Stress-strain curves of aluminum nanowires: fluctuations in the plastic regime and absence of hardening

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One of the most subtle issues in the increasingly broad area of nanoscience concerns the mechanical response of small systems. Mechanical devices are getting so small that quantum limits are already reachable [1]. Understanding how materials respond at such small scales is a need for the design of novel electromechanical devices.

Although technical difficulties inherent to the measurement of the mechanical response of small systems are enormous, nowadays tools are allowing to investigate both inorganic [2–5] and organic (biological) [5, 6] systems. Several issues are particularly attracting the interest of researchers, among which we mention the size dependence of mechanical moduli (Young modulus, yield stress, ...) [5], fracture at the nanoscale [3], and whether small systems do or do not harden [4]. No complete agreement has yet been attained on any of these questions.

We have carried out molecular dynamics calculations of stress-strain curves of aluminum nanowires using the interatomic potential proposed by Ercolessi and Adams [7]. Nanowires were stretched along the [001] direction at a constant rate of 0.01 Å/ps at 4.2 K, using as initial conditions fixed atomic positions and velocity at each atom randomly distributed according to Maxwell distribution. The stress tensor can be easily derived from molecular dynamics calculations as:

$$\sigma_{\alpha\beta} = \frac{1}{V}\left(\sum_{i=1}^{N} m_i v_{i\alpha} v_{i\beta} + \frac{1}{2}\sum_{i\neq j}^{N} r_{ij\beta} F_{ij\alpha}\right) \tag{1}$$

where V is the volume of the sample, $v_{i\alpha}$ is the component α of the velocity vector at atom i, $r_{ij\beta}$ is the component β of the vector that joins atoms i and j, and $F_{ij\alpha}$ is the component α of the force that atom i exerts on atom j. V was replaced by its initial value, thus giving the engineering stress.

Fig. 1 shows the results for a nanowire of 2645 atoms and an ab-initio result for a small cluster of 22 atoms. Both approaches show short quasi-elastic events followed by sudden drops of the total energy associated to major atomic rearrangements. Averaging over at least 1500 realizations on the streching of a 463 atoms nanowire allows to unambiguously conclude that, beyond the yield point, the system does not harden (see Fig. 2).

Another outstanding issue, is how fluctuations in the plastic, non-linear, regime are distributed [6]. Experimental data obtainedon polymers indicate that the work probability distribution has a Gaussian component plus long non-Gaussian tails. The origin of this deviation from the Gaussian distribution predicted by the Central Limit Theorem (CLT) is a matter of fundamental interest that is being intensively investigated. Whether this kind of deviations from the CLT is a characteristic common to any small system is something that has not yet been settled. The analysis over the around 1.5 million data indicate the presence of non-gaussian tails in the heat probability distribution but not in the engineering stress (Fig. 3).

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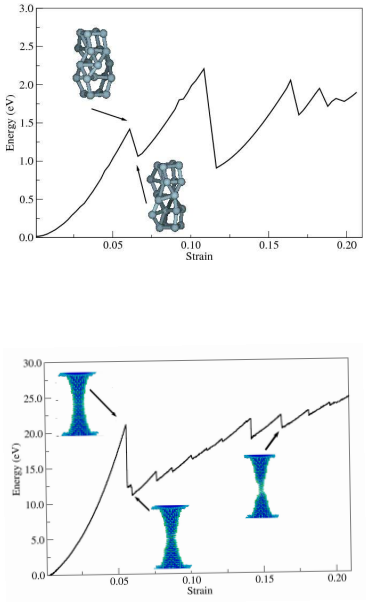

FIGURE 1: Energy vs engineering strain, calculated using either Density Functional Theory (upper panel) or molecular dynamics (lower panel), for aluminum nano-wires containing 22 and 2645 atoms, respectively: Actual atomic arrangements are also shown at different stages of the stretching process. The results correspond to single a realization (initial distribution of velocities)

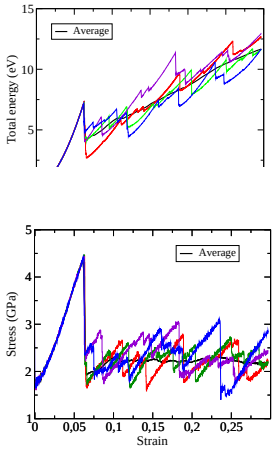

FIGURE 2: Total energy (upper panel) and stress (lower panel) versus engineering strain, as derived from molecular dynamics calculations on aluminum nanowires containing 463 atoms stretched at a constant strain rate. The results correspond to three individual realizations (different initial distributions of atomic velocities) and to an average that includes over 1500 (thick black line).

FIGURE 3: Probability distributions of the engineering stress and the heat evolved (ΔQ) in the non-linear (plastic) regime derived from molecular dynamics calculations on aluminum nanowires, containing 463 atoms, stretched at a constant strain rate. The distribution contains more than 1.5 million counts (1500 realizations by at least one thousand points along the stress-strain curve). The (red) continuous curves are Gaussian fits to the numerical data over the stress range [-0.5,0.5] GPa or the heat range [-0.02,0.02] eV.