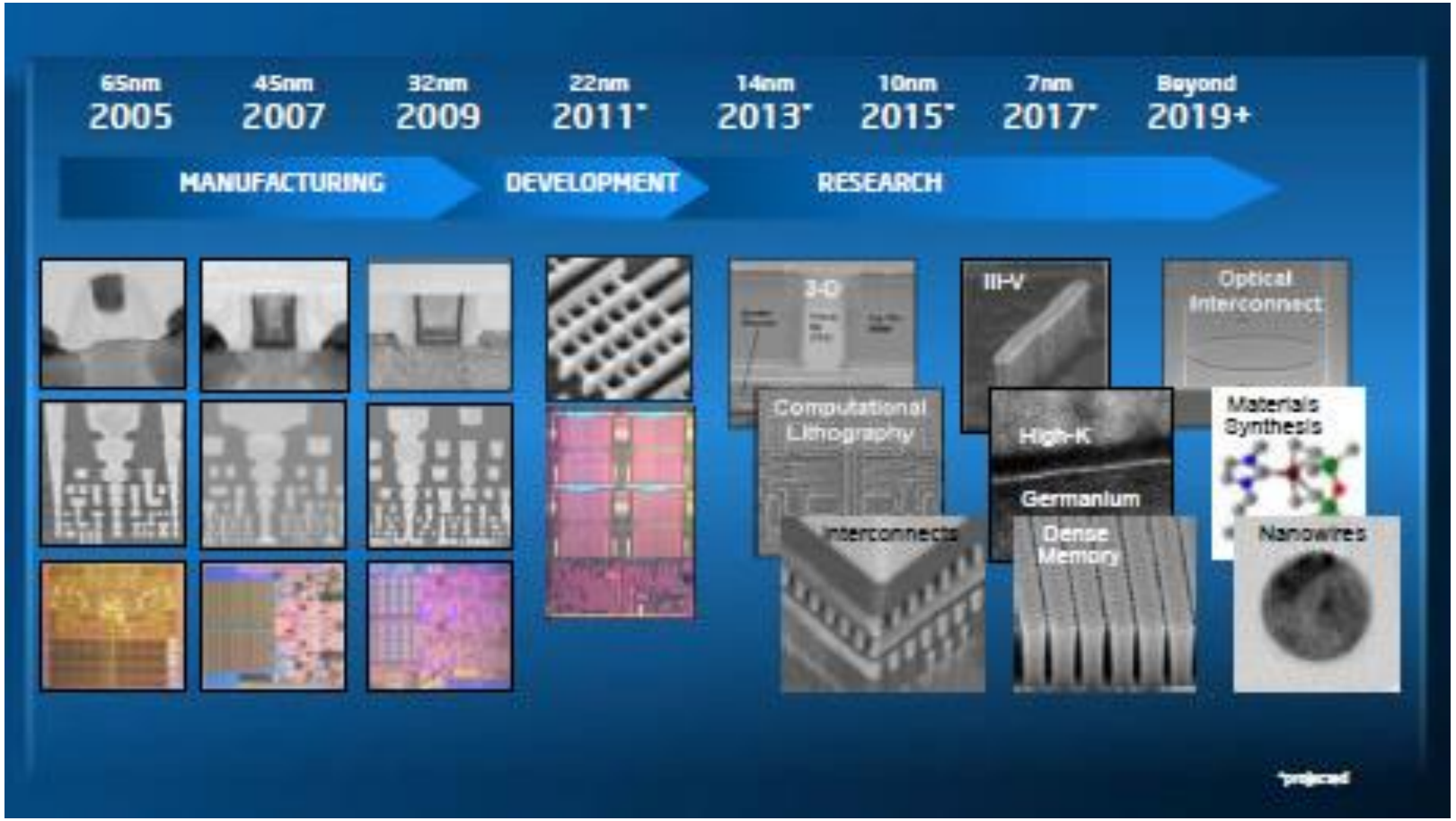
Outline

- Motivation
- Theoretical methods for modelling nanocontacts
- Jump to contact: Gold vs Copper
- More complex materials: BCC vs FCC and ferromagnetism
- Conclusion and outlook

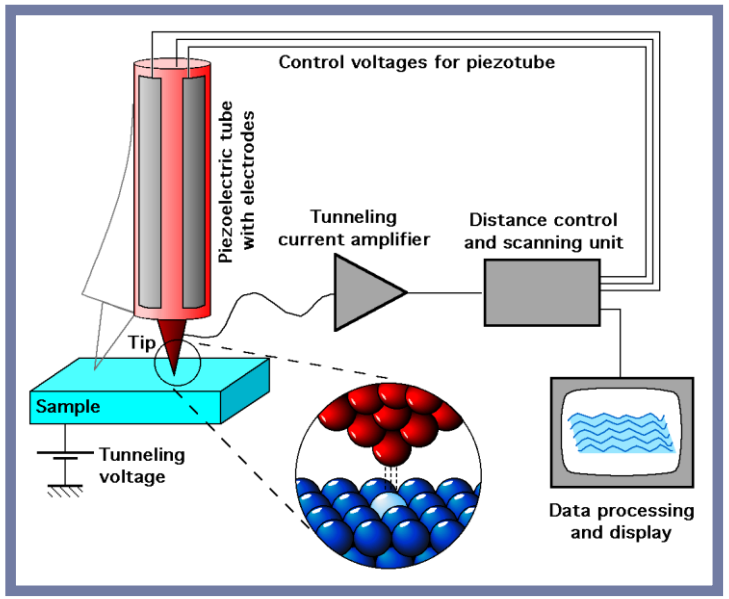
Limits to miniaturization of microelectronics



Source: www.cdrinfo.com/Sections/News/Details://.aspx?NewsId=30438

New approaches are needed at the nano-scale level

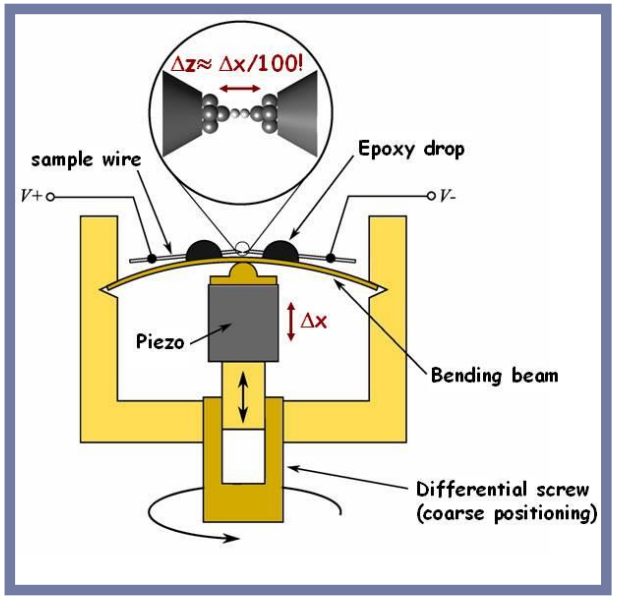
The nanoscale can be probed and manipulated by a scanning tunneling microscope (STM) or mechanically controllable break junction (MCBJ)



