A molecular dynamics study on deformation mechanisms and mechanical properties of $\{\bar{1}011\}\langle 10\bar{1}2\rangle$ nanotwinned magnesium

***L. Zhou [1], †Y.F. Guo [1]**

[1]Institute of Mechanics, School of Civil Engineering, Beijing Jiaotong University, China

*Presenting author: 150179734@qq.com

†Corresponding author: yfguo@bjtu.edu.cn

Abstract:

The strength and ductility of metal can be enhanced by embedding twin boundaries (TBs). However the deformation mechanisms responsible for the mechanical properties in $\{\bar{1}011\}\langle 10\bar{1}2\rangle$ nanotwinned magnesium is still unclear. In present work molecular dynamics (MD) simulations are performed to investigate the deformation behaviors of $\{\bar{1}011\}\langle 10\bar{1}2\rangle$ nanotwinned magnesium under compressive and tensile loadings. TBs spacing variation is also concerned to reveal the spacing effect. It is found that defects can hardly generate at TBs of $\{\bar{1}011\}\langle 10\bar{1}2\rangle$ nanotwinned magnesium under compressive or tensile loadings. After we employ vacancies in the models as the defects nucleation source, basal dislocation induced stacking faults and phase transformation are found to dominate the plastic deformation under compressive loadings. Meanwhile pyramidal slips which result from the basal dislocation transmission across TBs are also observed during the simulation process. In tension models basal partial dislocations firstly nucleate from vacancies and transmit across TBs quickly which also induces pyramidal slip in the neighboring grain. With strain increasing, trailing partials are generated by the interaction between pyramidal slip and basal slip in a same grain. A series of reactions involving the formation of perfect basal dislocations in the original grain and <c+a> perfect pyramidal dislocations in the neighboring grain are realized by the trailing partials emission and transmission across TBs. Thus basal slip and pyramidal slip both dominate the plastic deformation under tensile loadings. Because of the difference in deformation mechanisms a tension to compression asymmetry is observed. Tension models show better mechanical properties in yield strength and average flow stress than compression models. Moreover TBs spacing variation exerts a few influences in tension models. With the spacing reducing, flow stress in the initial stage of plastic state can be slightly enhanced.

Keywords: $\{\bar{1}011\}\langle 10\bar{1}2\rangle$ twin boundaries, tension to compression asymmetry, vacancies, twin boundaries spacing