ATOMISTIC SIMULATIONS AND MODELING OF PLASTIC DEFORMATION AND FRACTURE IN NANOTWINNED METALS

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Summary The rapid development of synthesis and characterization of nanostructured materials as well as unprecedented computational power have brought forth a new era of materials research in which experiments, simulation and modeling are performed side by side to probe the mechanical properties of nanostructured materials. Here we summarize some recent studies on plastic deformation and fracture mechanisms in nanotwinned metals. In contrast to conventional metals where there is plenty of space for dislocations to multiply so that the strength of material is often controlled by dislocations interaction with grain boundaries (Hall-Petch strengthening) and other obstacles, in nanotwinned metals there are plenty of dislocation nucleation sites while dislocation motion is not confined, and the twin boundaries can be significantly toughened by interaction with dislocations. Atomistic simulations reveal a number of interesting features of plastic deformation and fracture mechanisms in such materials.

Ultra-fine grained copper (grain size ~ 1μm) containing high densities of growth nanotwins with lamella thickness from a few nanometers to a few hundred nanometers exhibited an unusual combination of ultrahigh yield strength (~ 1GPa) and substantial ductility (~ 15% elongation to failure) [1-2]. This unique material system represents a novel class of hierarchically nanostructured metallic materials that opens up exciting possibilities in materials engineering at nanoscale.

Experiments have shown that the strength of nanotwinned Cu increases with decreasing twin thickness λ, reaching a maximum at λ=15 nm, followed by softening at smaller λ [2]. To understand the twin size-dependent softening, we note that reducing the twin thickness in the grains can produce more intersections between grain boundaries and twin boundaries (TBs), and thus more easy sources of dislocation, leading to an increased rate of dislocation nucleation under the same load, or equivalently decreased flow stress at the same plastic strain rate. Such twin size-mediated softening has been qualitatively confirmed by MD simulations [3,4]. Furthermore, a theory has been developed by considering the kinetics of dislocation nucleation and source density in such materials, which relates the strength of the material to TB spacing λ and grain size d as [3]

$$\tau = \frac{\Delta U}{SV^*} - \frac{k_B T}{SV^*} \ln\left(\frac{d}{\lambda}\frac{\nu_D}{\dot{\varepsilon}}\right) \tag{1}$$

where ΔU is the activation energy at zero stress, S is a factor representing local stress concentration and geometry, V^* is the activation volume, k_B is the Boltzmann constant, T is temperature, ν_D is the Debye frequency, and $\dot{\varepsilon}$ is the macroscopic strain rate. Fig. 1 compares the experimentally measured yield stress, the model predictions based on Eq. (1) and MD simulation results [3]. Both simulations and the theory consistently show TB spacing dependent softening in nanotwinned metals. Fig. 1 also indicates that the onset of softening depends on the grain size: the smaller the grain size, the smaller the critical twin-boundary spacing, and the higher the maximum strength of the material.

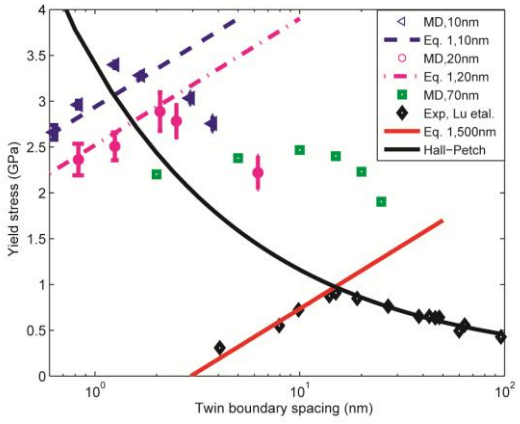

Figure 1. Yield stress of nanotwinned Cu as a function of TB spacing at different grain sizes. Experimental data [2] in the strength increasing region is fitted to the Hall-Petch equation $\sigma_y=\sigma_0+k\lambda^{-1/2}$, where σ_0=127.8 MPa, k=3266 MPa·nm$^{1/2}$ and λ is TB spacing in nm. Simulation results for yield stress (taken as the averaged flow stresses at strains larger than 6%) for d=10 nm, 20 nm (at strain rate of 2×10^8/s and temperature of 300 K), and experimental data for d=500 nm (at strain rate of 6×10^{-3} /s and temperature of 300 K), are shown together with the corresponding fitted curves from Eq. (1). The Quasi-3D simulation results for d=70 nm (at strain rate of 2×10^8 /s and temperature of 300 K) are shown but not fitted since Eq. (1) is based on dislocation nucleation in 3D nanotwinned metals.

