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Response to "Comment on 'Deformation mechanisms of face-centered-cubic metal nanowires with twin boundaries' " [Appl. Phys. Lett. 93, 086101 (2008)]

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In our recent study,[1] we performed molecular dynamics simulation on the tensile deformation of Cu nanowires with multiple twin boundaries to gain insight into the role of twin boundaries in the deformation mechanisms of Cu nanowires. Our calculations showed that twinned Cu nanowires show a significantly larger yield stress than twin-free wires. Our explanation for this observation is that the redistribution of interior stress owing to the presence of twin boundaries is responsible for the strengthening of the twinned nanowires. The concern raised by Sansoz and Deng[2] is about the origin of the strengthening effects of the twinned nanowires. They observed that the emission of the very first dislocation corresponding to the onset of plasticity in the five-twin nanowires is earlier than that in the twin-free wire and accordingly a lower yield stress of the five-twin wires. This observation leads them to the conclusion that the tensile yield stress should decrease with the addition of twin boundaries.

Firstly, we carefully re-examined our simulation for the three wires, twin-free, four-twin, and five-twin wires. The snapshots corresponding to the first dislocation nucleation are shown in Fig. 1. This figure clearly shows that the yield point in both the twin-free and twinned nanowires takes place at the stress level corresponding to the "precipitous drop" in the stress-strain curve. The yield stresses for the twinned wires are higher than those for the twin-free one. Once the first dislocation nucleated, a number of dislocation nucleation events are triggered to release the stored strain energy for their high instability, as shown in Fig. 1(d). After the dislocation emission, stress shows a precipitous drop as shown in Fig. 2(b) of Ref. 1. This makes us confidently believe that the yielding indeed occurs at the maximum point of the stress-strain curve rather than as suggested by Sansoz and Deng.[2] The difference in the plastic deformation mechanisms between the twin-free and twinned nanowires is that dislocations can freely leave out of the wires, causing "starvation" effects,[3] while the blockage of dislocation movements due to twin boundaries would cause some stress buildup, which will influence the next plasticity event. The blockage of dislocations definitely influences the behavior of nanowires after yielding. This is what we called "hardening," which is reflected by the small stress fluctuation of "flow stress" after yielding.

The perfect coherent twin boundaries are not the sources of dislocations, as in the case of grain boundaries. The difference in the roles played by twin boundaries and grain boundaries can be found in our recent simulations.[4]

Next, let us address some import issues that will cause confusion and error from the comments. According to the stress-strain curve (Fig. 1 of Ref. 2), similar to Fig. 2(b) in Ref. 1, the relationship between the stress and strains after "yielding" does not deviate from Hooker's law, i.e., stress linearly increase with strain, which means that they remain in the elastic region. Obviously, their statement of "tensile yield stress should decrease with the addition of twin boundaries" contradicts the observation of stress-strain curves. Then a natural question arises for Sansoz and Deng: Why stress drop after several continuing strains of the so-called yielding. What is the reason for the continuous increase in stress even after the so-called yielding. If the very first (single) dislocation nucleation could not relax the stress of the wire system?

The contradiction of our observation to that of the comment is not understood since they did not give any evidence and reasoning for the first yielding and subsequent harden-

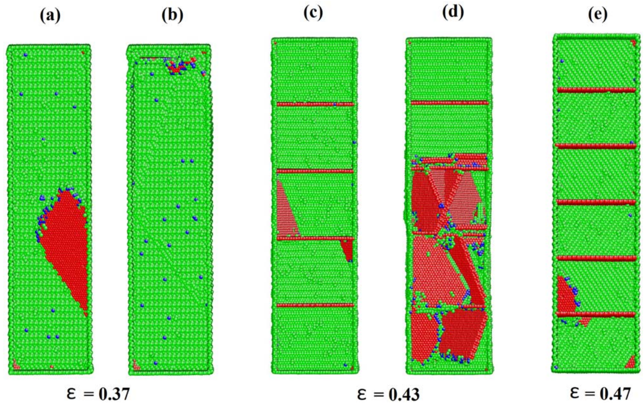

FIG. 1. (Color online) The snapshots correspond to the first yielding point of the stress-strain curve. (a) The first nucleation of dislocation; (b) several picoseconds later, dislocations move out of the wire in the twin-free single-crystal Cu nanowire, (c) and (d) are for the four-twin nanowire, and (e) is for the five-twin nanowire. This clearly shows that the first dislocation emission in twinned nanowires occur after that of the twin-free one. The plot also shows the "dislocation starvation" in the single-crystal wire, while a number of dislocations pile up at twin boundaries and stacking fault intersections, leading to some hardening effects after yielding.

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ing. Note that one needs to rule out the possibility of the observed lower yielding event due to the surface roughness or the geometry of the wire, which cannot be thought as the intrinsic properties of the materials.

Intuitively, the structure changes in the twinned wires due to the presence of twin boundaries cause the local stress state to change,[5] which is agreed by the calculation of Sansoz and Deng.[2] This is an indication of the difference in yield stresses, but may not be the essential origin. Structure determines the properties in materials. The variation in local stress state reflects the structure difference and can be a good indicator for their yield stress.

So we conclude that twin boundaries affect the mechanical properties of nanowires in two ways: (1) the structure (crystallographic orientation) changes in the twinned wires across twin boundaries, which consequently result in the local stress variation, are the reason for their higher yield stress; (2) the blockage of dislocation movement by twin boundaries after yielding could cause some hardening effects, as represented by the smaller drop in stress after yielding and smaller fluctuation in the flow stress.

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