Schematic representation of an STM

Source: Wikipedia

URL http://en.wikipedia.org/wiki/Scanning_tunneling_microscope

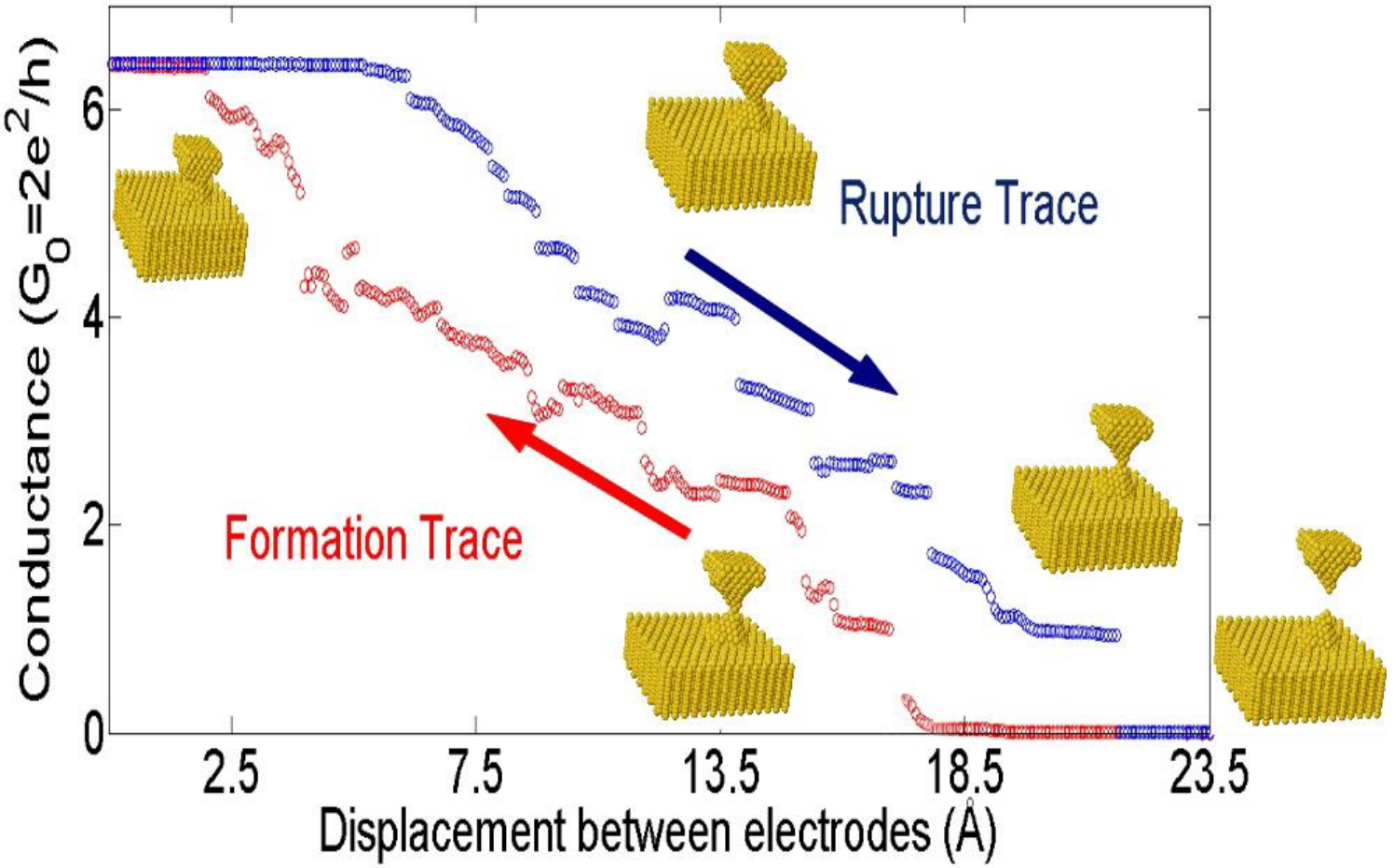


Schematic representationof an MCBJ.

Source: CINaM - Centre Interdisciplinaire de Nanoscience de Marseille

Conductance and IV characteristics can be measured with an STM or MCBJ as nano-sized contacts are made or broken

STM traces of conductance vs displacement between gold contacts at 4.2K



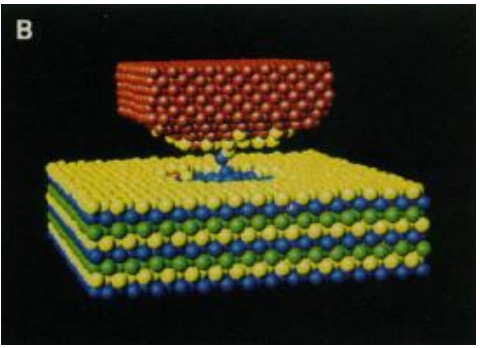
C. Sabater, PhD diss.,University of Alicante, 2013

It is not simple to interpret this behavior at the atomic level, merely by looking at conductance traces or IV characteristics. BUT, …

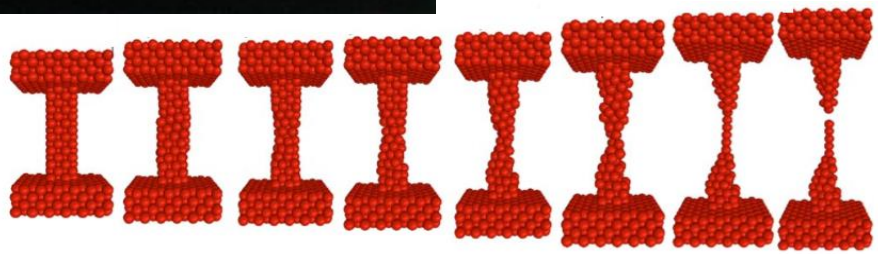
… atomistic simulations can model nanocontacts

