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Understanding Nanocontacts with atomic precision CARLOS SABATER, MARIA JOSE CATURLA, University of Alicante, JUANJOSE PALACIOS, University Autonoma of Madrid, CARLOS UNTIEDT, University of Alicante, UNIVERSITY OF ALICANTE TEAM, UNIVERSITY AUTONOMA OF MADRID TEAM — Measuring the variations of the conductance 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 observed as the first contact when the two metals approach 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 was 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.

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