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***Research article***

**Deformation mechanism of kink-step distorted coherent twin boundaries in copper nanowire**

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**Supplementary**

1. Atomic models of defective NWs before deformation

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**Figure S1.** Microstructure of the NWs with different kink densities. (a) 1 kink/ 4.4nm. (b) 1 kink/7.0nm. (c) 1 kink/8.8nm. (d) 1 kink/ 17.7nm.

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**Figure S2.** Microstructure of the NWs with different kink heights. (a) 0 nm. (b) 0.6 nm. (c) 1.2 nm. (d) 1.8 nm.



**Figure S3.** Microstructure of the NWs with distinct twin thicknesses. (a) 1.8 nm. (b) 3.1 nm. (c) 4.0 nm.

2. Nucleation site competition due to local stress state

To comprehend the underlying competition of ITB segments and surface atoms serving as nucleation sources, von Mises atomic stress contour is incorporated. Figure S2 reveals corresponding local atom contour of a defective NW after the initial elastic deformation. It is apparent that the ITB segments sustain significant high local atom stress, whereas the surface atoms attain a moderate local stress. From the existing publications on single crystal NW deformation, surface atoms are known to be the major sites for nucleation because of their predominant local stress state. Here, the same mechanism for dislocation nucleation applies. Local stress state promotes dislocation nucleation in both kink-steps and surface atoms, whereas the high local stress achieved at kink-steps makes them competitive in firstly nucleating dislocations. The first partial dislocation nucleates and transmits from a local stress-intensive region, referring in this case to the kink-step. This contour suggests that the induction of nucleation by stress concentration would be more likely at kink-step regions. The surface atoms in dislocation emission become insignificant due to their relatively low local atomic stress state.



**Figure S4.** Local atomic stress in parallel-twinned Cu NWs. The atomic stress contour clearly demonstrates that the kink-step is the preferential site for nucleation of dislocations.

Intense kink-steps account for improved local stress, as shown in Figure S5 (a) and (b). The local stress state becomes a predominant factor in the yielding mechanism when kink-step density reaches the critical value. By contrast, surface atoms may form nucleation embryos before all kink-steps do.



**Figure S5.** Local stress contour of the NW with kink density of (a) 4.4 nm per kink and (b) 7.0 nm per kink prior to initial yielding.

3. Shear localization of NWs of confined twin spacing



**Figure S6.** The morphology of defective NWs with different λ in [111] direction. Atoms are coloured associated with the local atomic shear strain. (a) 4.0-nm spaced NW. (b) 3.1-nm spaced NW. (c) 1.8-nm spaced NW.

Figure S6 shows the local shear strain map of specimens with distinct TB thicknesses. It is clearly seen that localized strain bands form in the progressive tension. The presence of shear bands implies that the NW undergoes ductile deformation. A thicker shear band, shown by the arrows, is seen from the 3.1-nm spaced and 1.8-nm spaced NWs, indicating substantially distorted structures and multiple dislocation activities along the shear path. There are many other shear paths in the course of the deformation, in accordance with the multiple activated slip systems <110>/{111} during deformation. At the yield point, the kink-steps serve as the major sites for dislocation emission. Once the critical deformation energy is reached, the surface atoms start involving the nucleation of partial dislocations. This process introduces surface ledges, which become the shear strain localized zone, as displayed in the contour. The NW with large twin thickness (4 nm) sustains much less shear localization than counterparts with confined spacing. Moreover, it is clearly evident that the location of the shear band shifts from the centre of the NW to the side of the NW, showing the most distorted region located on the edge of the NW. In refined-TB-spacing NWs, we find that multiple dislocation activities take place in the centre area. Confined spacing between TBs constrains the propagation of dislocations, increasing the likelihood of special events such as Lomer-Cottrell locks and kink migration.

Supplementary Movie 1: Deformation of the NW of 1 kink/ 17.7nm from ε=2% to 12%

Supplementary Movie 2: Deformation of the NW of 1 kink/ 4.4 from ε=2% to 12%

Supplementary Movie 3: Deformation of the NW of 0.6-nm kink height from ε=2% to 12%

Supplementary Movie 4: Deformation of the NW of 1.8-nm kink height from ε=2% to 12%

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