ON UNUSUAL TWIN MODES IN MAGNESIUM

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Abstract

The nucleation, propagation and growth mechanisms of twinning are extensively studied nowadays [1-3]. The deformation twinning in metals with hcp structure still not clearly understood [3]. Faceting of twin boundaries, non-schmid behavior, importance of disconnections are widely discussed in recent publications. The most frequent twin modes in magnesium is $\{10\bar{1}2\}$ twin. It was demonstrated that this twin can be bounded by basal-prismatic facets. Migration of such facets can lead to deformation, which is different from simple shear on $\{10\bar{1}2\}$ plane. The difference can be accommodated by declination settled in facet junctions.

In the current study, we analyze mechanisms of twin boundary migration by using of computer simulation and electron backscatter analysis, which was performed to verify the simulated results. We study unusual $\{11\bar{2}6\}$ twin modes, Such twins were observed in magnesium rolled at room temperature. The simulations were performed using LAMMPS with using of embedded atom method potential.

Motivation

- To study the migration mechanisms of rolled Mg under applied stresses for the development of light weight materials.
- To provide the evidence of asymmetrical $(0001)/(1\bar{2}12)$ interface associated with $(11\bar{2}6)$ boundary.

AIM

To investigate the twinning mechanism by twin boundary migration of unusual twin interfaces and to understand nucleation of such interface and their role in plasticity deformation.

Simulation Method

- The calculation were performed by LAMMPS software [4] using the embedded atom method (EAM) potential developed by Liu et. al. [5].
- The visualization software OVITO is used to realize the dynamic display in our study [6].
- Orientation of simulation block: *x* axis is oriented with $[11\bar{2}\bar{1}]$ direction, z axis is along normal to the $(11\bar{2}6)$ plane whereas, *y* axis is aligned with $[1\bar{1}00]$ direction.
- Periodic boundary conditions were applied in the x direction and y direction respectively and atomic position near z surface kept fixed.
- In order to study the twinning mechanism, stress should be applied in x-z plane.

Conclusion

- EBSD and HRTEM confirms the existence of $(11\bar{2}6)$ twins in magnesium rolled at room temperature.
- Misorientation between matrix and twin is approximately 55°.
- EBSD and HRTEM show presence of $(0001)/(1\bar{2}12)$ and $(1\bar{1}04)/(1\bar{2}1\bar{1})$ asymmetrical interfaces.
- MD simulation of $\{1\ 1\bar{2}6\}$ twin demonstrated that $(0001)_M/(1\bar{2}12)_T$ boundary and $(1\bar{1}04)_M/(1\bar{2}1\bar{1})_T$ twin can nucleated under applied stress by accumulation of defects gliding along $(11\bar{2}6)$ boundary.

