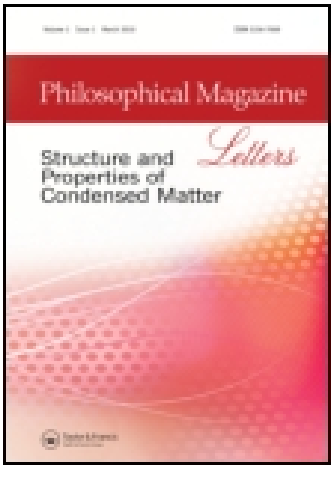

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Tensile deformation mechanisms of the hierarchical structure consisting of both twin-free grains and nanotwinned grains

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Tensile deformation mechanisms of the hierarchical structure consisting of both twin-free grains and nanotwinned grains

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A series of large-scale molecular dynamics simulations have been performed to investigate the tensile properties and atomistic deformation mechanisms for the nanostructured Cu with three typical microstructures: the hierarchical structure consisting of both twin-free grains ($d = 70$ nm) and grains with bundles of smaller nanotwins ($d = 70$ nm, $\lambda = 10$ nm), the fully nanograined structure and the fully nanotwinned structure. The average flow stress of the hierarchically structure is found to be higher than that calculated by rule of mixture. As compared with that of fully nanograined structure, the strength for the twin-free grains in the hierarchical structure is promoted and gives extra hardening due to the increased dislocation density and dislocation behaviours. It is also found that the nanotwin bundles are more deformable than the twin-free grains in the hierarchical structure according to the deviatoric strain invariant contour. This indicates that the fully nanograined structure cannot only be strengthened to a higher level, but also obtain better ductility by embedded with stronger bundles of smaller nanotwins. Thus, a superior strength–ductility synergy could be obtained in this kind of hierarchical structures, and this novel strategy has also been implemented in bulk austenitic steels or copper by recent experiments.

Keywords: molecular dynamics simulations; dislocation interactions; deformation mechanisms; nanostructured materials

1. Introduction

Superior strength–ductility synergy is always desirable for structural applications in modern industry. Such expectation has been realized through the emergence of several strategies in recent decades, such as, solid solution alloying, nanoprecipitate dispersion, transformation and twining-induced plasticity, engineering coherent twin boundaries (TBs) at the nanoscale, bimodal grain size distribution and gradient grained structure [1–11].

Recently, using low-temperature and high-rate severe plastic deformation and subsequent intercritical annealing, a novel strategy for strengthening austenitic steels or copper was introduced [12–15]. In this hierarchical structure, coarse or ultra-fine grains embedded with remaining nanotwinned (NT) regions are formed. The NT regions can be regarded as grains containing bundles of nanotwins, which are stronger than the

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surrounding recrystallized grains. In contrast to conventional strengthening strategies using hard foreign phases or structures, NT grain strengthening metals are single-phased and do not contain any phase boundaries, which are usually the sites for crack nucleation, resulting in superior strength–ductility synergy. The enhanced strength–ductility synergy is due to the fact that TBs are not only effective in blocking dislocation motion, but also can act as slip planes to accommodate dislocations [7,8,16–20]. However, the deformation and the interplaying mechanisms between the larger twin-free grains and smaller bundles of nanotwins in this hierarchical structure still remain unclear. For this perspective, using Cu as a model material, the focus of this paper is to investigate whether or not the dislocation behaviours and dislocation density for the larger twin-free grains in the hierarchical structure are promoted as compared with the corresponding fully twin-free structure, and find out how the plastic deformation is distributed and accommodated between larger twin-free grains and smaller bundles of nanotwins using large-scale molecular dynamics (MD) simulations.

