MICROSTRUCTURAL AND ATOMISTIC SIMULATION FOR DEFORMATION OF NANO-GRAINED METALS

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Summary The deformation of nano-grained metals is explored from three aspects: computation under a recently developed microstructural evolution algorithm; mechanics modelling for the cooperative insertion-rotation process under the 9-grain cluster model; and molecular dynamics simulation for fast isochoric stretching under large deformation.

Recently, experiment of rolling nano-crystalline copper at room temperature to an elongation of 5100% was reported [1]. Nano-grain metals of such small grain sizes deform mainly by neighboring grains sliding pass each other with insignificant distortion in the grain shape. We adopted a structural evolution algorithm to simulate the process. Accommodation mechanisms such as grain boundary diffusion, sliding and grain rotation control the kinetics of the process. Actual deformation minimizes the plastic dissipation and stored strain energy for representative steps of grain neighbor switching. Numerical simulations based on these principles are given for a representing cell composed of 200 non-uniform grains. The deformation process is portrayed in the snapshots shown in the left of Fig. 1, while the straight line in the log-log plot on the right indicates an inverse power dependence (-2.61) of the strain rate on the grain size under a sustained stress.

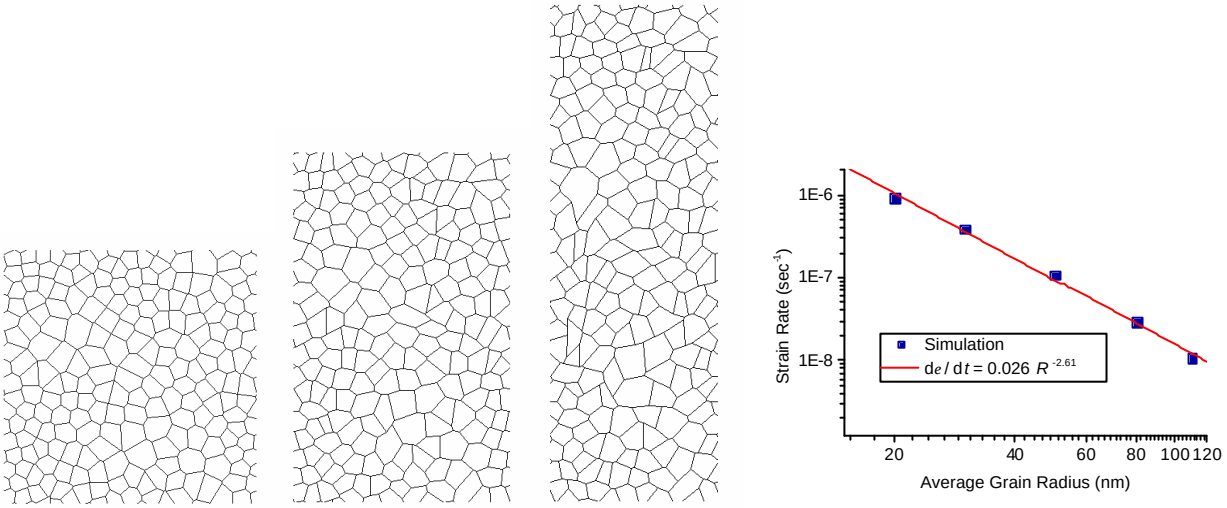
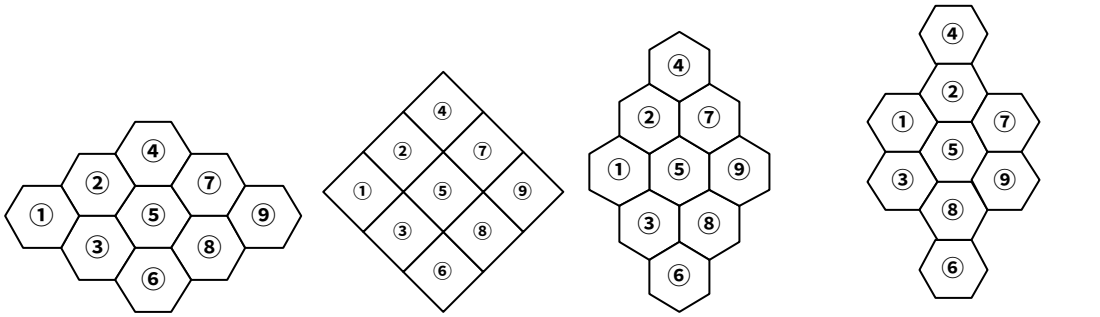


Figure 1 Simulated deformation process and scale dependence.

The 4-grain cluster model of Ashby and Verrall [2], with its concrete calculation and the perception of grains squeezing pass each other, should serve as the starting point for the mechanism model of nano-grained metals. Figure 2 illustrates an attempt to complete the Ashby-Verrall mechanism by adding a rotation of closely contacted grain pairs. The cell contains 9 regular hexagon grains and is termed the 9-grain cluster model.



