

PAPER • OPEN ACCESS

Temperature Effect on Dislocation Slip Mechanism of Nanotwinned Mg with Void Defect at the Twin Boundary

To cite this article: Kaixin Huang *et al* 2019 *IOP Conf. Ser.: Mater. Sci. Eng.* **484** 012018

View the [article online](#) for updates and enhancements.

Temperature Effect on Dislocation Slip Mechanism of Nanotwinned Mg with Void Defect at the Twin Boundary

Kaixin Huang, Junping Yao, Qiyao Hu, Letian Shao and Zhong Sun

School of Aeronautical Manufacture Engineering, Nanchang Hangkong University,
Nanchang 330063 China
Email: h13647096714@outlook.com

Abstract. In this paper, a molecular dynamics model is used to simulate the uniaxial tensile loading process at different temperatures of nano-twinned Mg with void defect at the twin boundaries. The dislocation slip mechanism during the stage of plastic deformation for different temperatures was studied. The results show that the initial edge dislocations formed from lattice misfit. It is found that the propagations of the slip bands emitted and the stacking faults also generated from Shockley partial dislocation.

1. Introduction

In recent years, many achievements have been made in the research on macroscopic defects of materials and breakthroughs have been made in microscopic defects. For example; Stella Brach [1] *et al.* used MD to study the effect of pore shape on the strength properties of nano-porous materials. The results show that the strength properties of nano-porous materials depend on all three Hagrid- Sigyard stress invariants. Xu[2] *et al.* studied the contraction of the spherical nano hole under the uniaxial compression load by using MD simulation, and found that the original defect of the model may shrink during the compression process. Tang [3] *et al.* used MD to simulate the expansion and fracture mechanism of single-crystal γ -Ti Alnanopores. The results show that the generation of dislocation nuclei and the propagation of shear rings expand the pores. Zhang [4] *et al.* simulated the effect of hole density of nickel single crystal on hole contraction mechanism based on molecular dynamics. The results showed that whole density could affect yield strain of nickel single crystal. However, they are mainly concentrated on the crack propagation of nano-single crystals, but there are few studies on the mechanism of the dislocation slip of twin boundaries (TB). Therefore, it is necessary to study the dislocation slip mechanism of the defect in the grain boundary of the TB. In addition, with the continuous development of classical MD and computer science and technology, we have been able to provide theoretical and technical support.

In summary, MD simulations are carried out with the Largescale Atomic Molecular Massively Parallel Simulator (LAMMPS) [5], and software OVITO [6] was used for visual processing to study the dislocation slip mechanism of the TB hole defects, to view the evolution of partial dislocations and slip bands during the tensile deformation, the Dislocation analysis (DXA) is adopted.

2. Model and Theoretical Method

In order to better observe the change process of dislocation slip mechanism, the model established should be of appropriate size. The size of the model is $320 \times 240 \times 12.8 \text{ nm}$, and it is divided into the upper part and the lower part, which are respectively $320 \times 240 \times 12.8 \text{ nm}$. The diameter of hole defect at the TB is $R=16 \text{ nm}$, and the total number of atoms is 84360. Periodic boundary conditions were applied in all three directions, and the EAM potential function developed by Sun [7] *et al.* was used to



describe the atomic potential of magnesium. The energy is minimized and 10,000 time step relaxation is performed before the uniaxial tensile load is applied, so that the total energy of the system reaches the equilibrium state. The uniaxial tensile load was then applied along the Y direction; the uniaxial tensile loading is applied with a constant strain rate of $2 \times 10^9 s^{-1}$, with a MD time step of 0.001 ps, the simulations are performed with NPT ensemble to erase the stresses of other two directions that are perpendicular to the loading direction at different temperature.

