Mechanical properties of twin lamella copper: Preliminary studies

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Abstract. The study of the mechanical properties of materials at nano- and sub-micrometer scales is motivated by increasing need for such materials due to miniaturization of engineering and electronic components, development of nanostructured materials, thin film technology and surface science. When the material volume is lowered, characteristic dimensions are reduced that control the material properties and this often results in deviation from the behavior of bulk materials. Using large-scale molecular dynamics, here we study the properties of nanostructured copper with ultra thin twin lamella structures, as investigated in experiment recently (Lu *et al.*, Science, 2004).

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‡ This is an excerpt of results related to modeling twin lamella copper as reported in my PhD thesis.

1. Plasticity of nanocrystalline materials with twin lamella

In previous studies, the properties of nanocrystalline metals were discussed [9, 10, 2, 16, 14, 15, 4]. Other studies focused on the mechanics of thin metal films [11, 7, 5, 3, 6, 1, 12]. The importance of reduction in dimensions, and its impact on the mechanical properties is further underlined by the studies reported in this report.

Here we focus on polycrystalline bulk copper, where the grain size is on the order of several nanometers to tens of nanometers.

We consider a polycrystalline microstructure with hexagonal grains, but with different grain orientations as in the previous case (see Figure 2 for details). To further study the effect of geometric confinement on plasticity, we introduce a sub-nano structure in the grains. This sub-nanostructure is established by assuming twin grain boundaries forming very thin twin-lamella. Such microstructure can be produced experimentally in copper [8]. With this model, we pursue two main objectives:

(i) We show that in bulk nanostructured materials, the type of the grain boundary plays a very important role for dislocation nucleation, as it was found for thin films.

(ii) We show that the sub-nanostructure composed of twin grain boundaries provides a very effective barrier for dislocation motion and therefore leads to a very "strong" nanostructured material.

2. Atomistic Modeling Method

To underline the first point regarding dislocation nucleation, we consider two samples. The first sample (i) has the following grain misorientations. Grain 1 is in the reference configuration ($[1\bar{1}0]$ in the x direction, $[11\bar{2}]$ in the y direction). Grain 2 is rotated counterclockwise by 7.4 degrees, grain 3 is rotated by 35 degrees, and grain 4 is rotated by 21.8 degrees with respect to grain 1. The model contains up to 35 million particles. With this procedure, a low-energy grain boundary is constructed between grains 3 and 4. After creation of the sample, the structure is relaxed for a few thousand integration steps using an energy minimization scheme. Figure 1 shows the atomistic model of the polycrystalline thin film. Only surfaces (yellowish color) and grain boundaries (bluish color) are shown.

We construct a second sample (ii) where all grain boundaries are of the same type.

We hypothesize that dislocation nucleation occurs predominantly from low-energy grain boundaries, the dislocation density in sample (i) should be higher in grains 3 and 4, and should be comparable in all grains in sample (ii).

The simulation geometry is depicted in Figure 2. The blue lines inside the grains refer to the intra-grain twin grain boundaries. The thickness of the twin lamella is denoted by d_{T}.

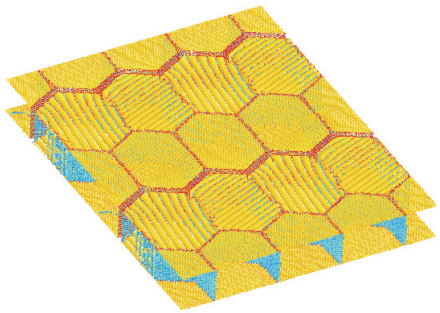

Figure 1. Atomistic model of the polycrystalline thin film. Only surfaces (yellowish color) and grain boundaries (bluish color) are shown.

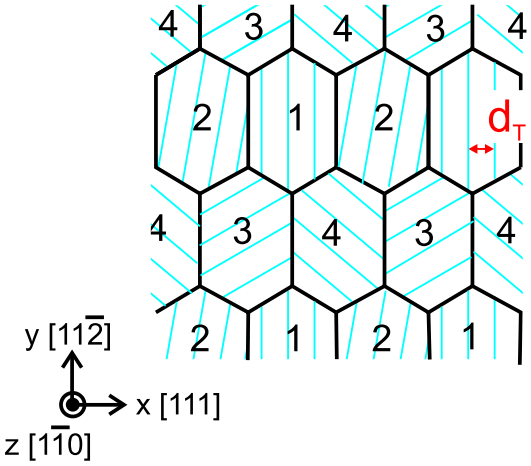

Figure 2. Nanostructured material with twin grain boundary nano-substructure. The blue lines inside the grains refer to the intra-grain twin grain boundaries. The thickness of the twin lamella is denoted by d_{T}.

3. Simulation results

The material is loaded uniaxially in the x-direction. We start with sample (i), and we consider is a grain size of 12.5 nm $\times$ 16.5 nm. The grains have the same misorientation as in the study described above. We perform the simulation for two different lamella sizes d_{T}. The results are shown in Figure 3.

