Improving the understanding of atomic-sized contacts' geometry through electronic transport in metals and semimetals.

C. Sabater[1], M.J. Caturla[1], J.J. Palacios[2] and C.Untiedt[1]

[1]Departamento de Física Aplicada, Universidad de Alicante, Campus de San Vicente del Raspeig, E-03690 Alicante, Spain

[2]Departamento de Física de la Materia Condensada, Universidad Autónoma de Madrid, Madrid E-28049, Spain

Carlos.sabater@ua.es

Abstract

Measuring the variations of the conductance in indentation experiments between two electrodes, we can obtain information on the changes in the atomic structure of the contact. We have analysed the Jump-to-Contact(JC) phenomenon which can be observed as the first contact when the two metals approach with respect each other. Moreover, we have studied the Jump-out-of-contact(JOC) phenomenon which is the last contact before breaking the two electrodes. Secondly, as we further approach the two electrodes and when the indentation depth is limited to a certain value of conductance, almost the exact behaviour in the evolution of the conductance can be obtained for hundreds of cycles of formation and rupture. That is, the same sequence of atomic configurations is followed. Both processes are rationalized using MD simulations together with DFT transport calculations, which show: a) the most probable atomic configurations in the first atomic contact following the JC or JOC processes; b) that after repeated indentations the two metallic electrodes are shaped into tips of a reproducible structure formed through a mechanical annealing process. These results improve our understanding of atomic-sized contacts and the evolution of their structural characteristics.

Finally using the same type of analisis for Bismuth Nanocontacts we have obtained a possible mechanism to exfolitate bismuth in bilayers at the crystallographic directions (111) showing a behavior wich these of Topological Insulators

References

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Figure 1

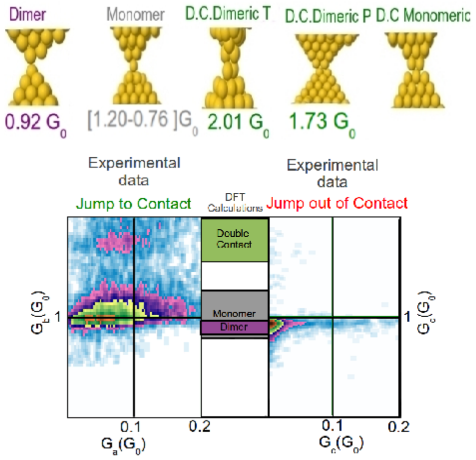

Figure 2