Received: 20 October 2019 | Revised: 18 November 2019 | Accepted: 19 November 2019

DOI: 10.1002/mdp2.122

WILEY

LETTER

Effects of the grain size gradient on the microstructural evolution in gradient nano-grained copper with initial central crack

Yaping Liu | Fan Yang | Jiarui Zhang

School of Aerospace Engineering and Applied Mechanics, Tongji University, Shanghai, China

Correspondence
Dr Fan Yang, School of Aerospace Engineering and Applied Mechanics, Tongji University, Shanghai, China.
Email: fanyang@tongji.edu.cn

Funding information
Shanghai Supercomputer Center; National Natural Science Foundation of China, Grant/Award Number: 11772231

Abstract

Due to the outstanding performances in both strength and ductility, gradient nano-grained (GNG) metals possess strong application potential. In this paper, a quasi-three-dimensional molecular dynamics model of GNG copper with initial central crack is established, and the effect of the grain size gradient on the crack evolution is investigated. The obtained results are helpful to reveal the cooperative mechanisms in the fracture process of the graded nanocrystalline needs.

KEYWORDS

central crack, fracture, GNG, gradient, molecular dynamics

1 | INTRODUCTION

Modern manufacturing industry raised increasingly strict requirements on the strength, ductility, and fatigue resistance of materials. GNG metals characterized with grain size decreasing from the surface to the bulk have recently received considerable attention for their high strength and high ductility.[1,2] Previous research reported that the strength of GNG copper could be increased by as much as three times while the homogenized ductility is comparable to that of the coarse-grained (CG) counterpart.[3] Study on the gradient structured steel shows that the strength enhancement is higher than that given by the mixing rule.[4,5] The excellent mechanical properties of GNG copper can be attributed to the synergistic mechanisms contributed by the surface nanocrystals and the internal coarse grains during the deformation,[6] in which the strain incompatibility between layers with different grain sizes promotes the dislocation activity and hence the plasticity of the whole structure.[4,7]

Mechanical surface treatments such as mechanical grinding[8,9] or shot peening[6] to refine the surface grains are the common methods to prepare GNG metals. However, on the one hand, although grain refinement could inhibit the initiation of cracks, it is not conducive to the propagation of cracks.[10] On the other hand, it would also cause stress concentration as a result of the increased surface roughness.[11] Both of these factors are ultimately reflected in the reduction of fracture resistance. The fracture of the gradient GNG metals exhibits a unique microscopic mechanism that is different from ordinary coarse crystals and uniform nanocrystals. In materials with uniform grain size or small gradient, cracks tend to propagate along the grain boundaries, and the deformation energy is mainly dissipated by the grain boundary cracking. While in materials with large gradient, the deformation energy is partially dissipated by the dislocation movement within the larger grains, which means that more atoms can be mobilized to resist fracture and thus improve the fracture toughness.[12] So far, existing efforts on GNG metal mainly focus on the deformation and the tensile ductility, and studies on the fracture behavior of GNG metals are still insufficient. It is necessary to systematically investigate the fracture behavior of GNG materials.

2 | MD MODEL OF GNG COPPER WITH INITIAL CENTRAL CRACK

Gradient nano-grained copper possesses a complex grain boundary topology. Figure 1A shows the topological structure of quasi-three-dimensional GNG copper with columnar grains. The geometric model of GNG was constructed using the Voronoi partition function of MATLAB.

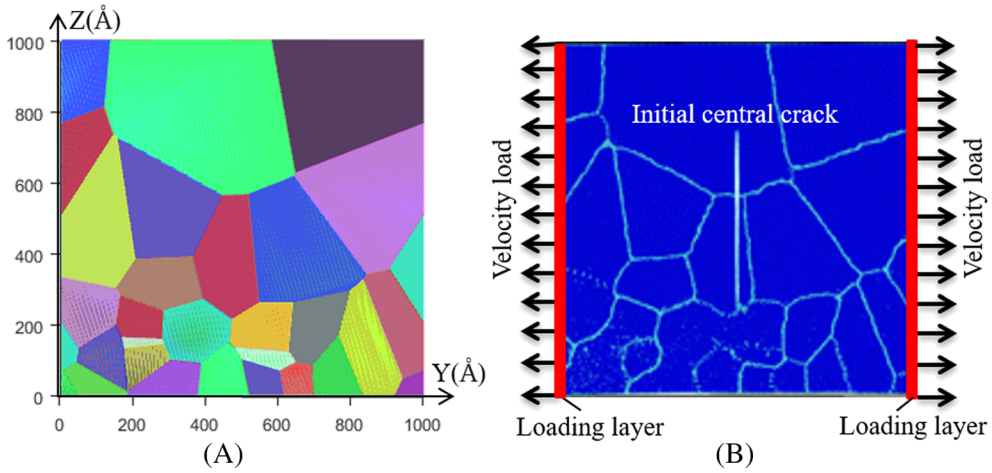

FIGURE 1 (A) Topological configuration of GNG copper with gradient of 5, and (B) loading scheme of GNG model with initial central crack

