Signature of clustering in Na nanocontacts

N. Zabala[1,2], A. Zugarramurdi[1,2], A.G. Borisov[3], E.V. Chulkov[2,4] and M.J. Puska[5]

[1]Department of Electricity and Electronics, FCT-ZTF, UPV-EHU, Bilbao, Spain.
[2]DIPC and CFM (CSIC-UPV/EHU), San Sebastian, Spain.
[3]CNRS, ISMO, UMR CNRS-Université Paris-Sud, 91405 Orsay CEDEX, France.
[4]Department of Materials Science, Faculty of Chemistry, UPV-EHU, San Sebastian, Spain.
[5]Department of Applied Physics, Aalto University, AALTO, Finland.

nerea.zabala@ehu.es

Nowadays, systematic studies of electronic and mechanical properties of nanocontacts are possible thanks to the mechanically controllable break junction (MCBJ) and scanning tunneling microscopy experiments [1,2]. In particular, the MCBJ is very well suited for conductance measurements, providing histograms for large sets of individual contact-breaking events as the basic input for further analysis. The electronic (atomic) shell structures of nanowires could be demonstrated with this technique [1] where the stable nanowire configurations are characterized by “magic radii” in analogy to the well-known “magic numbers” of abundance in metal clusters of different sizes [3].

Ogando et al. reported the formation of cluster-like arrangements of atoms, preceding the breakage of a stretched nanowire [4] using the ultimate jellium (UJ) model, in full agreement with previous first-principles molecular dynamics simulations [5]. The system considered in the simulations is sketched in the top of figure 1. It consists of two cylindrical UJ leads, whose potential is frozen after self-consistent calculations for an infinite wire of stable magic radius, and a central deformable part between the leads. Rearrangements upon stretching of the nanowire are only allowed in this central part. We have compared two cases in which 5 and 10 electrons are considered initially in the deformable region (this procedure is equivalent to the usual methodology followed in ab initio methods, where only a few atoms are allowed to relax. In the second case we observe the formation of a stable cluster of 8 electrons before the breakage.

Here we report on how the conductance of the elongated nanowire is affected by the formation of stable cluster-like arrangements of atoms in the break junction, by using a combined approach where the nanowire breakage is simulated with self-consistent electronic structure calculations within the density-functional theory (DFT). These self-consistent calculations provide an input for a follow-up wave packet propagation (WPP) study of the ballistic electron transport through the break junction [6,7].

We find that clustering leads to delayed and rounded conduction jumps upon the stretching of the nanowire (figure 1(a)). The results are analyzed in terms of the evolution of the transmission resonances originating from the cluster-localized electronic states [8]. The situation at hand then closely corresponds to the electron transport through molecular junctions studied in great detail in the context of molecular electronics, where the cluster would play the role of the molecular object. According to our results the resonant character of the transmission reveals itself particularly clearly in the bias voltage dependence of the differential conductance (figure 1(b)), suggesting experimental ways to evidence the presence of clusters in the break junction.

The main conclusions and results reported in this work are not determined by the specific choice of the nanowire material (Na) but rather by the very fact of the clustering at the break junction. The latter

phenomenon is of quite general nature, as it not only happens for the stretched Na nanowires but has also been reported for gold nanowires [9-11]. We hope that this work will stimulate further research on various aspects of the cluster formation during the contact breaking, such as the cluster appearance probability, stability and the effect on the conductance.