3. Results and Discussion

In order to explore the effect of temperature on the dislocation slip mechanism of void defects at the TB, three different temperatures 200 K, 300 K and 500 K, were set up respectively. As can be seen from Fig. 1(a), stacking faults (dark red cylinders in the Fig. 1(a)) and Shockley partial dislocations (yellow brown cylinders in the Fig. 1(a)) occur at the TB and the upper and lower boundaries of the model around the void defect. The reason for this is the Shockley partial dislocation caused by lattice misfit, and the partial dislocation will inevitably lead to stacking fault, that is, the partial dislocation line is the boundary line of stacking fault. In Fig. 1(b), due to the occurrence of plastic deformation, a large number of slip bands appear in the whole model. At the same time, the number of partial dislocation and stacking fault also increased. Fig. 1(c) as the plastic deformation increases, the TB of the upper and lower parts fuse with each other, resulting in small void defects at the left and right boundaries of the model. Fig. 1(d) it can be seen that the slip bands become denser and longer, and there is a slip network characterized by multiple slips. The number of partial dislocations and stacking faults increases continuously, indicating that the plastic deformation is very serious at this time.

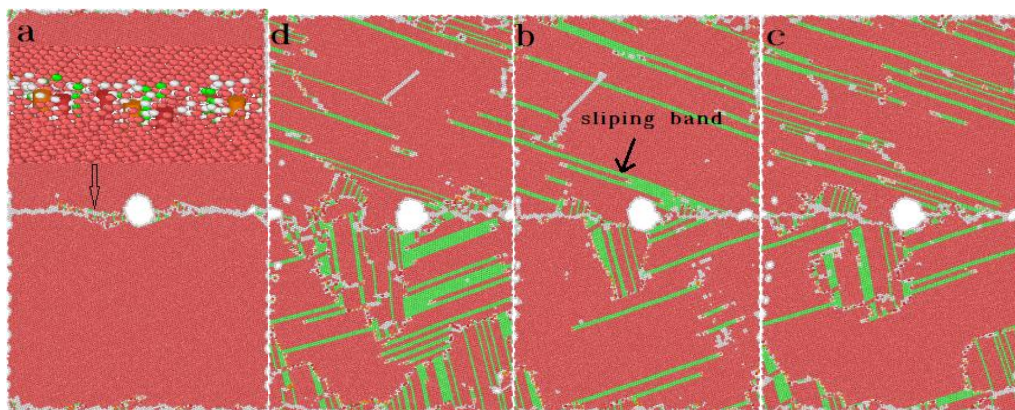


Figure 1. Dislocation analysis of the deformed atomic configurations at 200 K
(a) $\varepsilon=0.02$ (b) $\varepsilon=0.05$ (c) $\varepsilon=0.08$ (d) $\varepsilon=0.12$

As can be seen from Fig. 2(a), the distribution of partial dislocations and stacking faults in Shockley is similar to that in Fig. 1(a), which can be proved that temperature has no effect on partial dislocations and stacking faults. Fig. 2(b) compared with Fig. 1(b), the number of slip bands decreases but the number of twins increases. Fig. 2(c) shows that the grain boundary around the defect begins to break, indicating that the yield strength decreases with increasing temperature. Fig. 2(d) partial dislocations and stacking faults accumulate with the increase of deformation and form twin nucleation on the left side of the void defect, which hinder the fracture of the material.

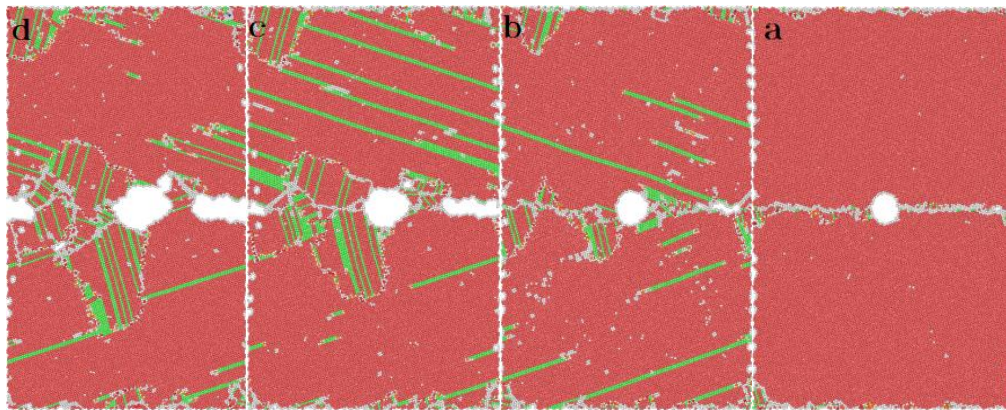


Figure 2. Dislocation analysis of the deformed atomic configurations at 300 K
(a) $\varepsilon=0.02$ (b) $\varepsilon=0.05$ (c) $\varepsilon=0.08$ (d) $\varepsilon=0.12$

