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Nucleation Mechanism for Shuffling Dominated Twinning in Magnesium

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Abstract

We observed nucleation of {10-12} twinning under tensile loading in magnesium rectangular rod system using atomistic molecular dynamic simulation. The rod axis is normal to basal plane of Mg crystal. The tensile deformation in c-axis nucleates {10-12} twinning starting at the corner of square of cross section of the rod. The twin boundary is spherical at the beginning and become a linear boundary in {10-12} planes as time goes by. The twinning and shuffling processes are described. The nucleation mechanism of the shuffling dominated twinning is explained.

Introduction

Twinning together with dislocation slip is a fundamental plastic deformation method. Many twinning nucleation mechanisms are proposed. Homogeneous twinning nucleation model in highly perfect crystals was first introduced by Orowan[5]. If the applied shear stress on twinning plane resolved along twinning direction reach theoretical strength of the material, homogeneous twinning occurs. Paxton et al.[4] considered the homogeneous twinning nucleation in this way against twinning- and anti-twinning shear stresses for five b.c.c. transition metals and for f.c.c. using density functional theory calculations. Thermal fluctuations are supposed to overcome the free energy barrier to the formation of a small twinned region.

The model of a lenticular twin consists of a series of loops of twinning dislocation. Each loop is in a lattice plane parallel to twinning plane. Loop diameter increases as the central plane of the lens is approached. The twinning dislocations in the loops are glissile and the embryonic twin could extend very rapidly in all directions contained within twinning planes. A possible mechanism for the thickening of a twin in the direction normal to twinning plane is the thermally-activated formation of a closed loop of twinning dislocation. The rate at which new loops form is big if the burger vector of twinning dislocation is small.

Defect-assisted twinning nucleation mechanisms are based on the dissociation of some dislocation which produce stacking fault for twin nucleus. The pole mechanism is one of defect-assisted twinning nucleation mechanisms.

Even though many theories of twin nucleation and dislocation loop in {10-12} twin planes are reported, none have reported a naturally occuring {10-12} tensile twin nucleation without artificial creation of twin structure in molecular dynamic simulations. The purpose of this article is to report the {10-12} twin nucleation, the nucleation mechanism, and structural analysis of twin in Mg crystal simulation.

Simulation setup

Figure 1 show the system configuration in the simulation. The system size is 9.33 nm by 5.51 nm by 5.09 nm. Total number of atom is 11520. The embed atom method magnesium potential of Sun et. al.[2] is used. No periodic boundary conditions are used in x, y, and z directions. The atoms in 1 nm of left and right ends of crystal are fixed after incremental strains are applied. The rest of atoms are free to move after strain applications. The constant NVE thermodynamics are applied where N represents the total number of atoms in system, V represents the volume of the system, and E represents the energy of system. Initial temperature are set to 100 K by assigning Gaussian random velocity on atoms. For 5 pico seconds equilibrium condition of system arrives. The ramping velocities are applied to all atoms correstponding to the strain rate of 1G/s.

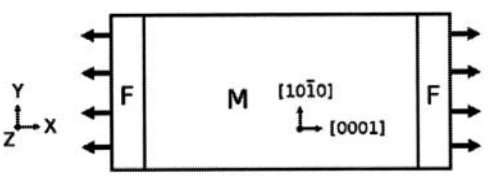

Figure 1. The schematic of the simulation configuration. Tensile strains are applied on Mg crystal in [0001] direction. No periodic boundary conditions are applied in all x, y, and z directions. The letter F indicates that atoms in the region are fixed and M indicates that atoms are mobile in the region in molecular dynamic steps after strains are applied.

Simulation results

The defect surface of quad sphere shape nucleates from the middle edge and propagates away from nucleation point. The defect surface leaves behind a HCP crystal structure which has different crystal orientation from parents. Figure 2 (a) shows three dimensional nucleation of twin. The colors represent the different structures classified by Ackland method[2]. Yellow represent h.c.p. structure and green f.c.c. The twin structure has the same h.c.p. as the parent and has different crystal orentation. The twin boundary is distinguished by different colors. The nucleated twin h.c.p. structure grows spherically from the nucleation point of a edge in the middle of simulation box.

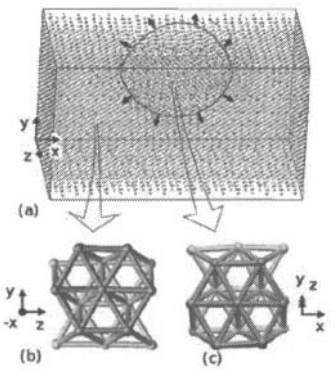

Figure 2. (Color online) (a) Twin nucleation and spherical growth of twin region from the middle edge. The colors of atoms are assigned by Ackland method[3]. The parent and twin structures are h.c.p. structures which represented yellow colors. (b) The structures of parent is magnified and viewed from x direction. The basal planes of parent is normal to x axis. (c) Twin region is magnified at specific view points to show the basal planes of twin. The colors in (b) and (c) represent depth.