Results

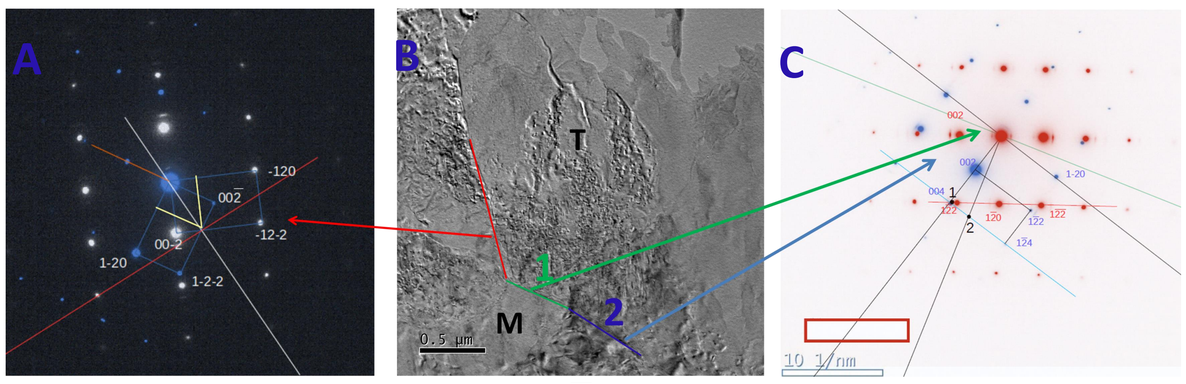

Figure 1: HRTEM Images of $(11\bar{2}6)$ feceted twin boundary.
Red line marks $(11\bar{2}6)$ symmetrical boundary, green line marks $(0001)/(1\bar{2}12)$ and blue line marks (1-104) $/(1\bar{2}1\bar{1})$

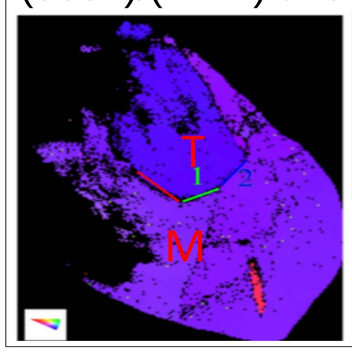

Figure 2: EBSD map shows twin embryo with misorientation angle approximately 55°.

Red line marks $(1\ 1\bar{2}6)$ symmetrical boundary, green line marks $(0001)/(1\bar{2}12)$ and blue line marks $(1\bar{1}04)$ $/(1\bar{2}1\bar{1})$

Observation of different stages of twins (LAMMPS)

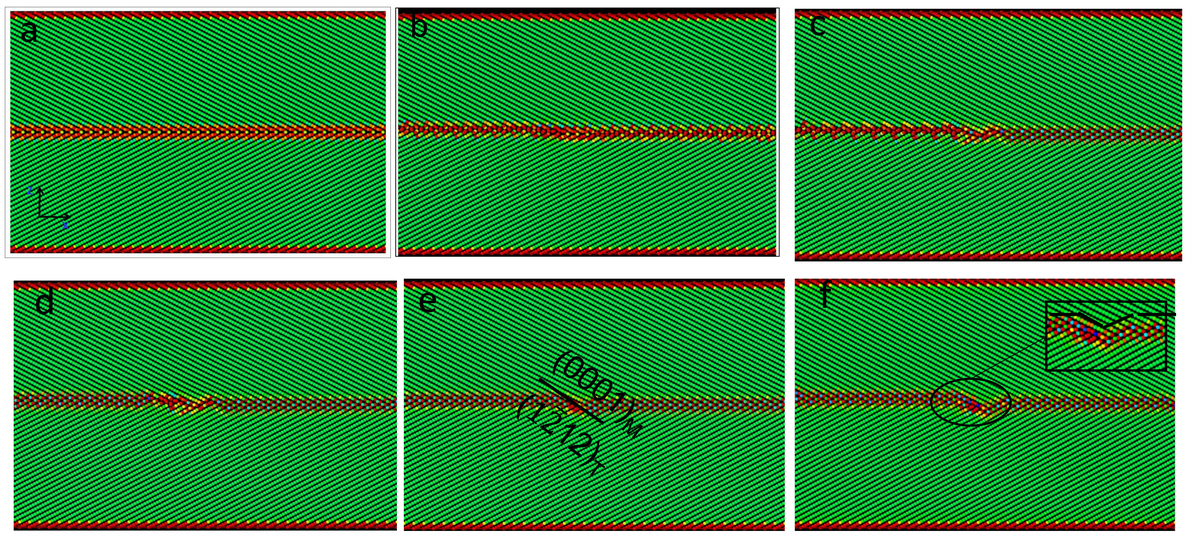

Figure 3 (a-f): Different stages of twinning performed by molecular dynamic simulation , represents nucleation of twin embryo

$(11\bar{2}6)$ (a) $\longrightarrow$ $(0001)/(1\ \bar{2}\ 12)$

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