SOME OBSERVATIONS ON THE SIZE EFFECTS IN NANOTWINED METALS AND THEIR THEORETICAL EXPLANATION

Yujie Wei[*]

[*]*State Key Laboratory of Nonlinear Mechanics, Institute of Mechanics, Chinese Academy of Sciences, Beijing 100190, P.R. China*

Summary When materials are deformed plastically via dislocations, a general finding is that samples with smaller dimensions exhibit higher strengths but with very limited amount of plasticity in tension. Here we report that one-dimensional coherent nanostructures with tilted twins exhibit anisotropic size-effect: their strengths show no apparent change if only their thicknesses reduce, but become stronger as the sample sizes are reduced proportionally. Large-scale molecular dynamics simulations show that such NWs deform primarily through twin migration mediated by partial dislocations in one active slip system, and a large amount of plasticity could be achieved in such nanowires via twin migration. Theoretical explanation on the abnormal size effects is supplied. The unique structure shown here is suitable to explore strengthening mechanisms in metals when plasticity is controlled by a single dislocation slip system. This study also suggests a novel approach to modulate strength and ductility in one-dimensional coherent nanostructures.

INTRODUCTION

Recent progress in fabrication and testing of micro- and nanoscale metallic or intermetallic pillars or wires have generally confirmed the notion of smaller being stronger – the strengths of materials tend to increase as either their sample sizes or microstructural dimensions decrease. The work of Uchic *et al.*[1] showed that single-crystal nickel and intermetallic Ni_3Al-Ta samples with smaller radii exhibit higher yield strengths. Subsequently, similar size effects were revealed in other metallic systems and discussed in recent review articles[2]. Here we report from large-scale molecular dynamics (MD) simulations that coherent Cu nanowires (NWs) with tilted internal twins (see Fig. 1 for illustration) show anisotropic size effect: their strengths are insensitive to the decrease in sample thicknesses in [**-110**] direction, but exhibit smaller-being-stronger effect as all dimensions of the sample are proportionally reduced[3]. Such NWs also show large amount of plasticity in tension, and plastic deformation is exclusively accommodated by twin migration, i.e. partial dislocation mediated detwinning.

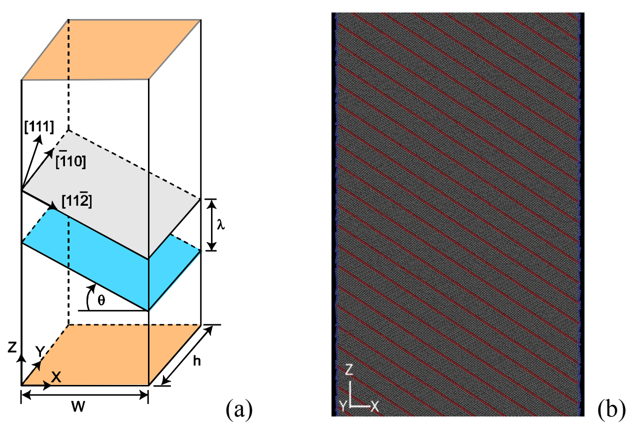


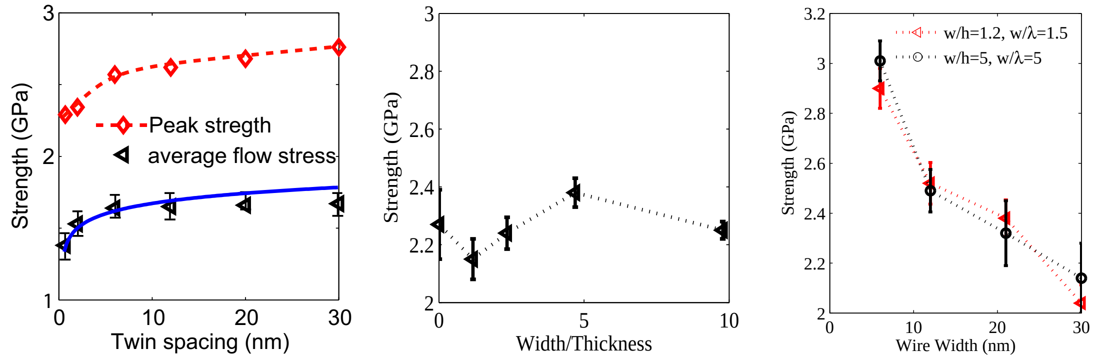
Fig. 1: (a) The geometry of a face center cubic nanowire with thickness direction along [**-110**]. Shadowed planes in the middle refer to twin boundaries, and twin planes are tilted by an angle θ w.r.t. the wire/loading axis. Twins are spaced by a uniform distance λ. Note the three characteristic dimensions: wire width *W*, wire thickness *h*, and *λ*. (b) The projected view of NWs with tilted twins. Atoms in the twin boundaries are in red.