References

[1] N. Agraït, A. Levi-Yeyati, and J. van Ruitenbeek, Phys. Rep., **377** (2003) 81.
[2] G. Rubio, N. Agraït, and S. Vieira, Phys. Rev. Lett., **76** (1996) 2302.
[3] W. D. Knight, K. Clemenger, W. A. de Heer, W. A. Saunders, M. Y. Chou, and M. L. Cohen, Phys. Rev. Lett., **52** (1984) 2141.
[4] E. Ogando, T. Torsti, N. Zabala, and M. J. Puska, Phys. Rev. B, **67** (2003) 075417.
[5] R. Barnett and U. Landman, Nature (London), **387** (1997) 788.
[6] A.G. Borisov, A.K. Kazansky, J.P. Gauyacq, Phys. Rev. B, **59** (1999) 10935.
[7] E. V. Chulkov, A. G. Borisov, J. P. Gauyacq, D. Sanchez-Portal, V. M. Silkin, V. P. Zhukov, and P. M. Echenique, Chem. Rev., **106** (2006) 41601.
[8] A. Zugarramurdi, A.G. Borisov, N. Zabala, E.V. Chulkov and M.J. Puska, Phys. Rev. B, **83** (2011) 035402.
[9] P. Jelínek, R. Pérez, J. Ortega, and F. Flores, Phys. Rev. B, **77** (2008)115447.
[10] L. Hui, F. Pederiva, G. H. Wang, and B. L. Wang, J. Chem. Phys., **119** (2003) 9771.
[11] F. Tavazza, L. E. Levine, and A. M. Chaka, J. Appl. Phys., **106** (2009) 043522.
[12] A. Nakamura, M. Brandbyge, L. B. Hansen, and K. W. Jacobsen, Phys. Rev. Lett., **82** (1999) 1538.

Figures

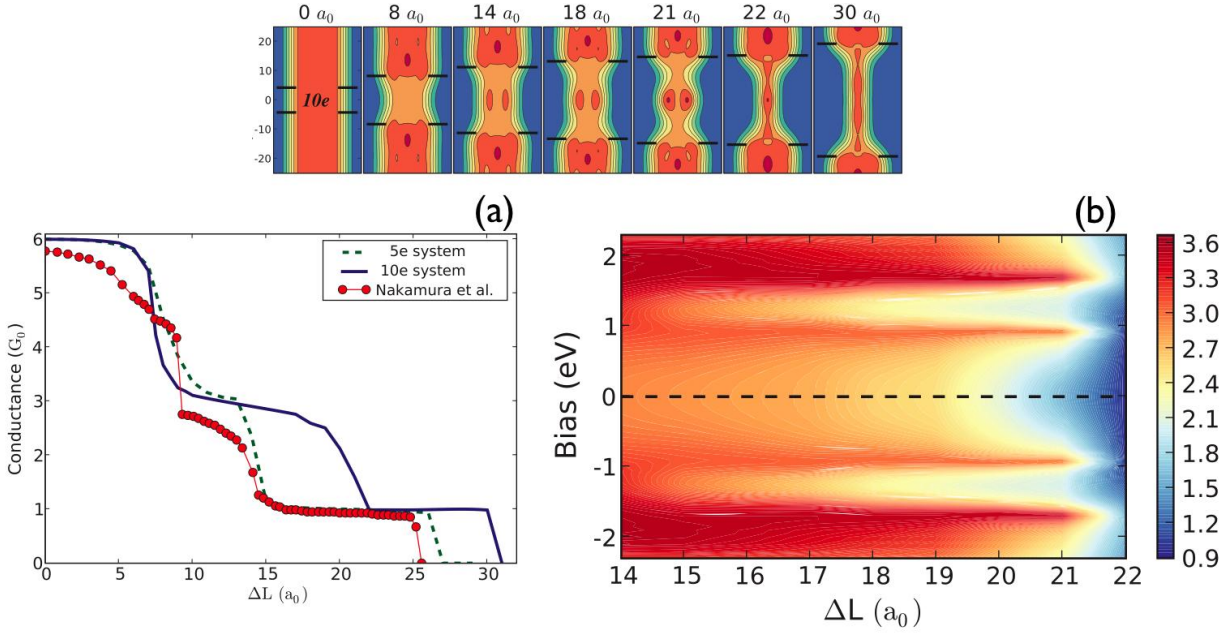

Figure 1: (Up) Snapshots of the charge density during the stretching of a Na nanowire of magic radius 10.7 a_0 and ten electrons initially in the deformable constriction for elongations $\Delta L = 0, 8a_0, 14a_0, 18a_0, 21a_0, 22a_0$, and $30a_0$. (a) Calculated conductance as a function of the nanowire elongation when 5 and 10 electrons are considered initially in the deformable part, together with ab initio data by Nakamura et al. [12]. (b) Differential conductance dI/dU map for the breakage of the same Na nanowire with ten electrons in the deformable constriction. The results are shown as a function of the applied bias voltage and nanowire elongation.