Creating nanowires with atomic precision

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Abstract
Measuring the conductance between gold electrodes and limiting the indentation depth between the two electrodes up to a conductance value of approximately $5G_0$ in the case of gold we can obtain the same conductance behavior for hundreds of cycles of formation and rupture of the nanocontact. Furthermore, when two metals approach, the first contact between them occurs abruptly in most cases. This phenomenon is called “jump-to-contact” . It is well known that the conductance in a nanocontact is related to the smallest area of the contact between the two electrodes. Therefore, variations of the conductance should be related to changes in the atomic structure at the contact. Similarly, a jump in the conductance is observed when the two electrodes are pulled apart and the contact is broken, in what is called "jump-out-of-contact". Both experiments are rationalized using molecular dynamics simulations together with density functional theory transport calculations which show how:

a) after repeated indentations (mechanical annealing), the two metallic electrodes are shaped into tips of reproducible structure.

b) certain atomic contact structures are most likely to occur.

These results provide a crucial insight into fundamental aspects relevant to nano-tribology or scanning probe microscopies

References

[1] C.Sabater, C. Untiedt, J.J.P, Phys. Rev. Lett. **108**, 205502 (2012).

[2] C. Untiedt, M. J. Caturla, M. R. Calvo, J. J. Palacios, R. C. Segers, and J. M. van Ruitenbeek ,Phys. Rev. Lett. **98,** 206801 (2007)

Figures

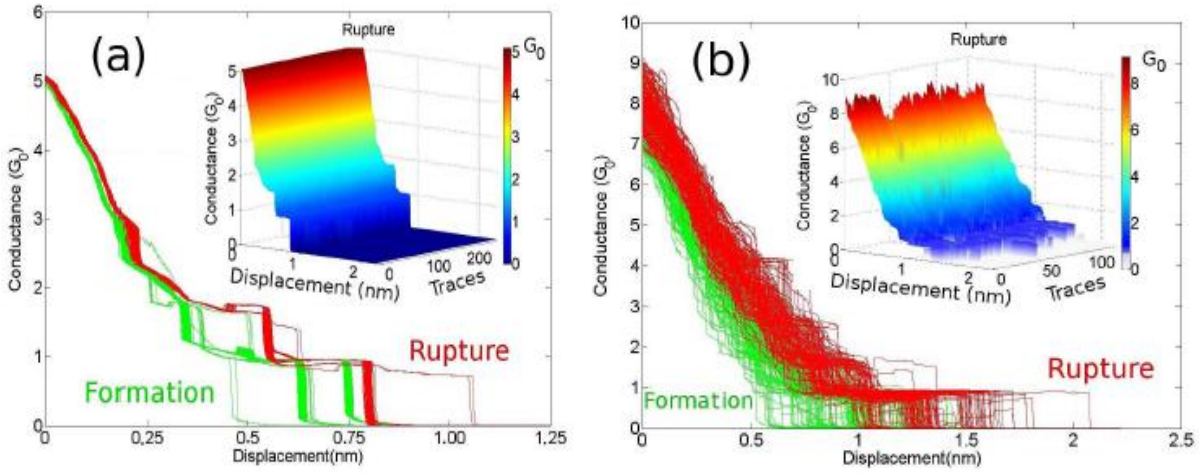

FIG. 1. Experimental traces obtained for Au nanocontacts during formation and rupture when limiting the conductance to (a) $5G_0$ and (b) $8G_0$. The inset shows a 3D figure of the rupture where the third axis is each individual trace

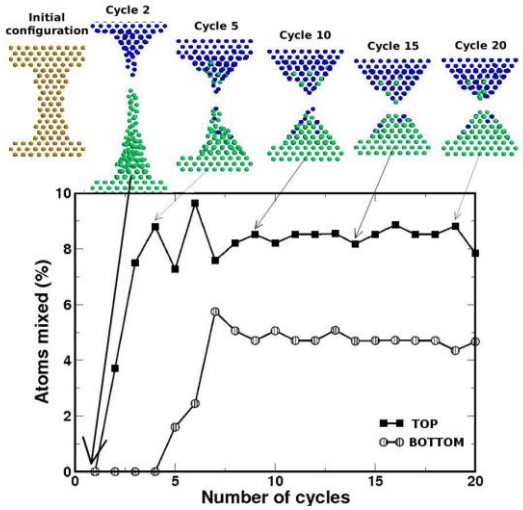

FIG. 2. Snapshots of the MD simulations of rupture and formation of a nanocontact in gold for the initial configuration and before cycles 2, 5, 10, 15 and 20 (top). Number of atoms in the top nanoelectrode (in %) that were initially on the second one, and viceversa, as a function of the number of cycles(bottom). Temperature was not fixed in this calculation.

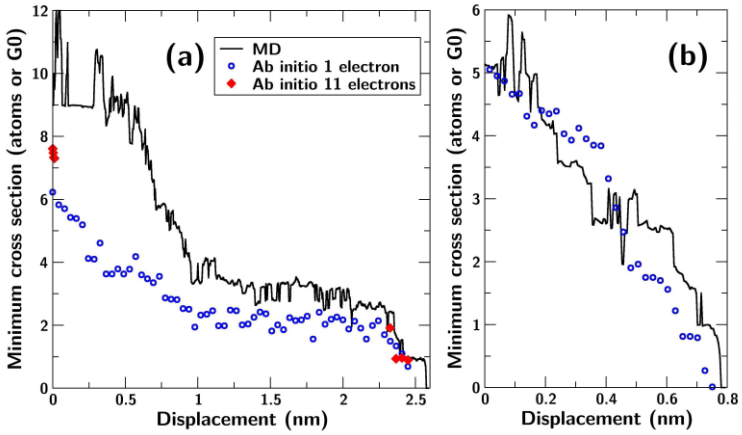

FIG. 3. Traces of conductance from DFT (open circles are calculations with 1 electron and diamonds are calculations with 11 electrons) and estimates from MD minimum cross section (lines) for calculations with 525 atoms. (a) Rupture trace during first cycle and (b) rupture trace for cycle number 10 for a maximum indentation of 5 atoms in cross section.

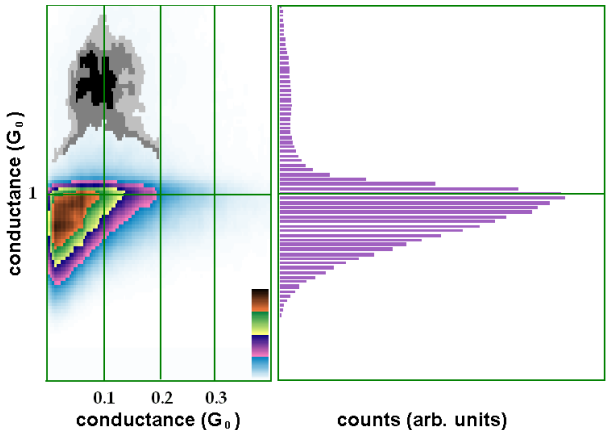

FIG. 4: (color online) Analysis of the steepest jump of conductance before the formation of a metallic contact for the case of gold, made from more than 300 000 conductance traces. The left panel shows a density plot, where the horizontal axes represents the conductance at which the jump takes place and the vertical axes shows the conductance of the contact formed. We have artificially changed the colors of the peak above (gray scale) to make it visible. The right panel shows the corresponding histogram of the conductance of the contact formed after the jump.