Figure 3 (a) shows two layers of parent basal planes including twin nucleation point colored by Ackland method. The twin nucleates from top right conner and propergates spherically toward bottom left conner. As the twin region grows, two prismatic planes in parent region are aligned and form one basal plane in twin region. The angle between parent basal plane and twin basal plane look like right angle. The angle between parent and twin basal planes in {10-12} twin are 87 degrees according to theory. The twin boundary in –z direction is faster in speed and wider in width than –y direction.

Figure 3 (b) one layer colored by x positions of atoms. The red color and + sign mean the atoms are close, and the blue color and – sign mean the atoms are far. The basal plane of parent become the corrogated prismatic plane of twin.

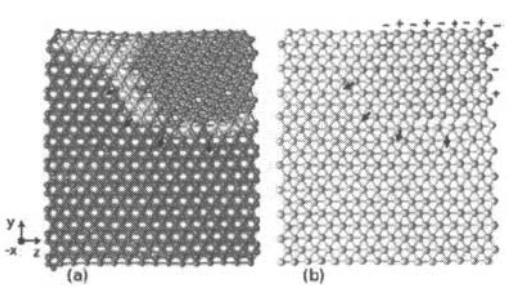

Figure 3. (Color online) (a) Two layers of parent basal planes including twin nucleation point colored by Ackland method[3]. (b) One layers of the same view point colored by coordinate x positions of atoms.

Figure 4 (a) shows a few layers of (1-210) planes slicing the forefront of simulation box. The twinning boundary toward –z direction is quite thicker than others. Figure 4 (b) shows a few layers of (10-10) planes slicing the upper part of simulation box. The three dimensional shape of twin boundary is a ellipsoid and the growing speed and thickness of twin boundary are different.

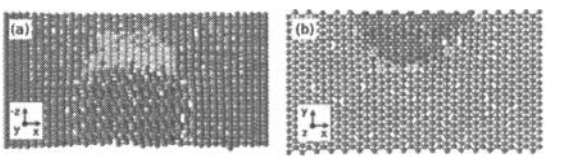

Figure 4. A few layers of top planes (a) and front planes (b) colored by Ackland method.

Figure 5 shows a few layers of (11-20) planes sliced to show the plane of shear for {10-12} twinning colored by Ackland method. In order to get rid of the interaction between surface and twin boundary more biger system is used for Figure 5. The twinning boundary shape in the plane of shear forms a retangle starting from a circle. The retangle consists of four twinning planes. The black solid line indicates the basal planes of parent and twin. The angle between parent and twin basal planes is consistant with the theoretic expectation.

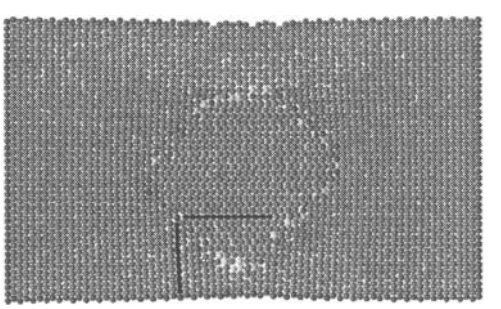

Figure 5. A few layers of (11-20) planes slicing the twinning structure are colored by Ackland method[3].

Discussion

Our early twin structure just after nucleation is very different from common expectation that a certain number of atomic layers of twin structure nucleate at a time by twinning dislocations[6]. The twin boundary shape is spherical. The twin nucleation point is always at the edge of retangular rod. The thermal Brownian motion of atoms at edge creates twin nucleation point because the atoms at edge have more freedom to move away from the crystal lattice position and form nucleation points. The spherical shape of the twin boundary surface doesn't continue because the growing speeds of the twin boundaries are not same. Each part of the twin boundary grows with different velocity which depends on boundary structures and growing directions. As the twin region grows it might form the experimentally observed lenticular shape of twin.

Our overall simulation results suggest a surprising idea that the driving force to {10-12} twinning is tensile stress rather than shear stress. The {10-12} twinning forms by shearing and shuffling. The burger vector of twinning dislocation is extremely small and the shuffling is dominent. The shuffling lower the energy of system which is increased by applied tensile load. When the shear stress is applied to a crystal, dislocations are nucleated to accomadate loading stress instead of whole crystal shear deformation. In h.c.p {10-12} twinning, the shearing load is not the main contribution to twinning nucleation but the tensile load is. The shear-dominent twinning nucleates and grows by resolved shearing load. The shuffling-dominent twinning nucleates and grows by the resolved loading stress which induce shuffling to lower the system energy, for example, tensile loading stress in the current system. More evidences will be investigated in future.

Conclusion

We found a {10-12} twinning nucleation in rectangular rod system of Mg crystal under tensile stress in molecular dynamic simulation. The twinning nucleates from the edge which have more freedom of atom motion by thermal activation. The nucleated twinning grows spherically at early stage. The growing speeds of each part of spherical twin boundary are different and depend on boundary structures and growing directions.

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