We observe that dislocations are generated exclusively from the low-energy grain boundaries between grains 3 and 4. This is in agreement with the results of the polycrystalline thin films. The fact that we use a different grain orientation in this study with different boundary conditions suggests that the nucleation conditions discussed previously is a more general concept. The results indicate that the twin grain boundaries are an effective barrier for further dislocation motion, since we observe dislocation pileups at the twin grain boundaries. An important consequence is that the thinner the lamella structure (small d_{T}), the less plasticity can transmitted via the motion

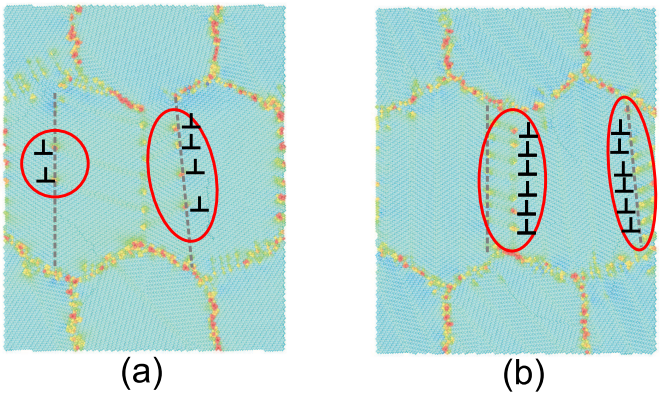

Figure 3. Simulation results of nanostructured material with twin lamella substructure under uniaxial loading for two different twin lamella thicknesses. Subplot (a) shows the results for thick twin lamella ($d_{\mathrm{T}} \approx 15\ nm > d$) and subplot (b) for thinner twin lamella ($d_{\mathrm{T}} \approx 2.5$ nm). Motion of dislocations is effectively hindered at twin grain boundaries.

of dislocations. This indicates that grains with a nano-substructure of twin grain boundaries is an effective hardening mechanism for materials.

We report another study with the same microstructure, but different grain misorientation angles, sample (ii). In this case, we choose the grain boundary misorientation identical in all grains. Grain 1 is in its reference configuration, grain 2 is rotated by 30°, grain 3 by 60° and grain 4 is misoriented by 90°. All grain boundaries are now high-angle grain boundaries.

The results of this calculation are shown in Figure 4 (a). Unlike in Figure 3, dislocations are now nucleated at all grain boundaries and the nucleation of dislocations is governed by the resolved shear stress on different glide planes. We observe that dislocations can easily penetrate through the stacking fault planes generated by motion of other partial dislocations, but build pileups at the twin grain boundaries. We also observe that dislocations with opposite Burgers vector annihilate. Further, dislocations cross slip (see highlighted region in the center of Figure 4 (b), region i.) in regions with high dislocation densities. The activated primary and secondary glide planes are highlighted in the plot. The primary glide planes are parallel to the twin grain boundaries so that dislocation glide is not restricted. In contrast, once dislocations have cross-slipped to the secondary glide plane their motion is restricted due to the twin grain boundaries (see Figure 4 (b) ii.). Figure 4 (b) iii. shows intersection of dislocations. A defect is left at the intersection of the stacking fault planes.

As in the previous studies of nanostructured materials [13], we also observe that partial dislocations dominate plasticity. Dominance of partial dislocations is verified by the fact that dislocations leave behind a stacking fault.

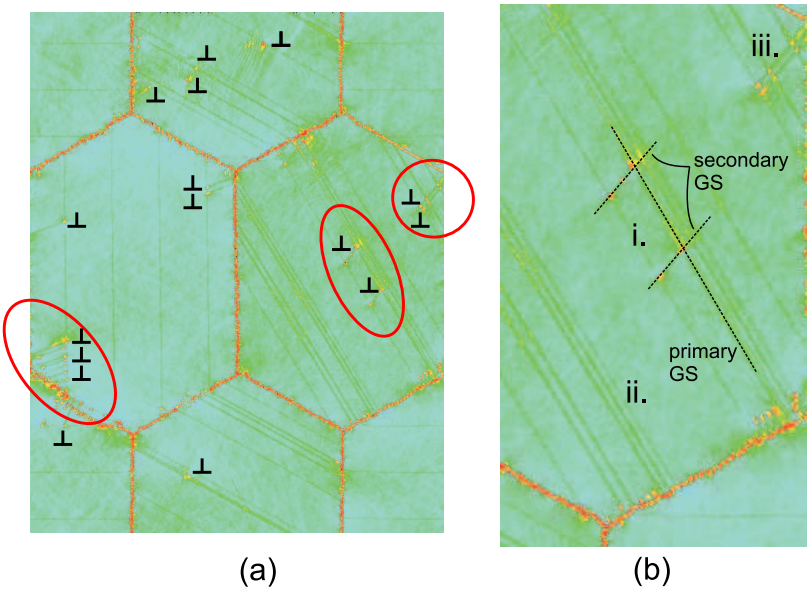

Figure 4. Simulation results of nanostructured material with twin lamella substructure under uniaxial loading for two different twin lamella thicknesses, all high-energy grain boundaries. Subplot (a) shows the potential energy field after uniaxial loading was applied. Interesting regions are highlighted by a circle. Unlike in Figure 3, dislocations are now nucleated at all grain boundaries. The nucleation of dislocations is now governed by the resolved shear stress on different glide planes. Subplot (b) highlights an interesting region in the right half where i. cross-slip, ii. stacking fault planes generated by motion of partial dislocations and iii. intersection of stacking fault planes left by dislocations is observed.

4. Discussion and conclusion

The preliminary study on nanostructured materials reported here showed that an intergranular nano-substructure constituted by twin lamellas could play an important role in effectively strengthening materials. Since twin grain boundaries are relatively poor diffusion paths (since they are low-energy grain boundaries), such materials could potentially be successfully employed at elevated temperatures where "usual" materials with ultra-fine grains can not be utilized since creep becomes the dominant deformation mechanism.

The study supports the notion that geometric confinement has strong impact on the deformation, and could potentially be utilized to create materials with superior mechanical properties.

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