Previous investigations on one-dimensional twinned NWs are for the case that twin planes are aligned to be perpendicular to the wire axes. When subjected to axial loading, the resolved shear stresses within the twin planes in such NWs remain zero. It deactivated three important slip systems parallel to the twin planes; only dislocations inclined to twin planes are activated, and deformation by dislocation motion within the twin planes are prohibited. In contrast, NWs with tilted internal twins (see Fig. 1) allow us to include dislocation activities in all slip systems. In fact, we will show that by choosing an appropriate twin orientation with respect to the wire axis, it is possible to design the behaviors of NWs such that its deformation is dominated by only one slip system parallel to the twin planes.

MAIN RESULTS

Figure 2a shows the average flow stresses in NWs of width W=30 nm, thickness h=25.6 nm, and twin tilt angle θ=30^o for different twin spacings. It indicates that when sample width and thickness are fixed, the average flow stresses decrease as twin spacings are reduced. This behavior is reminiscent of strength softening in nanotwinned Cu as the twin spacing is reduced to below a critical value[4]. To investigate the dependence of average flow stresses on sample sizes, we fix the sample width W=30 nm and twin spacing λ=20nm while changing the thickness h. The strength versus thickness curve is shown in Fig. 2b. There is no apparent change for average flow stresses as the wire thicknesses are reduced.

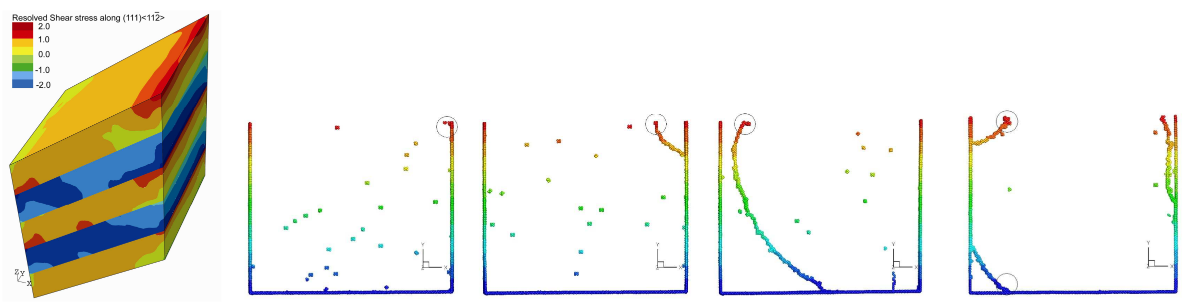
Strengthening in self-similar wires with sample width from 30nm to 6nm while keeping W/h and W/λ ratios constant is observed, as shown in Fig. 2c.



(a) (b) (c)

Fig. 2: Size effects for the three characteristic dimensions. (a) Both peak strength and average flow stresses decrease as twin spacing λ decreases. (b) Stress-strain behaviors for NWs with W=30nm and λ=20nm as their thicknesses decrease. No apparent size effect in strength is observed if we only reduce sample thicknesses. (c) Strengthening in self-similar wires with sample width from 30nm to 6nm while keeping W/h and W/λ ratios constant. A strong size effect is seen.

Nucleation site density is responsible for the slight size-effect as twin spacing λ decreases (Fig. 2a), but not regarded as the major course of size effects observed in Figs. 2b and 2c. Finite-element analysis show that there exists a strong stress concentration at the edge of NWs with rectangular cross sections (Fig. 3a). Such stress concentrations is speculated to be the course of the insensitive strength dependence on NW thickness along [-110] direction (Fig. 2b). Probably stronger surface pinning of partial dislocation in samples with smaller width could be the main reasons behind the size effects in those NWs (Fig. 2c). Our analysis on surface attraction to nucleated dislocations in the NW shows that surface attraction becomes stronger as wire width reduces. In addition, we show that NWs with tilted twins exhibit elastic, almost perfectly plastic behavior upon straining, and a large amount of plasticity could be achieved at room temperature by detwinning (Figs. 3b to 3e).



(a) (b) (c) (d) (e)

Fig. 3: Stress-concentration and dislocation nucleation at the edge. (a) Finite-element analysis to show the stress concentration at the edge of single-crystalline Copper NW with tilted twins. (b) Dislocation nucleation site at the edge. (c) Nucleation of a dislocation along the twin boundary. (d) Extension of the nucleated dislocation. (d) Absorption of the nucleated dislocation as it reaches the opposite free surface. Another dislocation nucleated at the edge again. A large amount of plasticity could be achieved via the continuous nucleation twinning partial dislocations.

CONCLUSIONS

We report that one-dimensional coherent nanostructures with tilted internal twins exhibit anisotropic size-effect: their strengths show no apparent change if only their thicknesses reduce, but become stronger as the sample sizes are reduced proportionally. This study suggests an alternative approach to modulating strength and stretchability/ductility in one-dimensional coherent nanostructures, e.

References

[1] Uchic M.D., Dimiduk, D.M., Florando, J.N., and Nix, W.D. *Science* **305**:986-989, 2004.
[2] Zhu T., Li, J. *Prog. Mater. Sci.* **55**, 710, 2010.
[3] Wei, Y., *Phys. Rev. B* **84**, 014107, 2011.
[4] Li, X., Wei, Y., Lu, K., Lu, L., Gao, H. *Nature* **464**, 877-880, 2010.