2. Simulation techniques

The MD simulations were carried out using the Large-scale Atomic/Molecular Massively Parallel Simulator code and a Cu EAM potential developed by Mishin et al. [21]. This potential was calibrated according to the *ab initio* values of stacking faults and twin formation energies. To explore deformation mechanisms of the hierarchical structure consisting of twin-free nanograins ($d \approx 70$ nm) and nanograins ($d \approx 70$ nm) with bundles of smaller nanotwins ($\lambda = 10$ nm), it is necessary to simulate grains larger than those possible in fully three-dimensional simulations. In this regard, similar to the configuration used by Yamakov et al. [22], quasi three-dimensional simulations with a columnar grain structure were considered. The thickness direction contains 12 atomic planes, and is along $[\bar{1}10]$. In the present study, three typical microstructures are

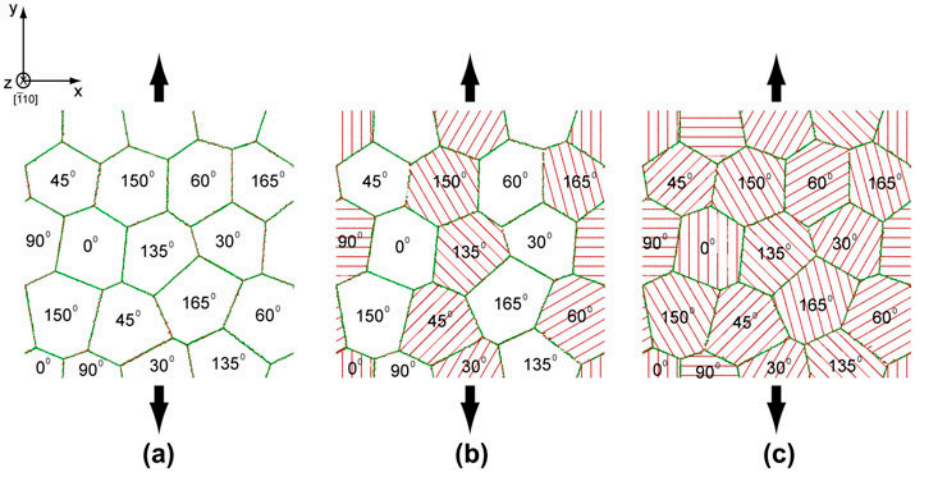

Figure 1. (a) The relaxed Cu sample with fully nanograined structure. (b) The relaxed Cu sample with hierarchical structure. (c) The relaxed Cu sample with fully NT structure.

considered: the fully nanograined structure, the hierarchical structure and the fully NT structure. The relaxed Cu samples for these three structures are shown in Figure 1, with atoms coloured according to common neighbour analysis (CNA) values. Grey colour stands for perfect fcc atoms (not shown in Figure 1), red colour stands for hcp atoms and green colour stands for grain boundaries (GBs), dislocation core, free surface and other atoms. The same CNA colour coding is used in the following figures. In all structures, polycrystalline samples with 16 grains were constructed by the Voronoi method, and the average grain size d was fixed as 70 nm (the samples have dimensions of $280 \times 280 \times 1.53\,\text{nm}^3$ and contain approximately 10,180,000 atoms). The TB spacing was fixed as 10.01 nm for the hierarchical structure and the fully NT structure. The same Voronoi grain structure and the same crystallographic orientations of all grains were retained for all the three structures. In the hierarchical structure, the crystallographic orientations of the eight twin-free grains were also kept the same as those of the eight grains containing nanotwins. Periodic boundary conditions were imposed along all three directions and the tensile loading was along y direction. Before tensile loading, the as-created samples were first subjected to energy minimization by the conjugate gradient method, then gradually heated up to the desired temperature in a stepwise fashion, and finally relaxed in the Nose/Hoover isobaric–isothermal ensemble (NPT) under both the pressure 0 bar and the desired temperature (1 K) for 100 ps. After relaxation, a 20% strain was applied to each sample at a constant strain rate of $5 \times 10^8\,\text{s}^{-1}$. During the tensile loading, Nose/Hoover isobaric–isothermal ensemble (NPT) was also used, and the pressures in the x and z directions were kept to zero in order to simulate the uniaxial loading. MD simulations have proven to be particularly useful for investigating the plastic deformation mechanism of nanostructured metals with carefully designed model system, in which the transient responses of the system and atomic-level stress and strain distributions can be examined [22–27].