1. Classical molecular dynamics (CMD) simulations give dynamical information at the atomic level: the motion of the atoms

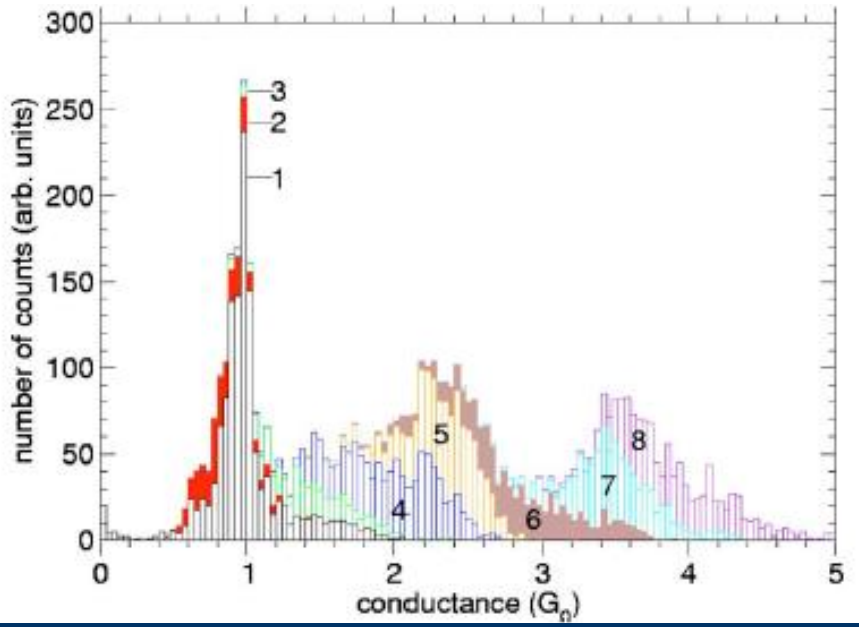
2. Quantum transport calculations on CMD structures yield charge transport across nanocontacts



Landman, U. *et al*. Science **248**, 454 (1990)



Dreher, M. *et al*., Phys. Rev. B **72**, 454 (2005)



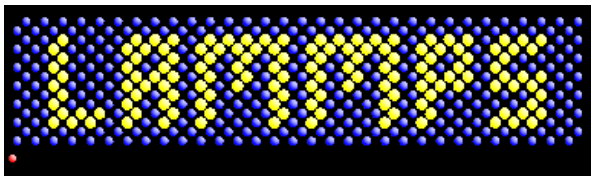
E.g., the quantization of conductance in metal nanocontacts was first convincingly explained with the help of CMD

Olesen, L. *et al.*, Phys. Rev. Lett. **72**, 2251 (1994)

Theoretical tools to model nanocontacts

LAMMPS (Large-scale atomic/molecular massively parallel simulator)

http://lammps.sandia.gov/



- Embedded Atom Method (EAM) potential:

  Daw, M. and Baskes, M., Phys. Rev. Lett. **50**, 1285 (1983)

$$U = \sum_{i} F(\rho_i) + \frac{1}{2} \sum_{\substack{i,j \\ (i \neq j)}} \phi(r_{ij})$$

- Forms of ρ_i, $F(\rho_i)$ and $\phi(r_{ij})$ from: Wadley, H. N. G., Prog. Mater. Sci., **46**, 329 (2001)

Besides bulk properties, also fitted to a surface property (heat of sublimation), for 18 metals

Theoretical tools to model nanocontacts

- Full **spin-lattice** dynamics (SLD) in **SPILADY** to model interactions between ferromagnetic atoms **more realistically**:

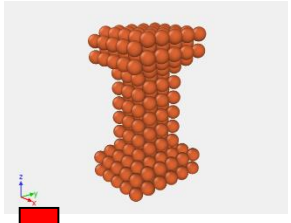
http://www.ccfe.ac.uk/spilady_code.aspx

$$H = \sum_i \frac{\mathbf{p}_i^2}{2m_i} + U - \frac{1}{2}\sum_{i,j} J_{ij}\mathbf{e}_i \cdot \mathbf{e}_j$$

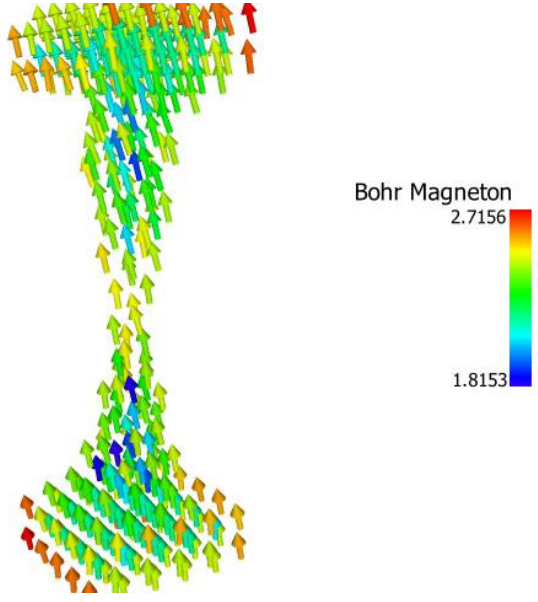
P.-W. Ma *et al*., Comput. Phys. Commun. **207** 350–361 (2016)

Scalar-magnetic part of (EAM) potential, ***U***, from:

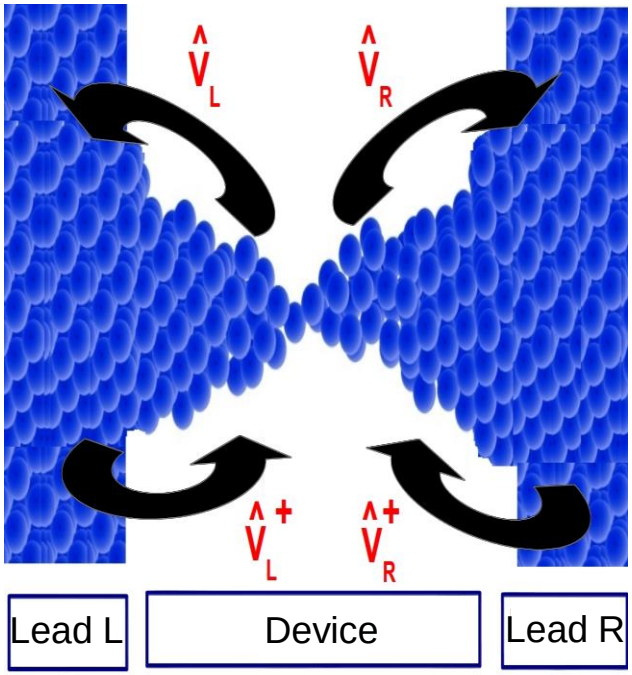
Dudarev S. L. And Derlet P. M., J. Phys.: Condens. Matter **17,** 7097 (2005)