Recent MD simulations [4,6] have also revealed an intrinsic capability of TBs to trap a high density of dislocations. In these simulations, a crack is introduced in front of a TB, as illustrated in Fig. 2(a). When the sample is loaded, the crack serves as a "dislocation gun" that shoots out a massive number of dislocations toward the TB. As these dislocations impinge on the TB, they either remain in, or slip across, or decompose into residual and transmission dislocations on the TB. In this way, the TB becomes decorated with a high density of dislocation debris, transforming into a dislocation wall, as illustrated in Fig. 2(b,c). Such dislocation wall blocks further dislocation motion, resulting in strain hardening [6], and becoming increasingly impenetrable to further slip transmission and more resistant to crack propagation [6]. Fig. 2(d) indicates that there exists a boundary layer near the TB where dislocation densities are much higher than elsewhere. The dislocation wall is found to span about 6 nm across the TB, irrespective of the local dislocation density and the strain level, which is consistent with experimental observations and the twin-boundary-affected-zone (TBAZ) model [7]. In-situ tensile experiments inside a transmission electron microscope have demonstrated that the dislocation-wall-strengthened TBs can strongly confine crack nucleation and resist crack propagation, leading to crack bridging by nanoscale twins [6].

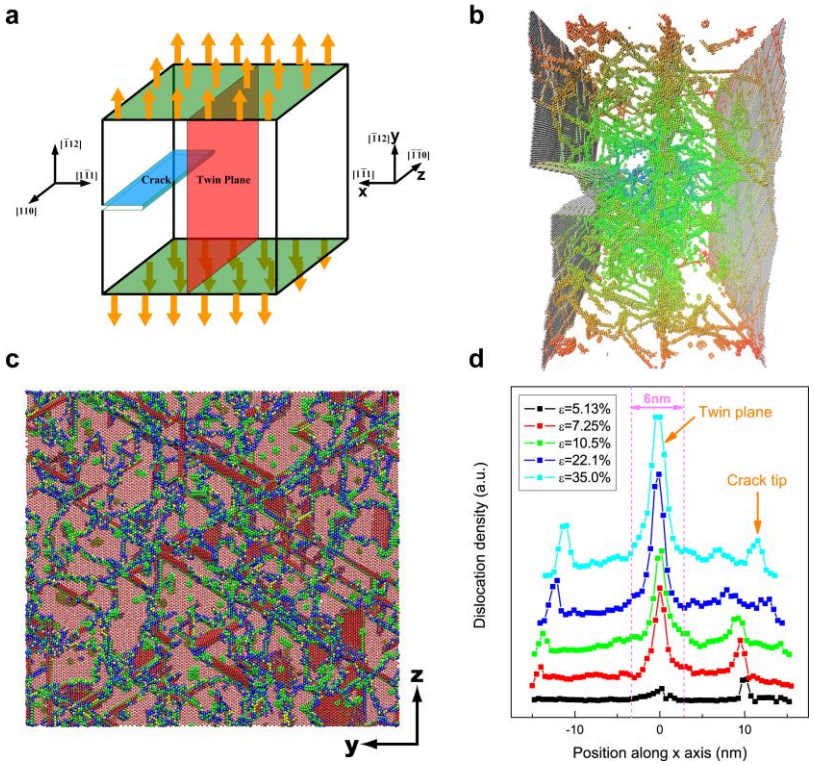

Figure 2. MD simulations for the transformation of TB into dislocation wall. (a) Schematic view of the simulation sample. (b) A snapshot of 3D dislocation structures at a total strain of 22.1%, showing that the TB has become a wall of high dislocation density; the gray atoms are on free surfaces, and other colors represent the distance of atoms near dislocation cores to the centre of the simulated sample. (c) Patterns of dislocation structures remaining on the TB after a large number of dislocations have impinged and slipped across the twin plane; atoms are rendered by the local crystalline order method. (d) Dislocation density distribution along the x-axis across the twin plane showing the characteristic thickness of the TBAZ to be around 2.5-3.5 nm on each side of the TB.

In summary, experimental studies and atomistic simulations have revealed that TB plays a significant role in the plastic deformation of nanotwinned metals. For polycrystalline nanotwinned bulk metals, dislocation nucleation from grain boundary-TB intersections induces a size-softening mechanism. Dislocations interaction with a TB can transform the TB into a dislocation wall which block further dislocation activity and resist crack propagation.

References

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