(a) initial configuration (b) critical configuration (c) completion of insertion (d) rotation of 30 degrees

Figure 2 Model of 9-grain cluster

The constitutive law for fully relaxed creeping behavior is [3]:

$$\dot{e} = C(s - s_{\text{th}}) \tag{1}$$

where the creep rate C is given by

$$C = \frac{\sqrt{3}\Delta e^2}{8D}\left[\frac{m^2 K_B T D}{3\Omega\left\{nD_V + D_B\sum_{i=1}^{n}\frac{d}{l_i}\right\}} + \frac{h_B}{d}s^2\right]^{-1} \tag{2}$$

and the threshold stress is:

$$s_{\text{th}} = \frac{1}{\Delta e}\left[\left(\sqrt{2\sqrt{3}} - \sqrt{3}\right)\frac{4\Gamma}{3D} + \left(1 - \frac{p}{2\sqrt{3}}\right)\Delta g\right] \tag{3}$$

The linear creep law in (1) agrees in form with the experimental data by Cai et al. [4] for nano-grained copper, as indicated in Fig. 3. An extension of the coorperative insertion-rotation mechanism to the plane strain and three-dimensional cases is achieved by Wang and Yang [5].

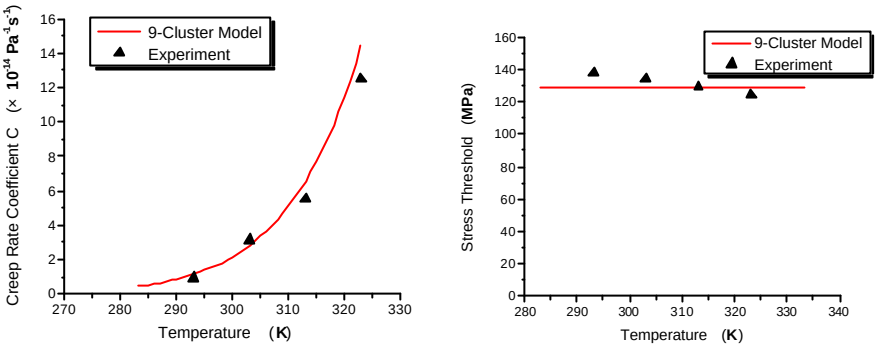


Figure 3 Creep rate (left) and threshold stress (right) for nano-grained copper.

The method of molecular dynamic simulation is only capable of the case of fast stretching. The previous works concerning on this subject were not conducted to the regime of large deformation. Here we only present a simulation for copper of 1,000,000 atoms under EAM potential. The loading is imposed by a quasi-homogeneous manner. The profiles of the local crystalline order are plotted in Figure 3. The sites where local fcc order are colored green, those of hcp order (stacking faults) are colored red, and those of amorphous state are colored blue. As the amount of tension increases, one observes the bursts of defects (in the disordered form of stacking faults) within the grains. Most stacking faults are arrested by the grain boundaries and rotate slightly toward the tensile direction. A different family of stacking faults may be observed during the later stages of tension, and some areas dissolve into sub-grains of smaller size.

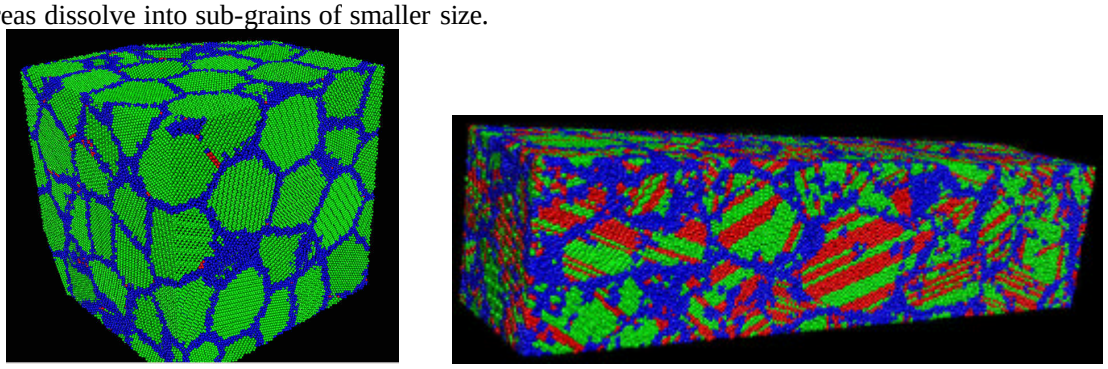


Figure 4 Profiles of local crystalline order for stretching nanocrystalline Cu. Left: initial configuration; right: elongated to a logarithmic strain of 100%.

References

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