3. Results and discussion

Figure 2a shows simulated stress–strain curves for various Cu samples containing the three different structures, in which the stress–strain curve for hierarchical structure based on the rule of mixture is also included for comparison. Tensile stresses are observed to increase with strain up to a certain peak stress, which is associated with the onset of plastic deformation, and then gradually decrease to a relatively steady-state value regardless of structures. It is physically more meaningful to compare the average flow stress over a certain plastic strain interval due to the peak stress overshoot induced by the high strain rate employed in MD simulations [7,28,29]. In view of this, the average flow stresses from a strain of 8–20% are calculated and indicated in Figure 2a. It is shown that the flow stress of the hierarchical structure is in between that of the fully nanograined structure and that of the fully NT structure, and is also higher than that calculated by the rule of mixture.

Atomic level analysis of the deformed configuration was conducted in order to understand the deformation mechanisms of the larger twin-free grains and grains containing smaller nanotwins in the hierarchical structure. The overall simulated deformation pattern at 10% strain for the hierarchical structure is shown in Figure 2b. It should be noted that, in the sample containing a large number of randomly oriented grains, deformation compatibility at GBs usually requires the simultaneous operations

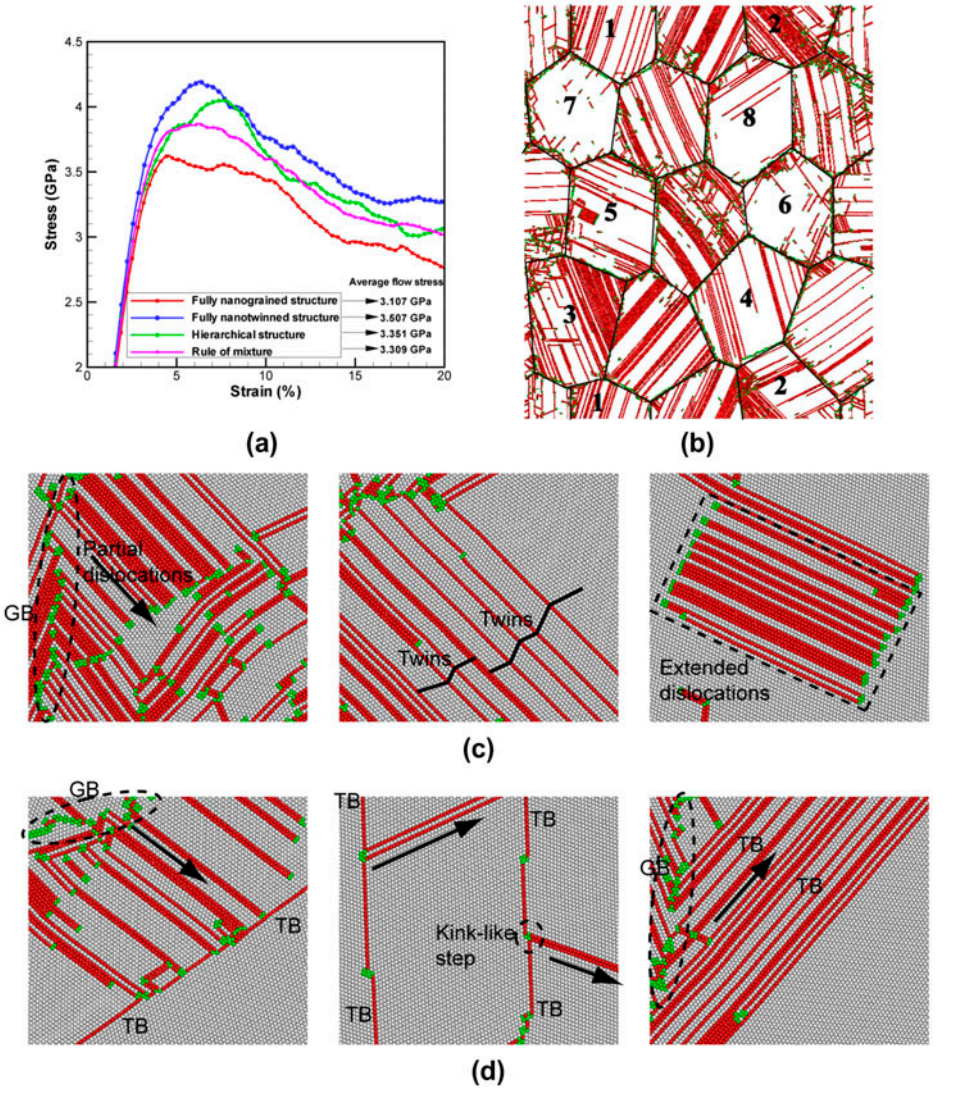

Figure 2. (a) Simulated stress–strain curves for various Cu samples. (b) Simulated deformation patterns at 10% strain for the hierarchical structure. The corresponding amplified configurations from Figure 2b showing the various deformation mechanisms: (c) In the twin-free grains; (d) in the grains containing nanotwin bundles.

of several slip systems. Figure 2c displays the corresponding amplified configurations from Figure 2b showing the various deformation mechanisms for the twin-free grains in the hierarchical structure. It is observed that the plastic deformation of the twin-free grains is accommodated by the following three mechanisms: (1) partial dislocation nucleated from GBs and interactions with stacking faults (SFs) from other slip planes (the dominating deformation mechanism); (2) formation of deformation twins;

