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ATOMISTIC STUDY OF PLASTIC DEFORMATION IN DEFECTIVE NANOTWINNED COPPER

Yonggang Zheng[1,]*, Yifei Fu[1], Hongwu Zhang[1] and Hongfei Ye[1]

[1] State Key Laboratory of Structure Analysis for Industrial Equipment, Department of Engineering Mechanics, Faculty of Vehicle Engineering and Mechanics, Dalian University of Technology, Dalian 116024, P. R. China

zhengyg@dlut.edu.cn; fuyifei@mail.dlut.edu.cn; zhanghw@dlut.edu.cn; yehf@dlut.edu.cn

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In the past few years, nanotwinned materials have attracted much attention due to their excellent mechanical properties and great potential applications [1,2]. These materials have been found to possess high strength and considerable ductility compared to their nanocrystalline counterparts without growth twins. To understand the deformation mechanisms and underlying physics of growth twin strengthening and toughening, a lot of experimental and atomistic studies have been conducted. Now it is commonly believed that the high strength is mainly a result of the inhibition effect of the twin boundaries (besides the grain boundaries) on the motion of dislocations and the toughening may be ascribed to the enhanced capacity of twin boundaries to accommodate dislocations [3-10]. However, most studies mainly focus on the plastic behaviors of relatively perfect nanotwinned structures. Only few work on the mechanical properties of defective nanotwinned materials has been reported [8,9]. There is still a lack of a clear and thorough understanding of the effect of defects on the mechanical properties and deformation mechanisms of these materials, especially the interplay and competetion between the defects and twin boundaries.

In this paper, we present atomistic simulations to study the tensile and shear plastic deformations of nanotwinned copper with crack-like defects [11,12]. Simulation results indicate that the defects and twin boundaries play different roles in determining the plastic deformation behaviors of nanotwinned copper during the tensile and shear loading processes. The cracks usually act as the sources for dislocation nucleation due to stress concentration at the crack tips and thus mainly influence the onset of the plastic deformation. The twin boundaries display inhibition effect on the motion of dislocations and meanwhile the joint actions of twin boundaries and cracks dominate the yield stress of the nanotwinned copper. During the plastic flow stage, together with the interactions between various dislocations, the interactions between twin boundaries and dislocations accommodate the plastic deformation. At this stage, the features of the stress-strain curve are different from the tensile test to the shear test, which can be attributed to the different forms of dislocation activities and dislocations-twin boundary interactions. Due to different loading directions, the deformation patterns are different. That is, the dislocations glide in the close-packed planes that intersect with the twin boundaries in the tensile plastic deformation in which the loading direction is perpendicular to the twin boundaries, while the dislocations mainly glide in the planes that parallel to the twin boundaries in the shear deformation process.

Furthermore, the effects of the crack length, temperature and loading rate on the mechanical properties have been investigated. Simulation results show that the crack length, temperature and loading rate have little influence on the elastic modulus and shear modulus. With the increase of the crack length or temperature, the yield stress decreases, while the influence of the loading rate shows an opposite tendency. Moreover, the dependence of the yield stress on the crack length is nonlinear, which is similar to that between the yield stress and the loading rate, but is different from the influence of the temperature.

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