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AN ATOMISTIC STUDY OF TWIN BOUNDARY MIGRATION BY THE MOTION OF DISCONNECTION

Abstract:
The deformation twinning in hcp crystals have been extensively researched nowadays due to the dominant role it plays in the plastic deformation and strengthening mechanisms of materials. The twin boundary migration plays a significant role in the microstructure evolution of metallic materials. The knowledge of migration mechanisms under applied stress can be considered as a basis for the development of nanostructured materials with improved mechanical properties. The deformation twinning in magnesium is a complex phenomenon and is still under intensive study. The most common twinning mode in hcp metals is takes place in {10-12} planes [1] and this mode accommodates tensile deformation along with [0001] direction. Some less common twinning modes such as {11-26} and {11-22} are also observed in Mg [2].
In the present work, we highlight the atomic-level study of the migration of {11-26} twin boundaries by conducting molecular dynamic simulation using of LAMMPS [3] using the embedded atom methods (EAM) potential developed by Sun et. al. [4]. The visualization software OVITO [5] is used to realize the dynamic display in our study [5]. Simulation shows the formation of twinning disconnection in {11$\bar{2}$6} twin boundary with subsequent gliding along this plane. Twinning disconnections are accumulated in simulation block with formation of basel pyramidal interfaces. Electron backscatter diffraction analysis and TEM analysis were performed to verify the simulated results.

References

1. Ostapovets A., Gröger R., Modell. Simul. Mater. Sci. Eng. 22 (2014) 025015.
2. Ostapovets A.; Bursik J., Gröger R, Phil. Mag. 95 (2015) 4106. 3.
3. Plimpton S. J., Comp Phys 117 (1995) 1.
4. Sun D.Y., Mendelev M. I., Becker C. A., Kudin K. , Haxhimali T., Asta M., Hoyt J. J., Karma A., and Srolovitz D. J., Phys. Rev. B 73(2006) 024116.
5. A. Stukowski, Modell. Simul. Mater. Sci. Eng. 18 (2010) 015012.

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