(3) nucleation of extended dislocations inside the grain interior due to the relatively large grain sizes ($d \approx 70$ nm). Figure 2d displays the corresponding amplified configurations from Figure 2b showing the various deformation mechanisms for the grains containing nanotwins in the hierarchical structure. However, it is indicated that the plastic deformation of the grains containing nanotwins is accommodated by the following three mechanisms: (1) partial dislocation emitted from GBs travelling inclined to TBs (the dominating deformation mechanism); (2) partial dislocation emitted from TBs travelling inclined to other TBs; (3) partial dislocation emitted from GBs travelling parallel to TBs. According to previous research [30], the first deformation mechanism (the dominating one) for the nanotwin bundles will generate SFs as well as dislocation locks associated with dislocation/TB reactions, which are immobile and cause the work hardening. The second deformation mechanism also generates SFs and dislocation locks associated with dislocation/TB reactions, causing the work hardening, except that the sources of dislocations are TBs instead of GBs. After nucleation of partial dislocations, kink-like steps are also created at the dislocation–TB intersection sites, generating defective TBs [31], as indicated in Figure 2d.

Stress contours of the deformed configuration at various strains for the hierarchical structure were analysed to illustrate why the average flow stress of the hierarchical structure is higher than that calculated by the rule of mixture. Figure 3a shows stress contour (σ_{yy}) at 10% strain for the Cu sample with hierarchical structure. And then, the average stresses for the twin-free grains in the hierarchical structure were calculated based on the stress contour and shown in Figure 3b. It indicates that the flow stress for the twin-free grains in the hierarchical structure is promoted, as compared with that of fully nanograined structure. Figure 3c shows fractions of HCP atoms as a function of strain for the twin-free grains in the hierarchical structure and the fully nanograined structure, in which fractions of HCP atoms are general indictors of partial dislocation activities. As shown in Figure 3c, the promotion of flow stress for the twin-free grains in the hierarchical structure is caused by the increased dislocation behaviours and dislocation density. Figures 3d and 3e show the corresponding amplified configurations in typical twin-free grains (grains 2 and 8), indicating increased dislocation behaviours in hierarchical structure, as compared with the fully nanograined structure. For grain 2, only partial dislocations in one slip system are observed in fully nanograined structure; however, partial dislocations in two slip systems and interactions between each other are observed in the hierarchical structure. The grain 8 is clean and no dislocation behaviours are observed in fully nanograined structure, while extensive partial dislocation behaviours are observed for the same grain in the hierarchical structure.

