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ATOMISTIC SIMULATIONS OF INCIPIENT PLASTICITY IN STEPPED SURFACES

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ABSTRACT

To exploit mechanical properties of materials in a controlled way, a profound knowledge of the defects generated during deformation is required. But atomic deformation mechanisms (specially at the very initial stages) have proven to be complex and many issues are not well known yet. Nanoindentation experiments, with both very high spatial and load resolution, allow to determine the defects emerging at the surface, and their relation to the discontinuities in the load *vs* penetration curve. But sub-surface defect morphology generally remains hidden, and quite often only indirect conclusions can be inferred. Simulations offer then a very valuable tool to unveil defect configurations and their generation mechanisms.

Here we present atomistic nanoindentation simulations (using molecular dynamics and static minimization approaches with up to several million atoms) performed in gold, both on flat and defective surfaces. The reliability of these simulations is proven by direct comparison with experiments from our own group [1], shedding light on them and showing a close match. We analyze the defect configurations during the local deformation of the surface, while monitoring their evolution. Generally speaking, the very first plastic events consist in the formation of dislocation half-loops that either glide or split into more complex dispositions. The gliding and further switch of these loops to other slip planes (cross-slip) give rise to step traces on the surface, which we propose as a generalized mechanism for the usual debris piling-up observed around nanoindentation traces.

To provide a closer insight into *real* surfaces, we have performed simulations on defective surfaces, which show a qualitatively distinct plastic behavior with respect to flat (*ideal*) ones. The role of pre-existing surface steps is studied, which is often ignored when analyzing surface mechanical properties. Controversial issues, such as plastic activity preceding *pop-ins* in the force *vs* penetration curves, is addressed in the present work. We show how surface defects determine the nucleation site and geometry of the generated dislocations (see Fig. 1), as well as the very incipient surface plastic properties. Moreover, the local critical shear stress prior to dislocation formation is reduced when the indentation is performed at a surface step. The present simulations provide a clear example of how heterogeneous defect nucleation during the deformation of a surface can influence the final plastic properties of the material at the nanoscale.

We also show that these atypical deformation events do not result in pop-ins and exhibit a large degree of reversibility. All these issues may have profound implications in plasticity models, as well as in contact mechanics and friction between rough solids.

REFERENCES

[1] E. Carrasco *et al.*, Surf. Sci. **572,** 467 (2004); E. Carrasco *et al.*, Phys. Rev. B **68**, 180102 (2003); O. Rodríguez de la Fuente *et al.*, Phys. Rev. Lett. **88**, 036101 (2002); V. Navarro *et al.*, accepted in PRL (2007).

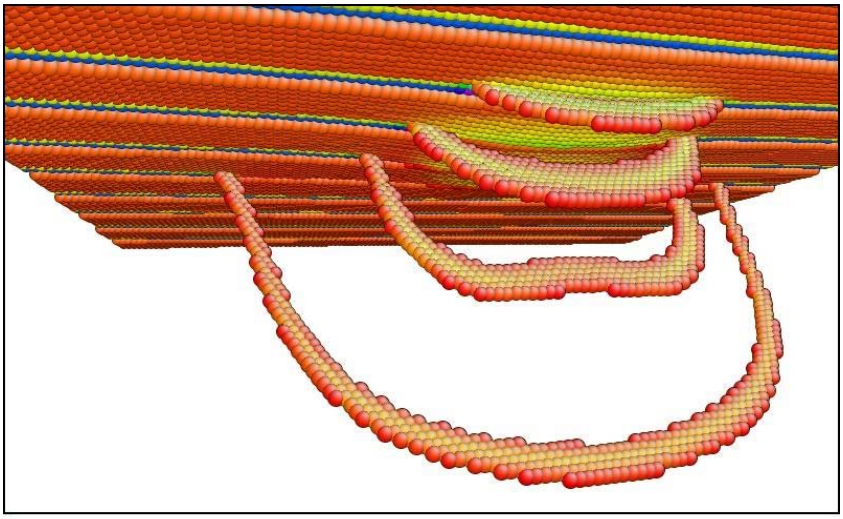

Figure 1: Sub-surface view of the dislocation half-loops nucleated below a stepped gold surface during nanoindentation. Just atoms belonging either to the surface or to volume defects are visualized. Every half-loop emerges from a surface step and glide along the same equivalent slip plane.