When the temperature is 500 K, the same distribution as that of Fig. 1 (a) and Fig. 2 (a) is observed in Fig. 3(a), which proves that the temperature has no obvious effect on the mechanical properties of the material during the elastic stage. It is shown from Fig. 3(b), 3(c) and 3(d) that the critical shear stress of slip decreases sharply with the increase of temperature, and the probability of slip initiation increases greatly, resulting in the increase of slip band and the decrease of twins. At the same time, the increase of temperature makes the thermal motion of atoms and the energy of atoms intensify, which leads to the increase of plasticity of materials and is not easy to fracture.

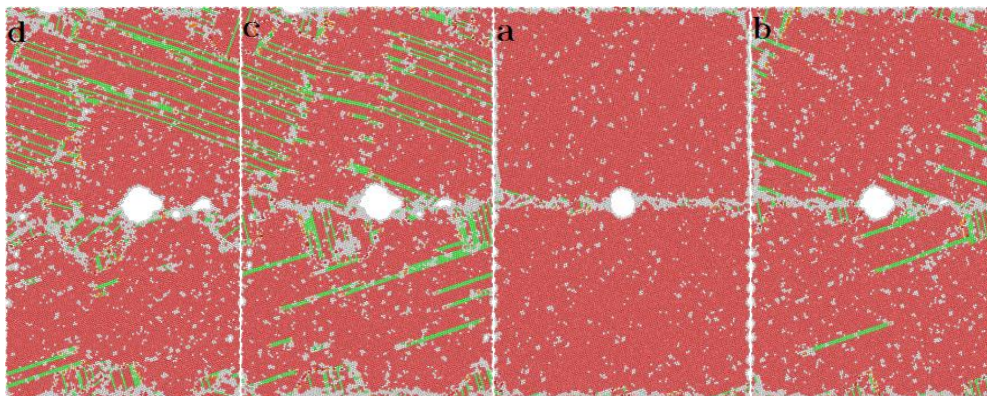


Figure 3. Dislocation analysis of the deformed atomic configurations at 500 K
(a) $\varepsilon=0.02$ (b) $\varepsilon=0.05$ (c) $\varepsilon=0.08$ (d) $\varepsilon=0.12$

4. Conclusions

In this paper, a molecular dynamics model is used to simulate the uniaxial tensile loading process at different temperatures of nano-twinned Mg with void defect at the TB. The following conclusions are drawn:

- (1) Temperature does not have a significant effect on the mechanical properties of the elastic deformation stage of the material, but it has a significant effect on the dislocation slip mechanism in the plastic deformation stage;
- (2) The number of partial dislocations and stacking faults is proportional to the material deformation, and then they accumulate to form twin nucleation, hindering the fracture of the material.

5. Acknowledgements

This work was financially supported by the National Natural Science Foundation of China (51164027, 51661024) and Key Science and Technology Project of Jiangxi Provincial Department of Education

(GJJ14502).

6. References

- [1] StellaB StefanoCDjmedoK2017J. Void-shape effects on strength properties of nanoporous materials *Mech .Res. Commu*86:11-17
- [2] XuX TTangF LXueH T2015JMolecular dynamics simulations of void shrinkage in γ -TiAl single crystal *Comput.Mater.Sci*107: 58-65
- [3] Tang F LCaiH MH WBao2014JMolecular dynamics simulations of void growth in γ -TiAl single crystal *ComputMater.Sci.*84:232-237
- [4] Zhang Y QJiangS YZhu X M2017JInfluence of void density on dislocation mechanisms of void shrinkage in nickel single crystal based on molecular dynamics simulation *Phy.E*90:90-97
- [5] Plimpton S J1995JFast parallel algorithms for short-range molecular dynamics *JCompuPhys* 117(1):1-19
- [6] Stukowsk A2010 JVisualization and analysis of atomistic simulation data with OVITO-the open Visualization Tool *Modell. Simul .Mater .Sci. Eng*18 (6):2154-2162