In order to check the detail strain distribution and deformability between twin-free grains and nanotwin bundles in the hierarchical structure, a local equivalent strain is calculated by using atomic local strain component: $\varepsilon_{eV} = \sqrt{J_2(\varepsilon)}$, where $J_2(\varepsilon)$ is the second deviatoric strain invariant. The atomic local strain tensor ε is computed as a best fit of the local affine transformation, and is obtained by running a least-square fitting procedure using the all local neighbour atom's information [24]. Figures 4a and 4b show the local equivalent strain contours for the Cu sample with hierarchical structure at 10% strain and 20% strain, respectively. As indicated, large local strains are observed at GB or SF areas. Figure 4c shows the average equivalent strain for twin-free grains and nanotwin bundles in the hierarchical structure as a function of the overall tensile strain. It should be noted that the nanotwin bundles are not only harder than twin-free

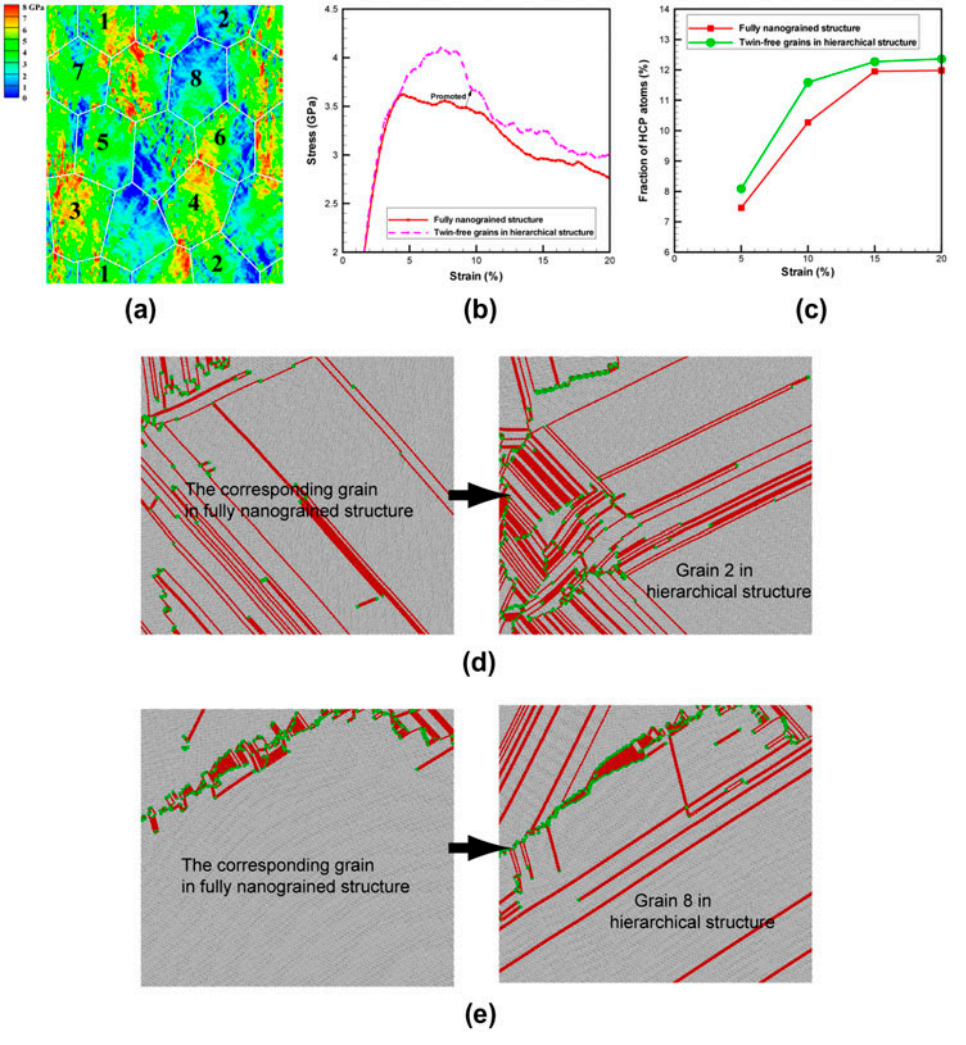

Figure 3. (a) Stress contour (σ_{yy}) at 10% strain for the Cu sample with hierarchical structure (twin-free grains are marked in the figure). (b) Simulated average stresses as a function of strain for the fully nanograined structure and the twin-free grains in the hierarchical structure. (c) Fractions of HCP atoms as a function of strain for the fully nanograined structure and the twin-free grains in the hierarchical structure. The corresponding amplified configurations in typical twin-free grains shows increased dislocation behaviours in hierarchical structure, as compared with the fully nanograined structure: (d) grain 2; (e) grain 8.