Stretched at 1 m/s



Landauer theory of Quantum Transport



C. Sabater, PhD diss.,University of Alicante, 2013

R. Landauer, J. Res. Dev. **1**, 223 (1957)

$$G(E_F) = \frac{2e^2}{h} T(E_F) = G_0 T(E_F)$$

Green Functions

Partitioning Method

$$T(E_F) = Tr\left[\widehat{G_D}(E)\widehat{\Gamma_R}(E)\widehat{G_D}^{d}(E)\widehat{\Gamma_L}(E)\right]$$

S. Datta, Superlattices and Microstructures, **28**, 253 (2000)

.G: **ANT.Gaussian** (Alicante atomistic computation applied to NanoTransport)

J. J. Palacios *et al*., Phys. Rev. B **64**, 115411 (2001)

Establishes a direct connection between calculated conductance (TB – tight-binding/DFT – density functional theory) and STM/MCBJ

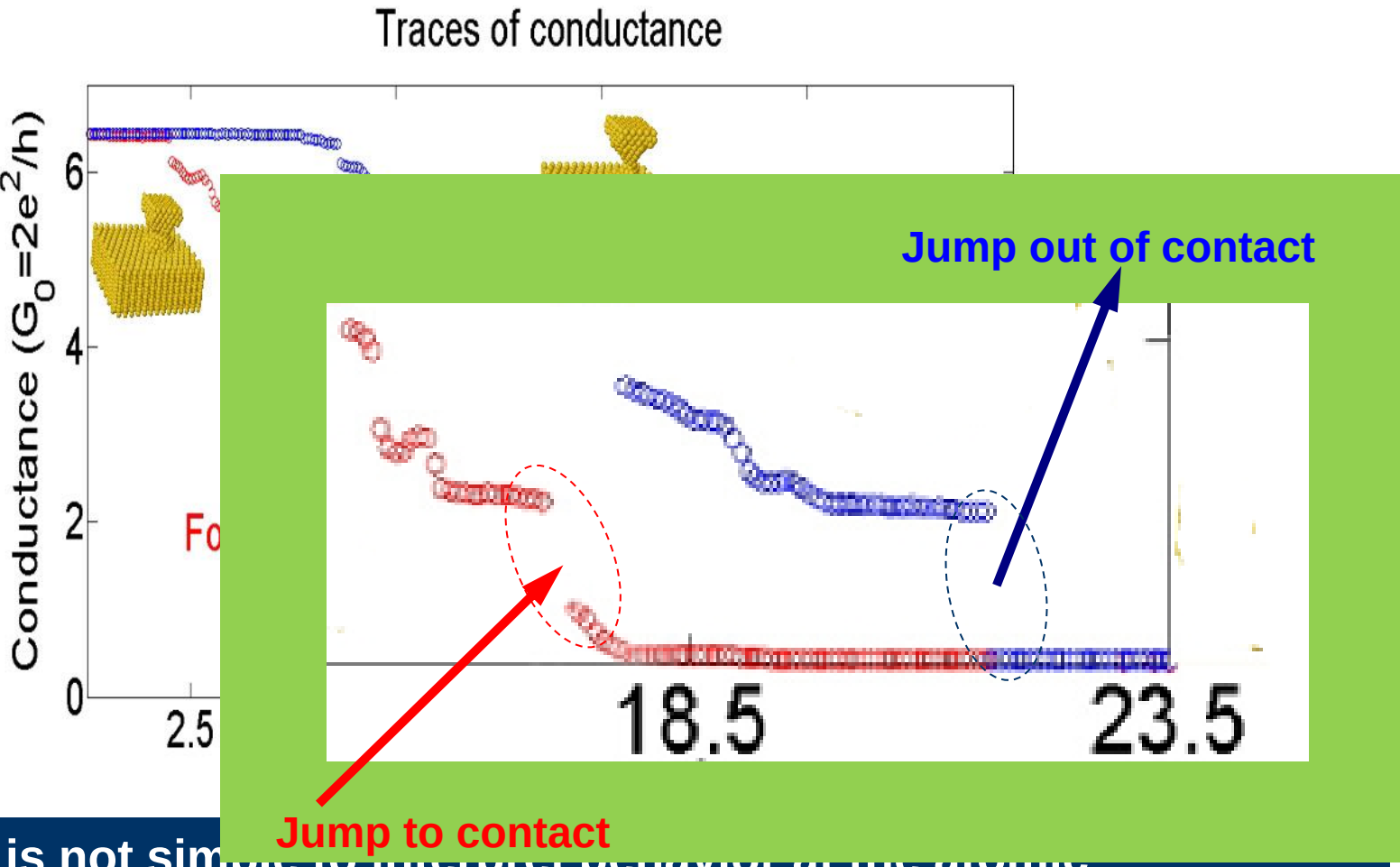
Examples of emergent properties that atomistic simulations can explain?

- The conductance **jump** at first contact between two gold nanoprobes, sometimes not exhibited by gold's isoelectronic analogues, copper (and silver).

- The **discrepancy** between experimental and theoretical peaks in conductance histograms of **BCC** ferromagnetic iron nanocontacts. (**FCC** ferromagnetic Nickel does not follow this trend).

