**Identifying stable atomic configurations by the correlation analysis of conductance traces**

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Break junction techniques have been proved to be a suitable method for the creation of high stability single-atom or single-molecule junctions. However, as the detailed configuration of the nano-scale junction cannot be traced by direct microscopic imaging, all the information must be collected from current and voltage measurements. Several techniques applying the toolbox of mesoscopic physics were developed for the study of atomic and molecular junctions [1], including the identification of stable atomic configurations by conductance histogram technique, the study of the transmission eigenchannels by conductance fluctuation [2], shot noise [3], or superconducting subgap structure measurements [4,5], as well as the detection of the vibrational modes by point-contact spectroscopy [2].

Conductance histogram technique had a pioneering role in understanding electron transport on the single-atom scale [1], and presently it is widely applied in the field of molecular electronics to identify well-defined single molecule structures [6,7]. However, it is obvious that conventional conductance histograms – measuring statistical averages – can only provide limited information about the studied nanostructures. In several fields of physics it is well known that going beyond averages can supply fundamentally new information, as demonstrated by the success of quantum noise studies in mesoscopic systems, or correlation spectroscopy in NMR studies [8]. Implementing these ideas we have developed [9] a novel statistical method based on the 2D cross-correlation analysis of conductance versus electrode separation traces. This method is capable of resolving several features of nanocontact formation dynamics, which are completely hidden in traditional conductance histograms.

This analysis can show, whether two configurations are always occurring together, one configuration is excluding the other, or their occurrences are independent events. Furthermore, the correlation analysis can resolve fine structures related to different atomic configurations, which are smeared out in the conductance histogram.

Applying this method we have studied the formation of atomic-scale nanocontacts in transition metal junctions, Ni, Fe, V [9]. In these metals low-symmetric *d* orbitals give an important contribution to the conduction, introducing an extreme sensitivity of conductance to precise junction geometry. Accordingly, traditional conductance histograms cannot show much more information than the conductance of a single-atom contact. Our analysis overcomes this difficulty, and opens a new window for resolving the typical evolutions of the conductance staircase starting from rather large contact diameters, and finding several, yet undetected stable atomic configurations. According to our novel analysis, Ni, Fe & V nanowires exhibit a very regular, atom by atom narrowing of the minimal cross section (figure 1), in contrast to the rather unordered rupture of Au junctions.

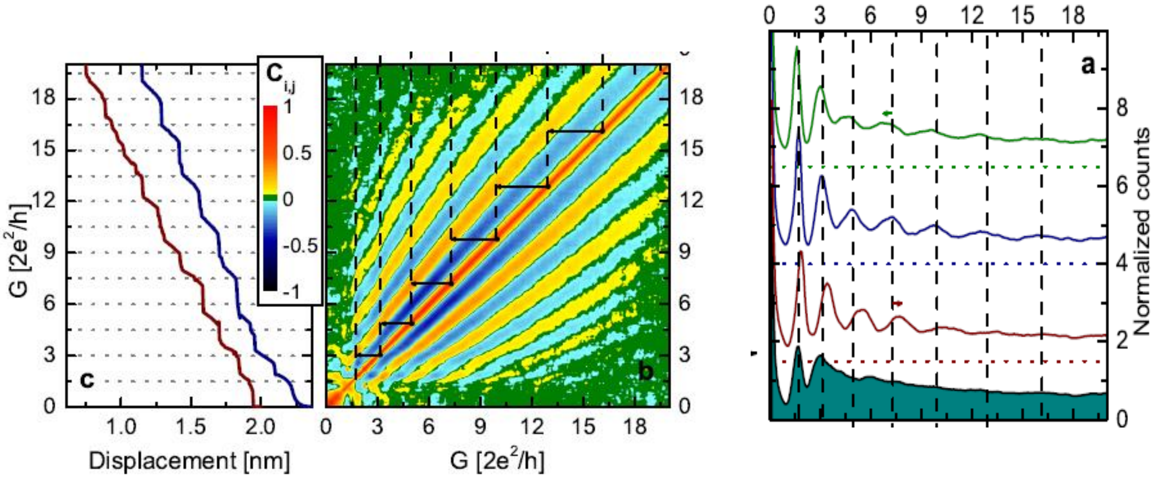
**References**

[1] N. Agrait, A. Levy Yeyati, J. M. van Ruitenbeek, Quantum properties of atomic-sized conductors, *Physics Reports* 377, 81 (2003).
[2] R. H. M. Smit, Y. Noat, C. Untiedt, N. D. Lang, M. C. van Hemert, J. M. van Ruitenbeek, Measurement of the conductance of a hydrogen molecule, *Nature* 419, 906 (2002).
[3] D. Djukic and J.M. van Ruitenbeek, Shot noise measurement on a single molecule, Nano Letters, 6 (2006)
[4] E. Scheer, N. Agrait, J. C. Cuevas, A. Levy Yeyati et al., The signature of chemical valence in the electrical conduction through a single atom contact, *Nature* 394, 154 (1998).
[5] P. Makk, Sz. Csonka, A. Halbritter, Effect of hydrogen molecules on the electronic transport through atomic-sized metallic junctions in the superconducting state, *PRB* 78, 045414 (2008).
[6] S. Wu, *et al.,* Molecular junctions based on aromatic coupling.
*Nature Nanotechnology.* 3, 569-574 (2008).

[7] L. Venkataraman, Jennifer E. Klare, Colin Nuckolls, Mark S. Hybertsen, and Michael L. Steigerwald, Dependence of singlemolecule junction conductance on molecular conformation. *Nature.* 442, 904-907 (2006).
[8]  R. R. Ernst, G. Bodenhausen and A.Wokaun, *Principles of Nuclear Magnetic Resonance in One and Two Dimensions*, (Oxford Univ. Press, Oxford 1987)

[9] A. Halbritter, P. Makk, Sz. Mackowiak, Sz. Csonka, M. Wawrzyniak, J. Martinek, Atom by atom narrowing of transition metal nanowires resolved by 2D correlation analysis.  arXiv:1006.1811v1, submitted to *Phys. Rev. Lett.* (2010).

**Figures**




*Measurements on Ni junctions. Left: Representative conductance traces and 2D correlation histogram for the data set. Right: Refocused histogram for Ni contacts (arXiv:1006.1811v1)*