grains (with higher flow stress), but also more deformable than twin-free grains. This should be due to the fact that TBs are not only effective in blocking dislocation motion, but also can act as slip planes to accommodate dislocations.

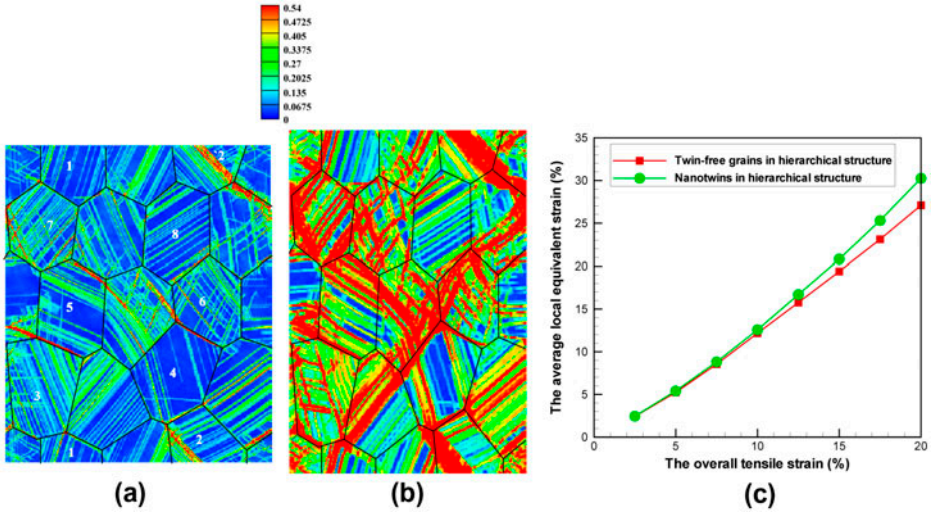

Figure 4. The local equivalent strain contour for the Cu sample with hierarchical structure (twin-free grains are marked in the figure): (a) at 10% strain; (b) at 20% strain. (c) The average deviatoric equivalent strain for twin-free grains and nanotwin bundles in the hierarchical structure vs. the overall tensile strain.

4. Summary

A series of large-scale MD simulations have been performed to investigate the tensile properties and atomistic deformation mechanisms for the nanostructured Cu with three typical microstructures: the hierarchical structure, the fully nanograined structure and the fully NT structure. The average flow stress of the hierarchically structure is found to be higher than that calculated by the rule of mixture. As compared with that of fully nanograined structure, the strength for the twin-free grains in the hierarchical structure is promoted and gives extra hardening due to the increased dislocation density and dislocation behaviours. It is also found that the nanotwin bundles are more deformable than the twin-free grains in the hierarchical structure according to the deviatoric equivalent strain contour. This indicates that the relatively larger nanograins ($d = 70$ nm) can not only be strengthened to a higher level, but also obtain better ductility by embedding with stronger bundles of smaller nanotwins ($\lambda = 10$ nm). Thus, a superior strength–ductility synergy could be obtained in the hierarchical structure consisting of relatively larger twin-free grains embedded with bundles of smaller nanotwins.

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