ATOMISTIC EXPERIMENTAL AND SIMULATION STUDIES OF THE INCIPIENT PLASTIC DEFORMATION MECHANISMS AROUND NANOINDENTATIONS IN Au(001)

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The nature and configuration of the dislocations generated during the incipient stages of plasticity in nanoindentations are still to a large extent unclear. In previous studies we have recognised and characterised by STM a number of novel surface defects in the surface of *fcc* metals generated by nanoindentation. We have analysed [1] the generation and kinetics of two types of dislocation configurations in Au(001): (i) *mesas* resulting from the splitting of perfect loops with Burgers vector **b** parallel to the surface and (ii) 'screw-loops', short name for half-loops with two segments in a screw orientation, their vector **b** being along a $\langle 110 \rangle$ direction inclined to the surface. In the present work we report a subsequent STM investigation, complemented by calculations based on the elastic theory of dislocations and by molecular dynamics simulations, of the mechanisms of generation, glide and cross-slip of these two types of dislocation configurations. In particular, it is shown that 'mesas' can glide under the action of local stresses originating in successive nanoindentations performed in the neighbourhood of the original one, the characteristics of that glide supporting the model which we proposed earlier for the *mesa* configuration. We also show that cross-slip of screw loops across the various {111} planes is the underlying mechanism for the generation of terraces winding around the nanoindentation and a main contributor for the permanent traces which are left behind in the sample surface once the tip has been retrieved.

More generally, our dislocation-based mechanism is able to account for the complex anisotropic surface structure, including crystallographically-oriented pile-ups of dislodged matter (figure 1), observed after nanoindentation by both our and other groups [2].

The STM experimental data are compared with molecular dynamics simulations, with up to a few million atoms. It is observed that in the first stages of plastic deformation, among other defects, dislocation loops are generated under the surface, below the nanoindentor (figure 2). Their properties and subsequent gliding are analyzed and monitored. With these simulated results we establish a quite direct comparison with experiments, since spatial ranges and defect configurations are equivalent. By combining both kinds of approaches, we elucidate some of the deformation processes during the onset of plastic activity on (001) *fcc* surfaces.

References:

[1] E. Carrasco et al., *Surface Science*. **572,** 467 (2004); O. Rodríguez de la Fuente et al., *Phys. Rev. Lett*., **88**, 036101 (2002)
[2] J.D. Kiely and J.E. Houston, *Phys. Rev. B* **57,** 12 588 (1998); A.Gouldstone et al. *Acta mater*. **48**, 2277 (2000); Y.Wang et al. *Acta mater*. **52**, 2229 (2000)

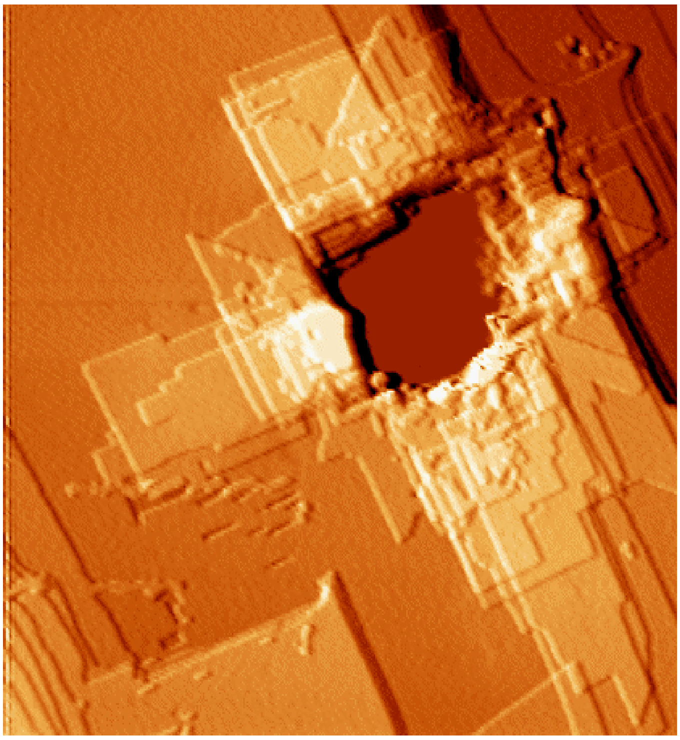

Figure 1: (680x680 nm^2) STM image of the Au(001) surface showing terraces around a nanoindentation, originated from the cross-slip of dislocation segments with screw character.

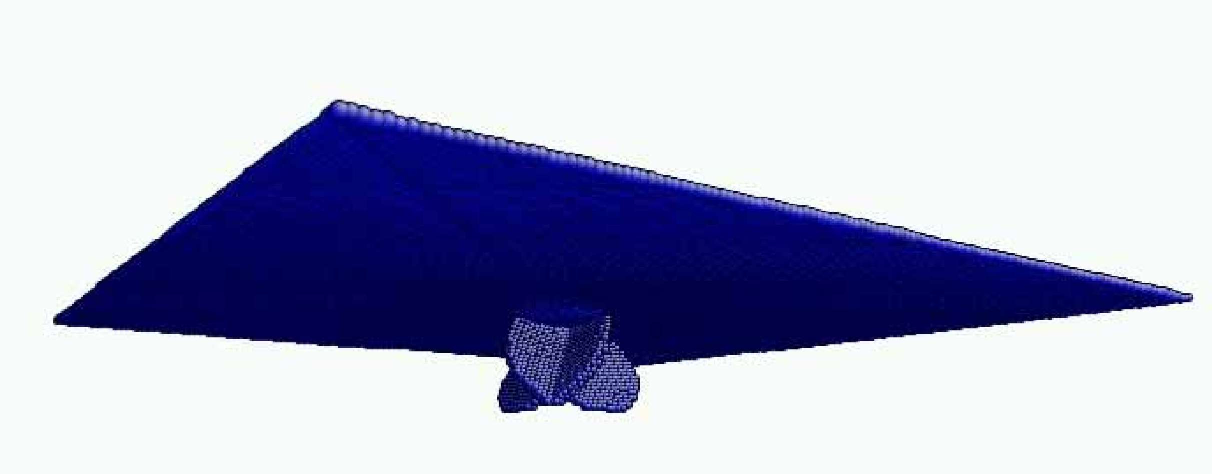

Figure 2: Molecular dynamics simulation of sub-surface dislocation half-loops generated below the Au(001) surface at the very initial plastic stages. These loops extend and glide under the external increasing force applied by the nanoindentor, giving rise to the experimentally observed screw-loops and pile-up terraces (see figure 1). Only atoms at dislocations and at the surface are visualized.