11th International Conference
on Advanced Materials

Rio de Janeiro Brazil
September 20 - 25

Elongation and rupture of nanoscale metal wires

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Abstract – The understanding of the mechanical properties of nanoscale materials is mostly on the results derived from computational simulations, where deformation rate is orders of magnitude higher than similar processes studied in experiments; then, temperature activated mechanisms or rate limited events can not be analyzed in depth. At present, nanomaterial deformation mechanisms are frequently described using models which have not been compared or are supported by laboratory measurements. As a consequence, the essential basic physics related to a stressed volume of matter is not yet fully understood. Here, we present studies of the tensile deformation of ~nm-wide metal wires studied by time-resolved HRTEM. The deformation processes were studied at different temperatures compatible with atomic resolution imaging. We have observed a size-dependent elastic-plastic transition of individual nanosystems. Our results provide fundamental quantitative data to improve atomic potentials used to model the mechanical properties of nanostructures.

Most of available knowledge on the deformation mechanism of nanomaterials has been derived from computational modeling and simulations, which in most cases are not be supported by experimental validation and, as a consequence, the underlying physics is not yet well understood. Future nanoscale device fabrication requires the fundamental understanding of friction, fracture, adhesion, etc. of nano-objects and, it is imperative to realize predictions of mechanical performance and reliability.

We have experimentally and theoretically addressed the tensile deformation of ~1-nm-wide metal wires by an atomic resolution time-resolved electron microscopy study and theoretical calculations. By directly observing the positions and displacement of atoms during the mechanical stretching of 1-nm-wide metal rods at different temperatures (see example in Fig. 1), we have determined how size and shape influences the mechanical behavior. We have derived by the first time, quantitative physical understanding of the size dependence of the elastic-plastic transition of individual nanosystems. This study provides fundamental quantitative data to improve models and atomic potentials used in future temperature dependent simulations of the mechanical properties of nanostructures. Also, the high surface/volume ratio of these nm wide metal rods may generate unexpected metastable atomic arrangements (ex. hollow wires) during deformation, which is quite different from macroscopic matter.

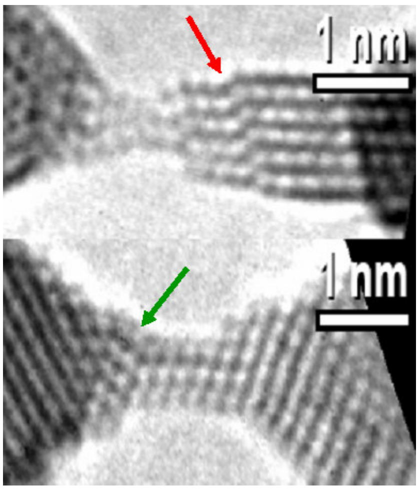

Figure 1: HRTEM image of gold nanorods being stretched at ~150K. Stacking faults and twin and frequently observed at low temperature. At room temperature the wire stay free of defects