Comment on "Deformation mechanisms of face-centered-cubic metal nanowires with twin boundaries" [Appl. Phys. Lett. 90, 151909 (2007)]

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The article by Cao *et al.*[1] provides some insight into the role of twin boundaries in the deformation mechanisms of Cu nanowires. There are, however, several statements in this letter that could cause considerable confusion for the understanding of mechanical behavior in twinned metal nanowires, if not clarified.

Our comment is related to conclusion (2) in the letter of Cao *et al.*: "(2) The smaller the TBS [i.e., twin boundary size], the higher the twinned nanowire yield stress. The redistribution of interior stress owing to the presence of TBs is responsible for the strengthening of the twinned nanowires." Such conclusion is drawn on the basis of the stress-strain curves presented in Fig. 2(b), in the analysis of which the authors state that "the precipitous drop of the curve implies the yielding." This analysis is inaccurate for the case of twinned fcc metal nanowires, because plastic yielding should be characterized by the point when the first partial dislocation is emitted. Later in the paper, the authors provide a contradictory conclusion as follows: "(3) TBs act as barrier for dislocation movements and consequently lead to hardening effects." According to this, we conclude that the blockage of dislocation movements by the twin boundaries would make the stress continue to increase even after plastic yielding. Therefore, the maximum stress shown in the stress-strain curves presented in Fig. 2(b) cannot possibly represent the yielding stress in all twinned nanowires without further examination. To support our comment, we have repeated the atomistic simulations of Cao *et al.* on a twin-free nanowire and a five-twin nanowire in Cu using the same procedure and parameters (wire shape, relaxation steps, applied boundary conditions, strain rate, temperature, etc.) as described in their original work. The simulated stress-strain curves are represented in Fig. 1, where the step corresponding to the onset of plasticity and the emission of the very first dislocation is indicated by an arrow. This figure clearly shows that the yield point in the twin-free nanowire takes place at the stress level corresponding to the "precipitous drop" in the stress-strain curve (7.42 GPa). In the five-twin nanowire, however, there is clear evidence that the emission of the very first dislocation occurs at a much smaller stress (6.08 GPa) than the maximum stress (8.24 GPa). This observation also suggests that the tensile yield stress should decrease with the addition of twin boundaries. This hypothesis is supported by a past atomistic study,[2] where it was found that the stress required for the nucleation of the dislocations in twinned gold nanowires was 18%–22% less than that of perfect wires with corresponding diameter.

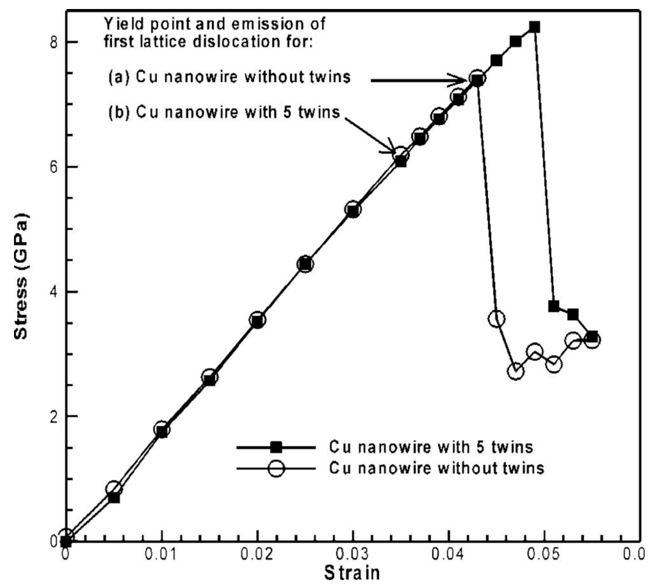

FIG. 1. Tensile stress-strain curves for single crystal and five-twin Cu nanowires as obtained from the same computational procedure used by Cao *et al.* The yield point corresponding to the emission of the very first lattice dislocation is indicated by an arrow.

Furthermore, the authors have provided no evidence showing that the presence of twin boundaries would alter the distribution of interior stress. While repeating the atomistic simulations of the Letter of Cao *et al.*, we found that the vicinity of twin boundaries does show a more compressive stress than the twin-free lattice after the energy minimization step, but such a difference may be considered negligible during the following elongation process in tension. The yielding mechanism of metal nanowires remains an open debate[3–5] and, therefore, the conclusion by the authors that "the redistribution of interior stress owing to the presence of TBs is responsible for the strengthening of the twinned nanowires." is too early to be drawn without further evidence.

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