Then, each grain was filled with the face entered cubic (FCC) copper atoms with the lattice orientation following a uniform random probability function in different grains. In this process, the [111] direction was always kept normal to the screen plane. Grain boundaries with different misorientation angles were formed between adjacent grains due to different lattice orientations of the grains. The dimension of the MD sample is $18.75 \times 1000 \times 1000$ Å^3 with about 1 600 000 atoms. Three MD samples with gradients of 1, 5, and 20 were created, and the gradient of the model is defined as the ratio of the maximum grain size to the minimum grain size. Correspondingly, the grain size of these samples varies linearly from 50 nm on the upper end to 50, 10, or 2.5 nm on the lower end. Finally, by shielding the interaction between the two sets of atoms on each side of the crack, a quasi-three-dimensional GNG copper model with an initial central crack was established.

The computations were carried out using the open source code LAMMPS. The embedded atom potential (EAM) was used to model the interaction between atoms. A 0.2-nm-thick atomic group was taken as the loading layer at both the left and the right ends of the sample, and a tensile velocity of 0.05 nm/picosecond (corresponding to a strain rate of 1.0×10^9 s^{-1}) was applied to the loading layers. All the simulations were carried out in the isothermal-isobaric (NPT) ensemble with the temperature controlled at 100K.

3 | RESULTS AND DISCUSSIONS

The cracking process in GNG copper is often accompanied by the formation and development of intragranular dislocations. Taking the sample with the largest gradient (gradient 20) as an example, the dislocation activities were shown in Figure 2 with different colors indicating different lattice types in Figure 2A-2D, or different dislocation types in Figure 2E-2H. During the loading process, Shockley partial dislocations begin to emit from the crack tip at strain of 0.024 (Figure 2A) and slip into the interior of the grains, leaving a large number of stacking faults behind. Different phenomena were observed when the dislocations meet the grain boundaries on the opposite side. In the upper region with larger grain size, the dislocation will be absorbed by the opposite grain boundary, leading to disappearance of the stacking fault. While in the lower region with smaller grain size, the dislocations will pass across the grain boundary until the next grain boundary is encountered and a stacking fault is left inside the grains.

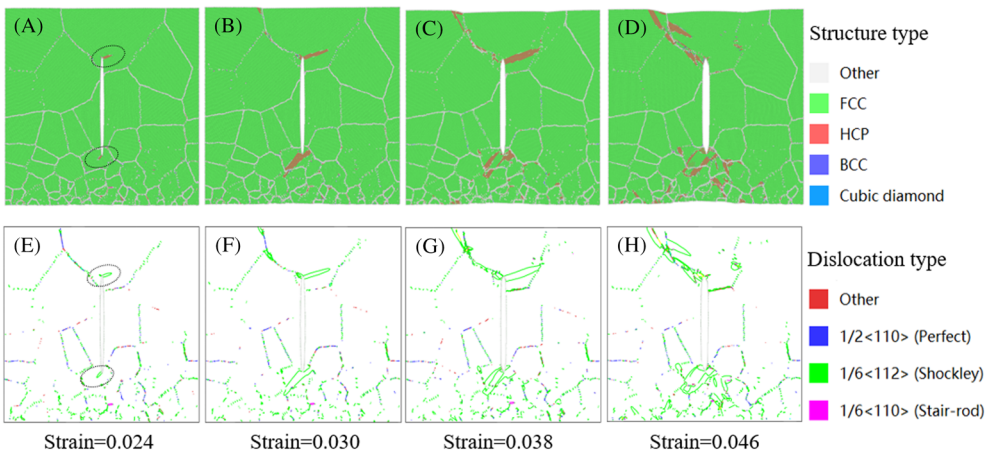

FIGURE 2 The formation and development of intragranular dislocations in the GNG copper during the cracking process (gradient = 20)

To investigate the effects of the grain size gradient on the crack evolution, we prepared three specimens with gradients of 1, 5, and 20 and the same initial central crack length of 50 nm. In order to compare the microstructural evolutions near the upper crack tip and near the lower crack tip, two rectangular regions of 400 × 300 Å^2 were selected as the comparison regions for the calculation of the dislocation density and the ratio of the hexagonal close packed (HCP) atoms, as shown in Figure 3.