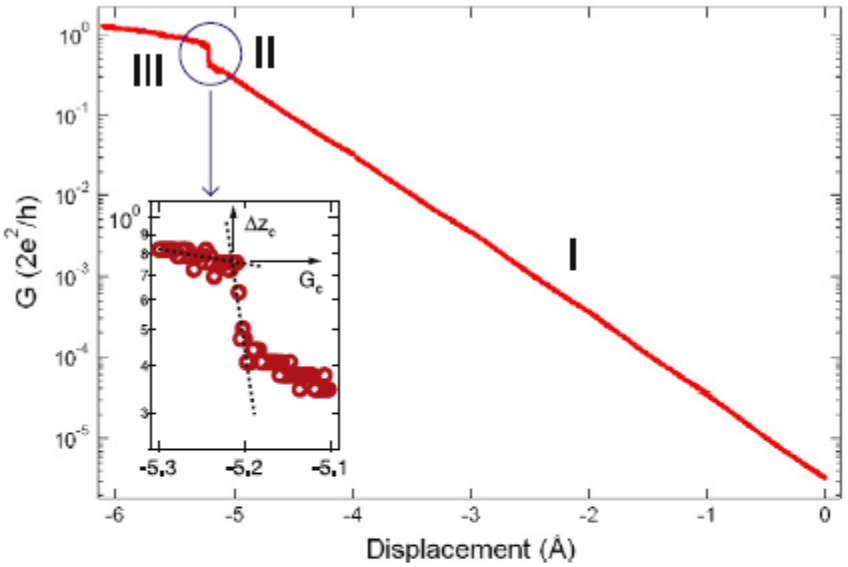
Jump to or out of contact

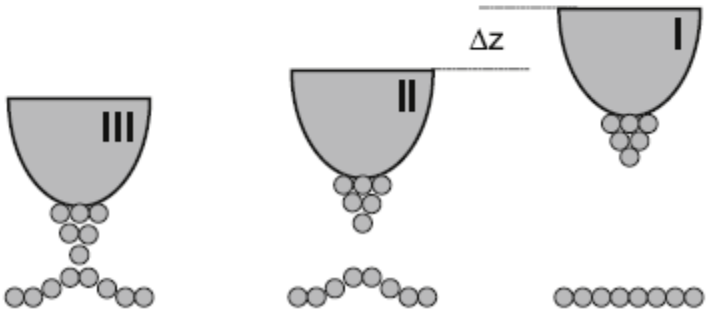
Traces from an STM measurement of conductance between gold contacts



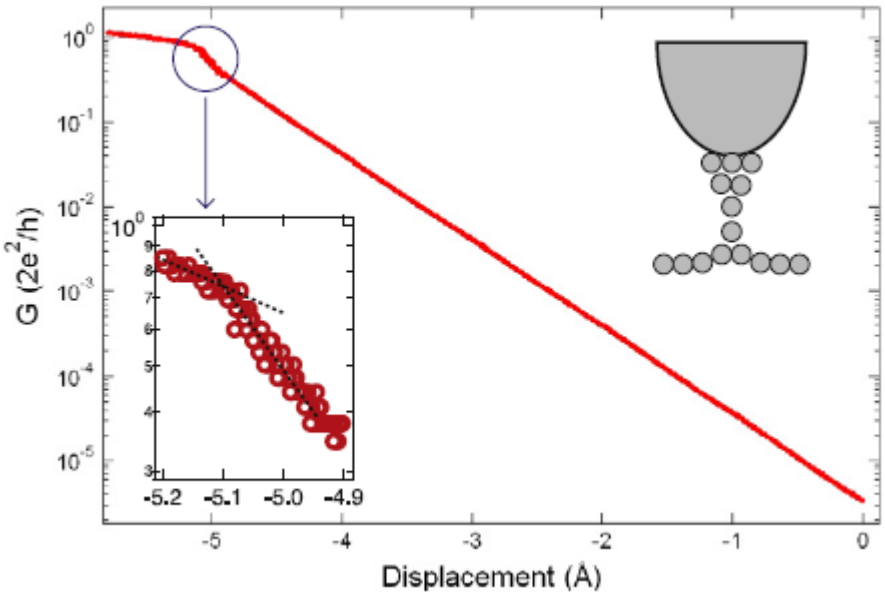
It is not simple to interpret behavior at the atomic level merely by looking at conductance traces

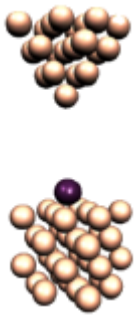
Jump to contact (experiment): Copper





Kröger J., Néel, N. and Limot, L.
J. Phys.: Condens. Matter **20** (2008) 2230010

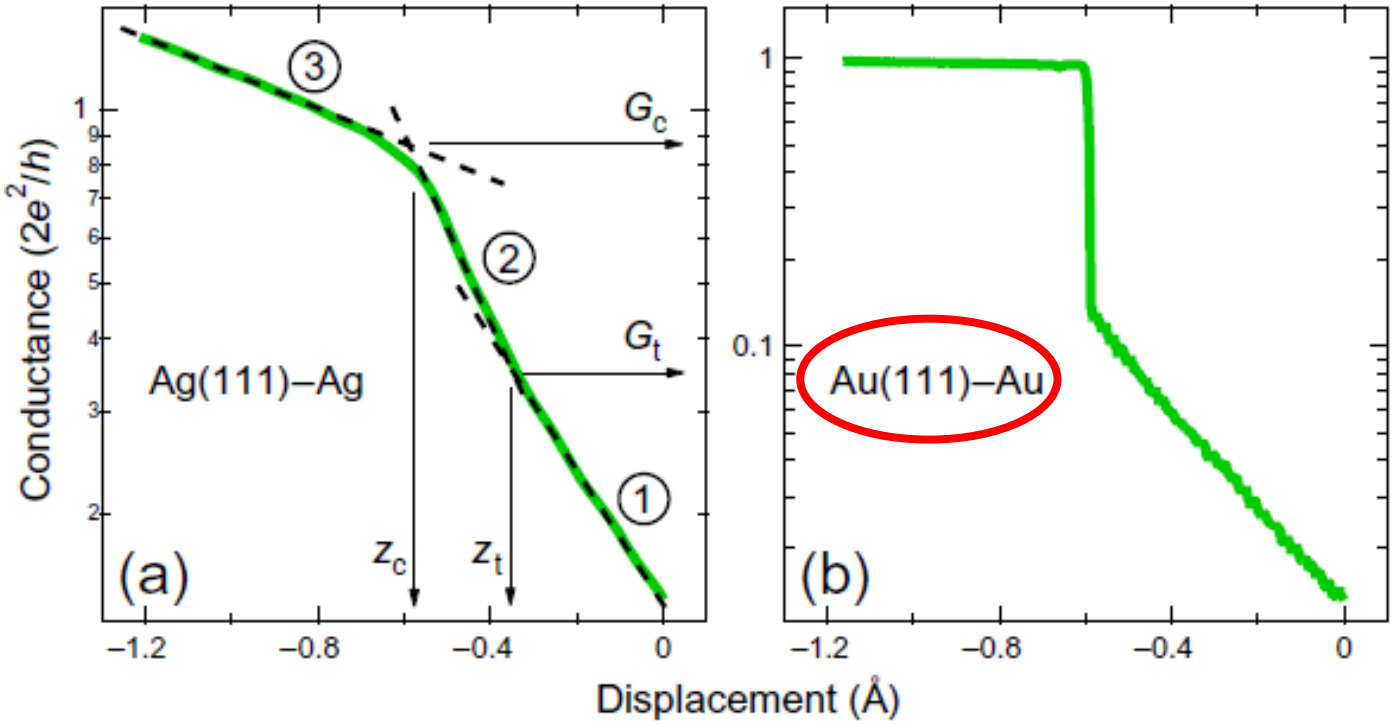


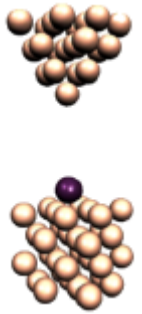


Neél, N. *et al*.
PRL **98,** 016801
(2007)

