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Mechanical Deformation of Gold Atomic-size Wires

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Abstract – We present a study related to the mechanical deformation of gold atomic-size wires at different temperature conditions. Experimental studies were developed by *in situ*-high resolution transmission electron microscopy. Our results revealed that nanowires deformed at 150 K display the formation and aniquilitation of planar defects (stacking faults and twins), in contrast to the structural behavior observed at 300 K (crystalline and free of defects). This reveals clearly that temperature plays a central role during mechanical elongation. *Ab initio* calculations of total energy associated with stacking fault formation showed that contribution from surface overrule stacking fault energetics.

The mechanical properties of a strained nanoscale volume of matter represent a fundamental issue for understanding phenomena such as friction, fracture, adhesion, etc [1]. Miniaturization levels are raising the need of accurately characterizing nanodevices and nanomaterials, to develop models and predictions of their mechanical performance and reliability. But, we must also consider that the deformation of macroscopic matter continues to be a very interesting and dynamic research field displaying open questions and polemical issues.

In this work, we have analyzed the atomistic aspects of the elongation of one-nm-wide metal rods using in-situ electron microscopy. For gold nanorods (NR) no extended defect could be observed at room temperature (figure 1), while at 150 K stacking faults (SF) are generated frequently (figure 2) [2]. In fact, we have observed that as their size is reduced, the energy barriers became very small that thermal ambient energy is sufficient to overcome them. Then, NRs display an extended elastic regime until a mechanism with high enough blocking barrier can be nucleated.

We have also developed *ab initio* calculations to derive the total energy changes associated with SF formation in NRs. *Ab-initio* calculations revealed that contribution from surface steps overrule staking fault energetics in NRs, in such a way that system size and shape determines preferred faults gliding directions. The relation between morphology and surface steps can produce anisotropic behavior and, even large differences in elastic or plastic response for elongation or compression [3].

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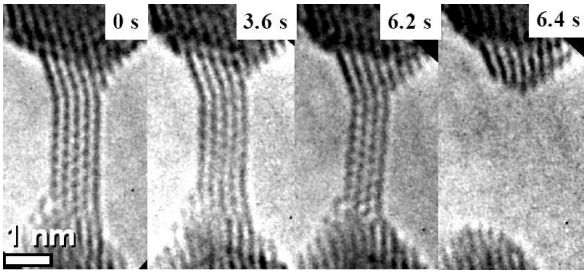

Figure 1: Thinning of a Au nanorod being elongated along the [110] axis at 300 K. Note that the structure keep its crystalline character and is free of defects during the deformation process. Atomic positions appear dark.

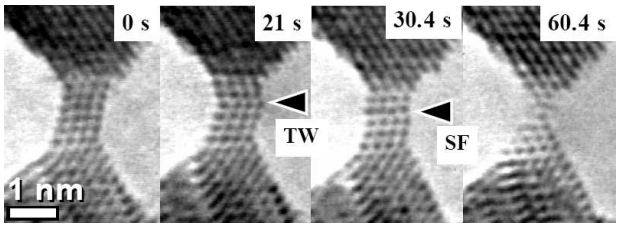

Figure 2 : Thinning of a Au nanorod being elongated along the [110] axis at approximately 150 K. Note that planar defects (stacking falults and twins) are formed during mechanical deformation process. Defects are indicated by arrows and atomic positions appear dark.

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