Figure 4A shows the evolution of dislocation density in the upper region of different specimens. It indicates that when the strain is less than 0.06, the dislocation density has negligible difference. When the strain is larger than 0.06, the dislocation density decreases rapidly for the specimen with the gradient of 1, while remains relatively stable for the other two specimens. Figure 4B shows the evolution of dislocation density in the lower region. It indicates that when the strain is less than 0.1, the dislocation density increases evidently with the strain for all specimens. When the strain is larger than 0.1, the dislocation density continues to increase for the specimen with the largest gradient 20, while starts to undulate for the other two specimens. Generally, a larger grain size gradient corresponds to a larger dislocation density for the lower region from Figure 4B.

HCP atoms are closely related to the stacking faults, and the change of their proportion can reflect the dislocation activities. Figure 5 shows the evolution of the ratio of the HCP atoms, with Figure 5A,B corresponding to the upper region and the lower region, respectively. It shows that when the strain is less than 0.02, almost no HCP microstructure is observed in the investigated regions. As the strain increases, the number of HCP atoms increases rapidly in both the upper region and the lower region, especially for the specimen with uniform grain size distribution (gradient equaling to 1). After reaching the peak value, the proportion of HCP atoms decreases and fluctuates violently as the straining continues,

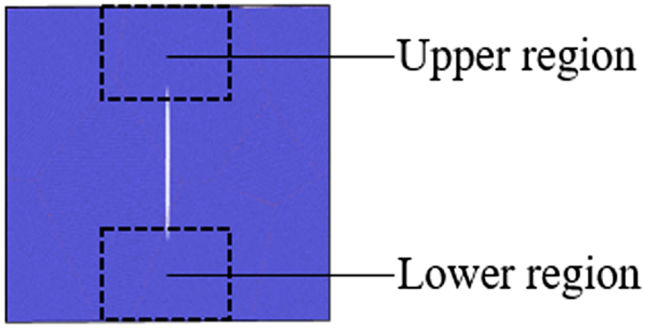

FIGURE 3 Schematic diagram of comparison regions in each specimen

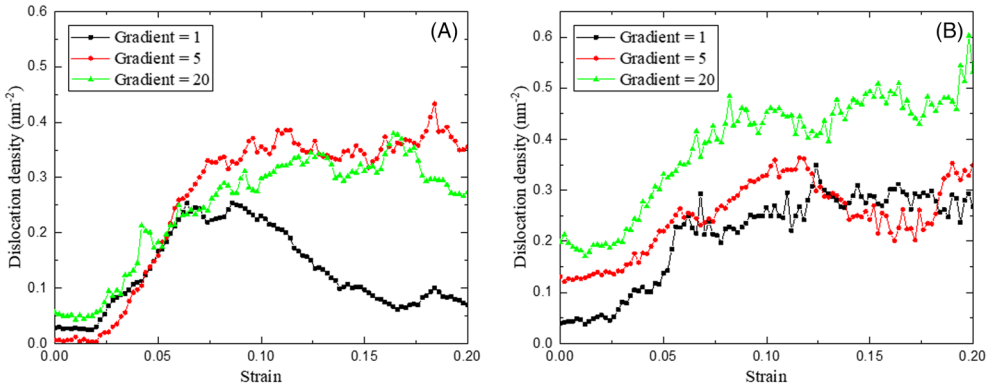

FIGURE 4 Comparison of dislocation density between different specimens in (A) the upper region and (B) the lower region