Even the same material (Cu) can exhibit jump to contact or NOT

Jump to contact (experiment): Gold





Neél, N. *et al*. PRL **98,** 016801 (2007)

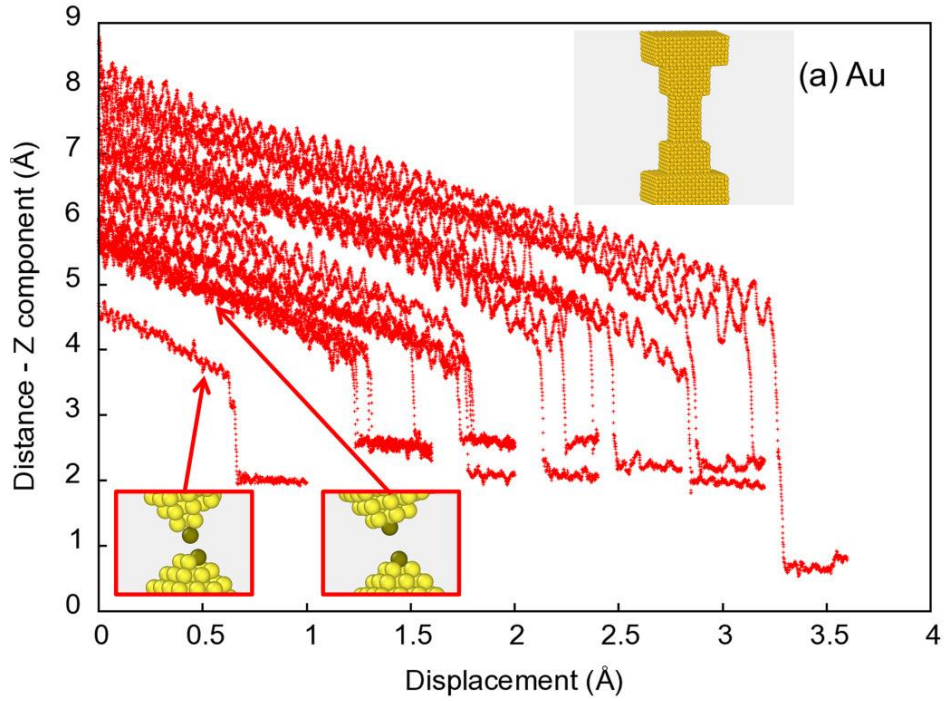
Kröger J. *et al*. New J. Phys. **11**, 125006 (2009)

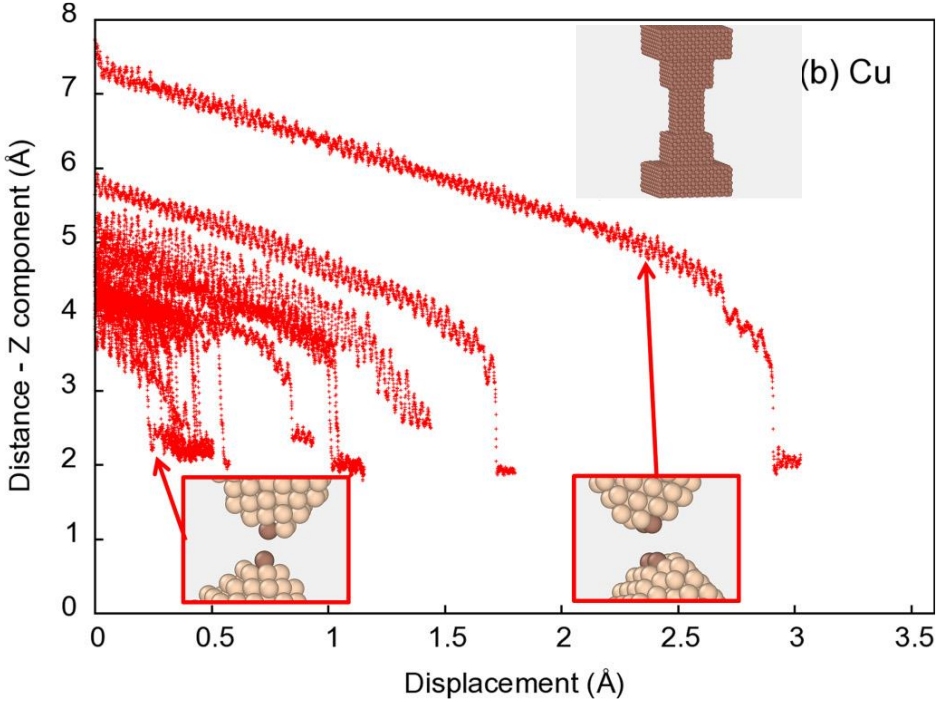
Gold, unlike Copper and Silver, ALWAYS exhibits jump to contact!

Untiedt C. *et al*., PRL **98**, 206801 (2007)

Jump to contact (theory): Gold vs Copper

- Classical molecular dynamics (CMD) results from **Cyclic Loading** of **MCBJ**-type (001) Au and Cu nanocontacts at **4.2K**:



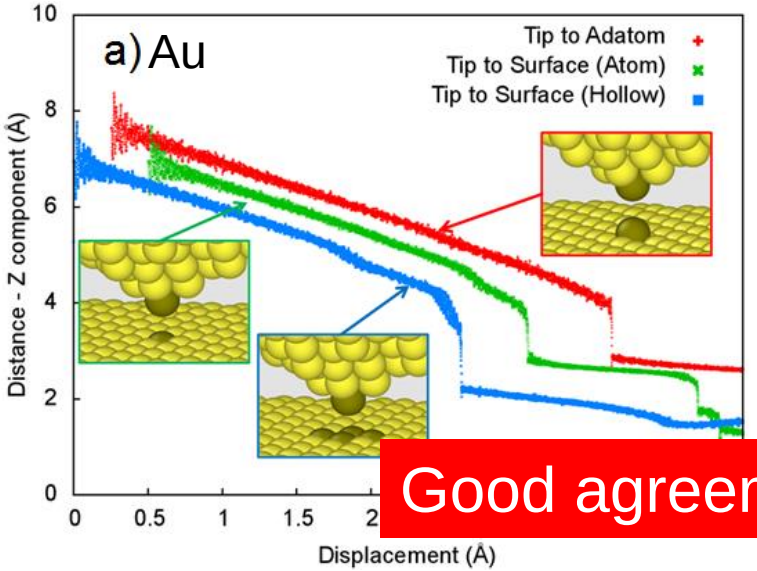


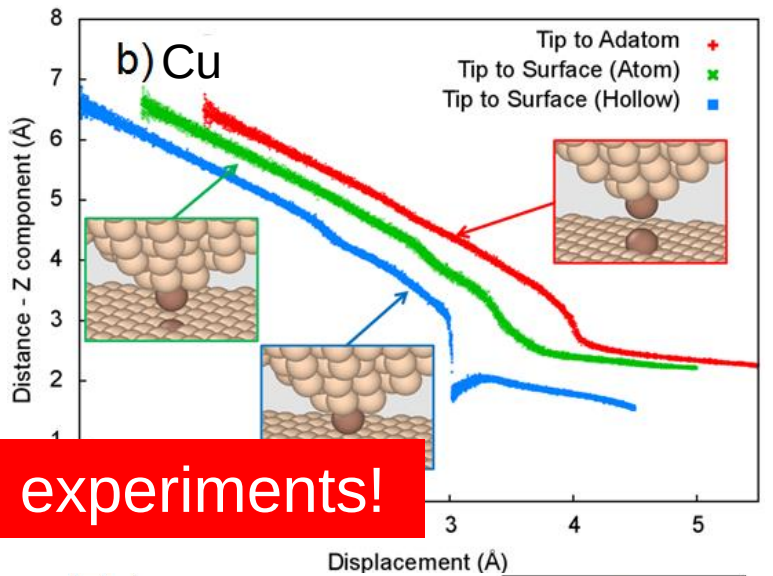
Fernandez M. A., *et al*., PRB **93**, 085437 (2016)

ACTUAL jumps in CMD simulations resemble conductance jumps in experiments. How about the SPECIAL GEOMETRIES in the previous slides?

Jump to contact (theory): Gold vs Copper

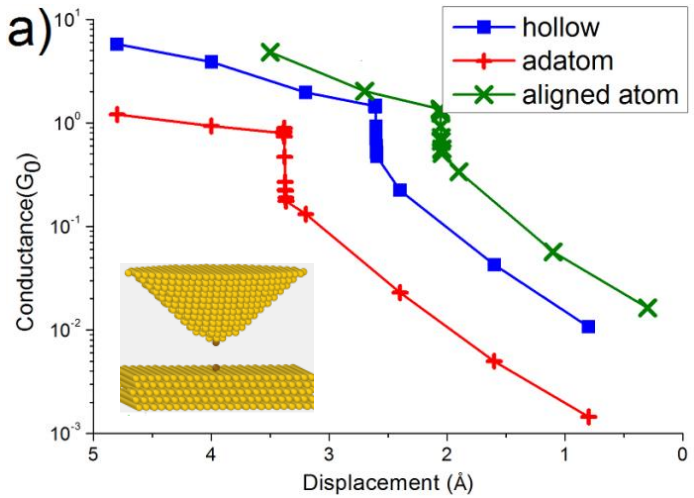
- CMD and **REFINED** DFT/TB transport results (from **ANT.Gaussian**) for **STM**-type (001) Au/Cu contacts at **4.2K**:

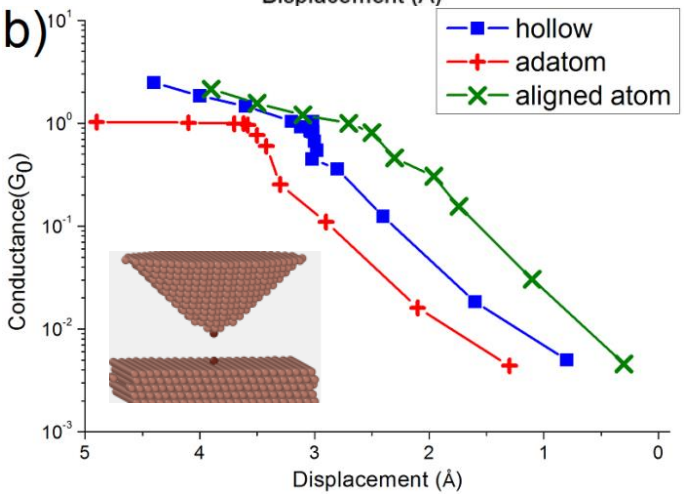




Good agreement with the experiments!

085437 (2016)

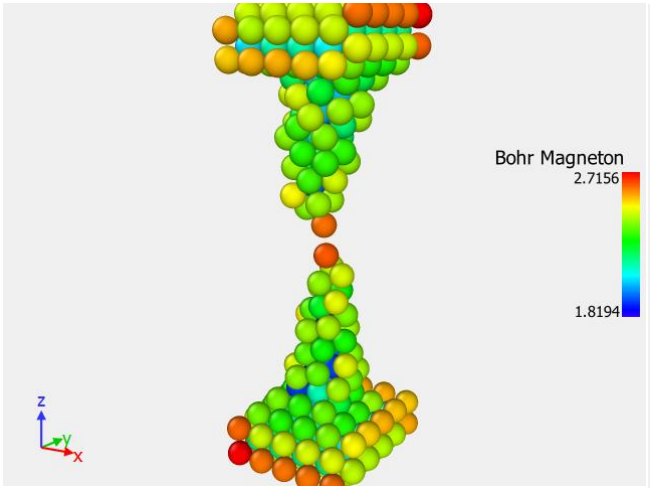




More complex materials: BCC vs FCC and magnetism

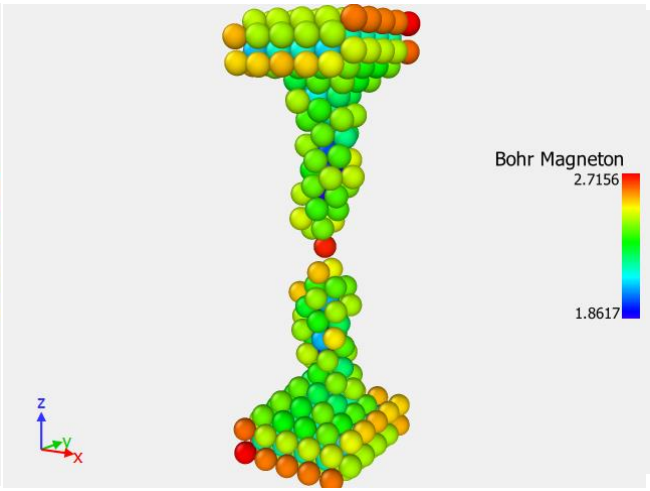
- What about **more realistic** (SLD) simulations on ferromagnetic **BCC** Fe(001) nanocontacts?
- The most common **last**-contact structures in **30** SPILADY **rupture** simulations:

