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Simulating mechanical annealing of atomic-sized gold surfaces via classical molecular dynamics and density functional theory transport calculations

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Abstract content
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The ability to probe interactions at the atomic level via scanning tunneling microscopy and other techniques has led to great interest in contact formation between atomic-sized metal electrodes [Agrait N et al. 2003 Phys. Rep. 377 81]. For example, achieving ever smaller electronic circuit sizes is still a very important practical goal of nanotechnology [Lu Y et al. 2010 Nature Nanotechnology 5 218]. In the present work, it is demonstrated by two complementary simulation techniques that atomic-sized gold surfaces can be sharpened reproducibly, or mechanically annealed, until they are stable and no longer change. Experimentally, stable sharp gold tips may be achieved by repeatedly indenting into a surface with the tip of a scanning tunneling microscope. Such a process can be simulated by classical molecular dynamics (CMD), which describes the dynamics of the gold atoms as the two atomic-sized surfaces make and break contact [Sabater C et al. 2012 Phys. Rev. Lett. 108 205502]. To account for the interactions between the atoms in simulations, semi-empirical potentials fitted to various material parameters of the metals are used. The second simulation method, density functional theory (DFT) transport calculations [Palacios J J et al. 2002 Phys. Rev. B 66 035322], serves to obtain the electronic properties of the CMD-simulated system, such as the transmission across the electrodes when they first make contact. This paper presents the CMD results of the repeated indentation of a gold tip into a flat gold surface, with and without adatoms on the surface beneath the tip. The quantized conductances of a large number of CMD snapshot configurations of these surfaces, at various points during the process of contact formation, are also presented. These results permit a better understanding and interpretation of the experimental observations.

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