STUDY OF THE INITIAL STAGES OF PLASTICITY IN NANOINDENTED Au(001) SINGLE CRYSTAL AND THIN FILMS.

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Dislocations are line defects in plastically deformed crystalline regions. It is generally accepted that dislocations can strongly affect not only nanostructural properties, but macroscopic mechanical properties. During last decades, microindentation has been widely used to characterize the mechanical properties of solids, with the aim of elucidating the underlying physical properties.

Nanoindentation is the penetration of the surface to nanometer sizes (in depth or area) using an appropriate nanoindenter device [1]. In this work, we present a detailed analysis of the nanoindentation process by using an AFM (Atomic Force Microscope) as the nanoindenter. At variance with other experimental techniques, an AFM is particularly useful in that kind of research, as it is able to provide a direct measurement not only of the load values involved in a nanoindentation process, but also of the defects produced in the surface due to the localized deformation [2].

Nanoindentation in metals produces a load *vs* penetration depth response that has two well defined separated regions: the elastic region and the plastic deformation region (Fig. 1.a). We have performed a series of nanoindentations in single crystal Au(001) and in gold thin films in order to elucidate dislocations generation mechanisms as well as other mechanical properties. In our series, we increased in a controlled way the load applied to the AFM silicon nitride tip. From these measurements we characterize the limiting region between the elastic and the plastic response of the material, which strongly depends on the material, particularly on the existing defects concentration.

The experimental data obtained with the AFM are analyzed and compared with atomistic simulations. Computations are performed with semiempirical potentials, the number of atoms ranging from a few hundred thousands to about 2 million. During nanoindentation, again, an elastic regime is observed, followed by irreversible deformation (see Fig. 2). In the first stages of plastic deformation, dislocation loops are generated under the surface, close to the nanoindentor. Their properties and subsequent movement are analysed and monitored. Every discrete jump in the nanoindentation curve corresponds to the formation, under the tip, of dislocations under different configurations. These considerations for the simulated results allow us to obtain a quite direct comparison with experiments, since spatial ranges are similar.

References:

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[2] J. D. Kiely and J. E. Houston, Phys. Rev. B **57**, 12 588 (1998); J. Li et al. Nature (London) **418**, 307 (2002).

Figures:

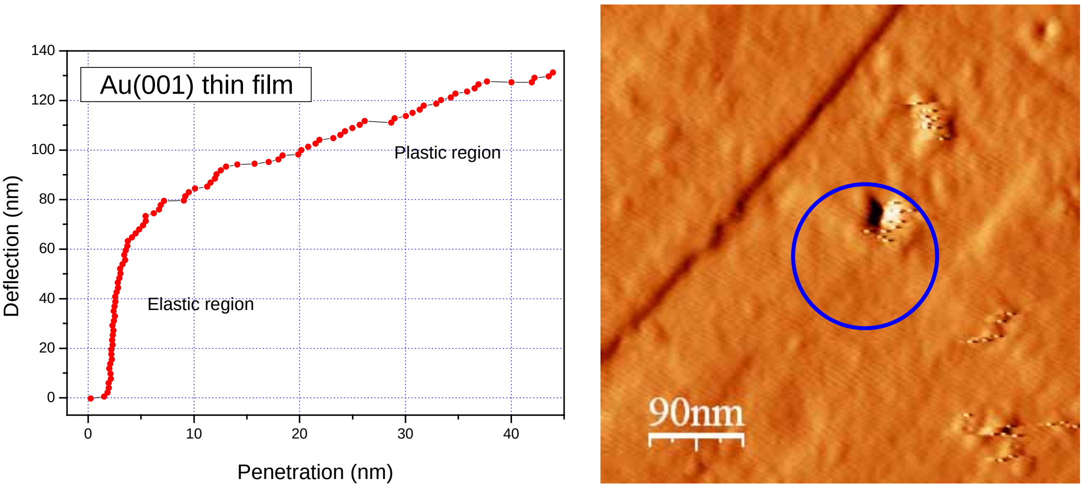

Fig. 1. Left: Tip deflection *vs* penetration depth directly extracted from an AFM experiment on Au(001) thin film. Right: AFM image taken immediately after the nanoindentation process. Only when plastic region is reached, a trace is observed in the image (blue circle).

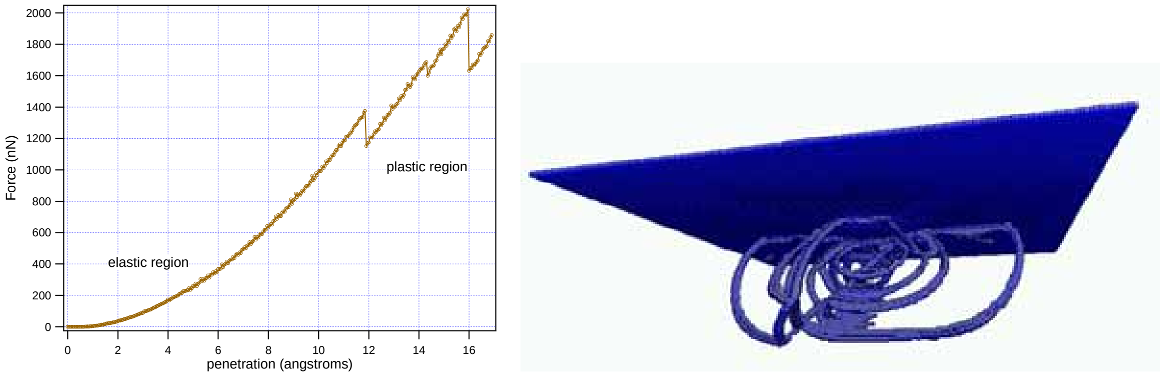

Fig. 2. Atomistic simulation of a nanoindentation process with 2.3 million atoms. Left: Force *vs* penetration curve. As in the experiments, two main regions are observed. The different shape of the steps observed in the plastic region between experiment and simulations depends on which parameter (strain or stress) is kept constant. Right: Resulting atomic positions on the last point of the nanoindentation curve. In the figure, only atoms located at dislocations are represented. Sub-surface dislocations loops generated under the nanoindenter are visible.