VERTICAL DIMER



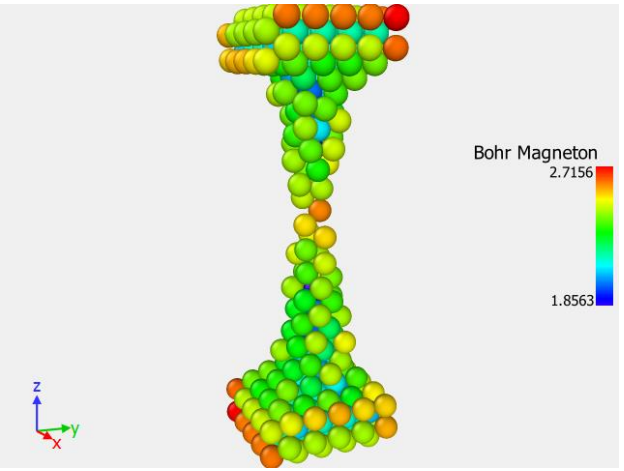
30%

MONOMER



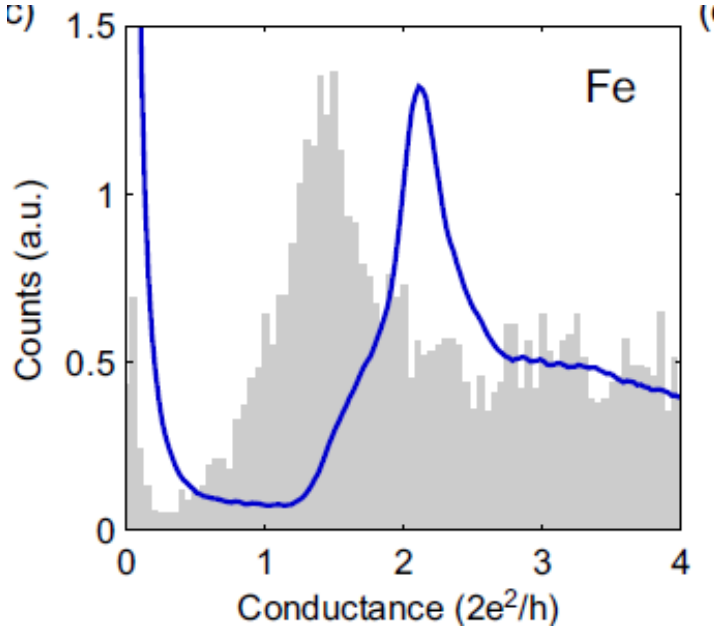
37%

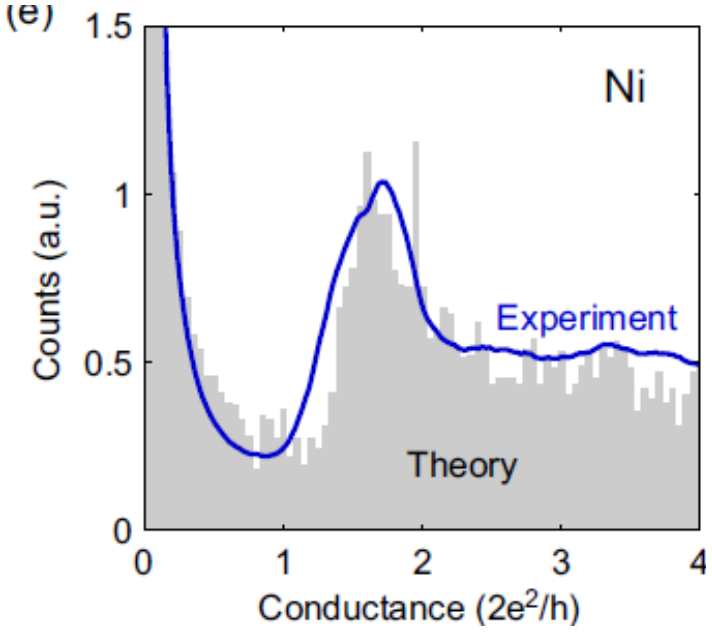
DOUBLE CONTACT

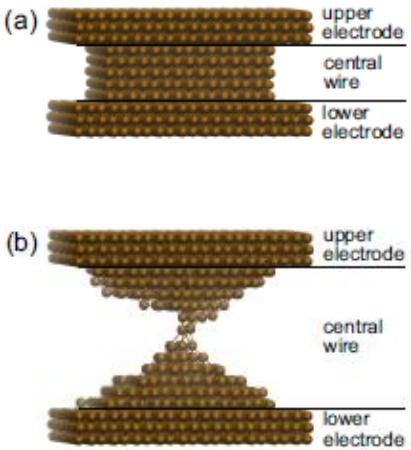


27%

More complex materials: BCC vs FCC and magnetism







Vardimon, R., *et al.*
PRB **93**, 085439 (2016)

Could **more realistic** SLD simulations narrow the gap between theory and experiment for ferromagnetic **BCC** iron?

Notice that **FCC** Ni (ferromagnetic) does not exhibit such a discrepancy. What is the role of the parent crystal structure (**BCC** vs **FCC**)?

Conclusion and outlook

- Combining CMD and **fine-tuned** DFT/TB transport simulations can reproduce the **emergent** and **geometry-dependent adhesive** properties of few-atom Au and Cu nanocontacts.

- Work-in-progress: unravelling the influence of parent crystal structure (**BCC** vs **FCC**) and ferromagnetism in SLD simulations of Fe nanocontact rupture.

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- Collaborators: **C. Sabater, M. A. Fernandez, C. Untiedt** (UA); **J. J. Palacios** (Dpto. de Fisica de la Materia Condensada, Universidad Autonoma de Madrid, Spain); **E. B. Lombardi** (School of Graduate Studies, UNISA).

THANK YOU!