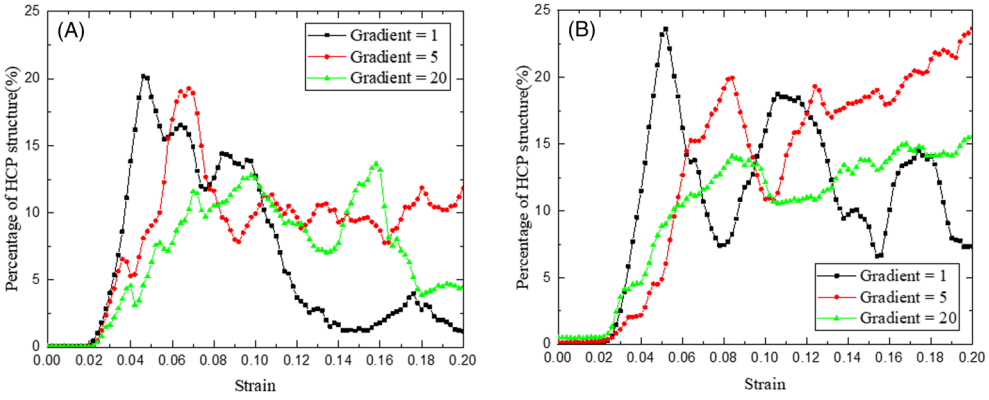

FIGURE 5 Comparison of HCP atom percentages between different specimens in (A) the upper region and (B) the lower region

indicating the abundant activities of partial dislocations and the resulting generation and annihilation of stacking faults. From Figure 5A,B, the proportion of HCP atoms is the highest in the uniform specimen at a small strain below 0.05. On the contrary, the proportion of HCP atoms is higher in the gradient grain-size specimens and the lowest in the uniform specimen when the strain exceeds 0.12. These results indicate that when the strain is small, the smaller grain-size gradient is beneficial to suppress the propagation of cracks, while as the strain increases, the larger grain-size gradient is advantageous in suppressing the crack growth.

4 | CONCLUSIONS

In the present work, the effects of the grain size gradient on the microstructural evolution in the GNG copper with initial central crack are studied. As a summary of a series of simulations, several key findings are listed as follows:

a. During the tensile deformation, a larger grain size gradient generates more dislocations near the crack tip.
b. When the deformation is small, the smaller grain size gradient is more effective in inhibiting the crack propagation, while as the deformation increases, the larger grain size gradient is more favorable in suppressing the crack propagation.

ACKNOWLEDGEMENTS

This work was supported by the National Natural Science Foundation of China (11772231) and Shanghai Supercomputer Center.

ORCID

Fan Yang https://orcid.org/0000-0003-4801-763X

REFERENCES

1. Lu K, Lu J. Nanostructured surface layer on metallic materials induced by surface mechanical attrition treatment. Mater Sci Eng A. 2004;375-377(1):8-45.
2. Lu K. Gradient nanostructured materials. Acta Metall. 2015;51(1):1-15.
3. Fang TH et al. Revealing extraordinary intrinsic tensile plasticity in gradient nano-grained copper. Science. 2011;331(6024):1587-1590.
4. Wu X, Yang M, Yuan F, et al. Heterogeneous lamella structure unites ultrafine-grain strength with coarse-grain ductility. Proc Natl Acad Sci U S A. 2015;112(47):14501-14505.
5. Fang Q, Li L, Li J, Wu H. Strengthening mechanism of gradient nanostructured body-centred cubic iron film: from inverse Hall-Petch to classic Hall-Petch. Comput Mater Sci. 2018;152:236-242.
6. Wang Y et al. Synergetic deformation-induced extraordinary softening and hardening in gradient copper. Mater Sci Eng A. 2019;752:217-222.
7. Li Z, Yang F. Grain rotations during uniaxial deformation of gradient nano-grained metals using crystal plasticity finite element simulations. Extreme Mech Lett. 2017;16:41-48.
8. Wang L et al. High tensile ductility and strength in a gradient structured Zr. Mater Lett. 2018;228:500-503.
9. Long JZ et al. Abnormal grain coarsening in cyclically deformed gradient nanograined Cu. Scr Mater. 2018;145:99-103.
10. Zhou P et al. Effect of grain size and misorientation angle on fatigue crack growth of nanocrystalline materials. Mater Sci Eng A. 2016;663:1-7.
11. Hassani-Gangaraj SM et al. Experimental assessment and simulation of surface nanocrystallization by severe shot peening. Acta Mater. 2015;97:105-115.
12. Wang P, Yang X, Tian X. Fracture behavior of precracked nanocrystalline materials with grain size gradients. J Mater Res. 2015;30(5):709-716.

How to cite this article: Liu Y, Yang F, Zhang J. Effects of the grain size gradient on the microstructural evolution in gradient nano-grained copper with initial central crack. *Mat Design Process Comm*. 2019;e122. https://doi.org/10.1002/mdp2.122