Lab for Multiscale INterfaces Design in Solids (MINDS)

NEBRASKA CENTER FOR ENERGY SCIENCES RESEARCH

Interface Facilitated Crystal Reorientation of Mg Nanolayers in Mg-Nb Multilayers

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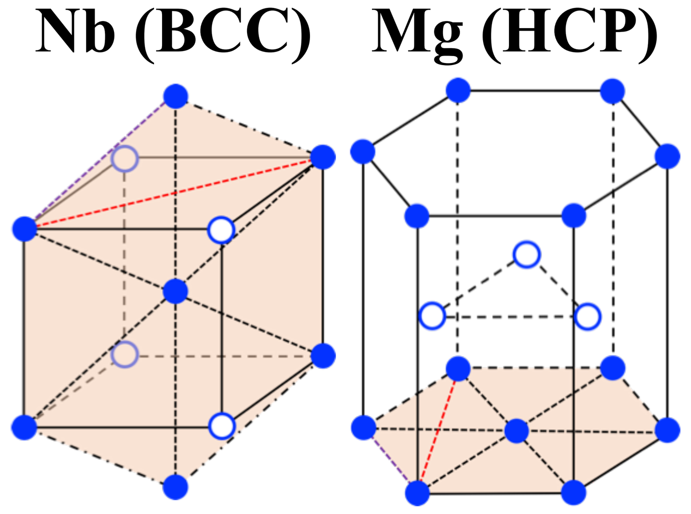
Magnesium (Mg) and its alloys, the lightest structure materials, have a huge potential in weight sensitive applications. However, with hexagonal close packed structure, Mg lacks the ductility and formability. One strategy to improve mechanical properties of Mg is to form heterogeneous interfaces within the system. In this work, with Molecular Statics (MS) and Molecular Dynamics (MD), we systematically characterize interface dislocations on Mg/Nb interfaces with Nishiyama-Wassermann (NW) orientation, which facilitates $\{\bar{1}012\}$ twinning involving three processes: nucleation, propagation and growth. Twin nucleation occurs with a critical volume and is accomplished by pure-shuffle mechanisms. Twin propagation and growth is accomplished by the migration of BP interfaces, which requires higher stress and will induce higher strain hardening rate.

Background

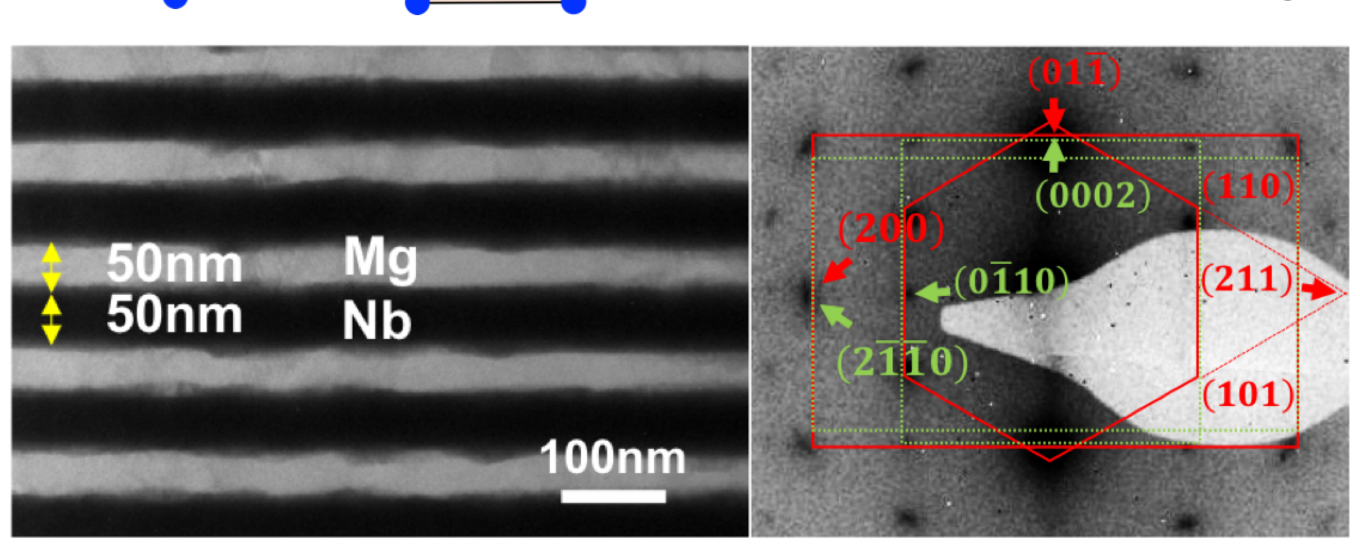
Mechanical properties of Mg and its alloys have been extensively studied because of the important applications for automobile and aerospace industries. However, one major problem for Mg is the **low inherent strength**. For instance, the yield strength of bulk Mg is ~65 MPa. **Forming heterogeneous interfaces** within the Mg based system is one effective way to improve the mechanical properties. Ham and Zhang [1] found the mechanical strength of the Mg/Nb multilayers could achieve a high value of ~1.0 GPa when the layers are a few nanometers thickness.

Orientation

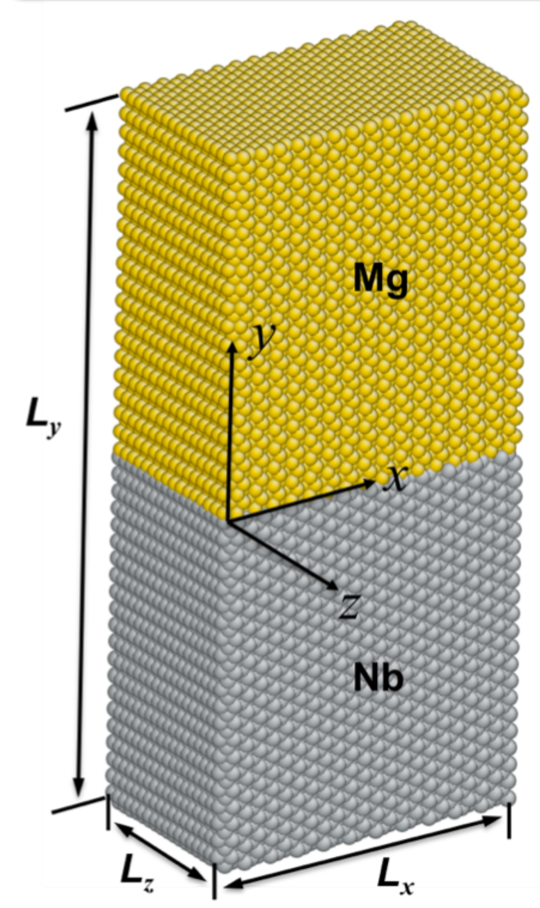


❖ **NW Orientation:**
- $(110)_{Nb}||(0002)_{Mg}$
- $[\bar{1}10]_{Nb}||[1\bar{1}00]_{Mg}$

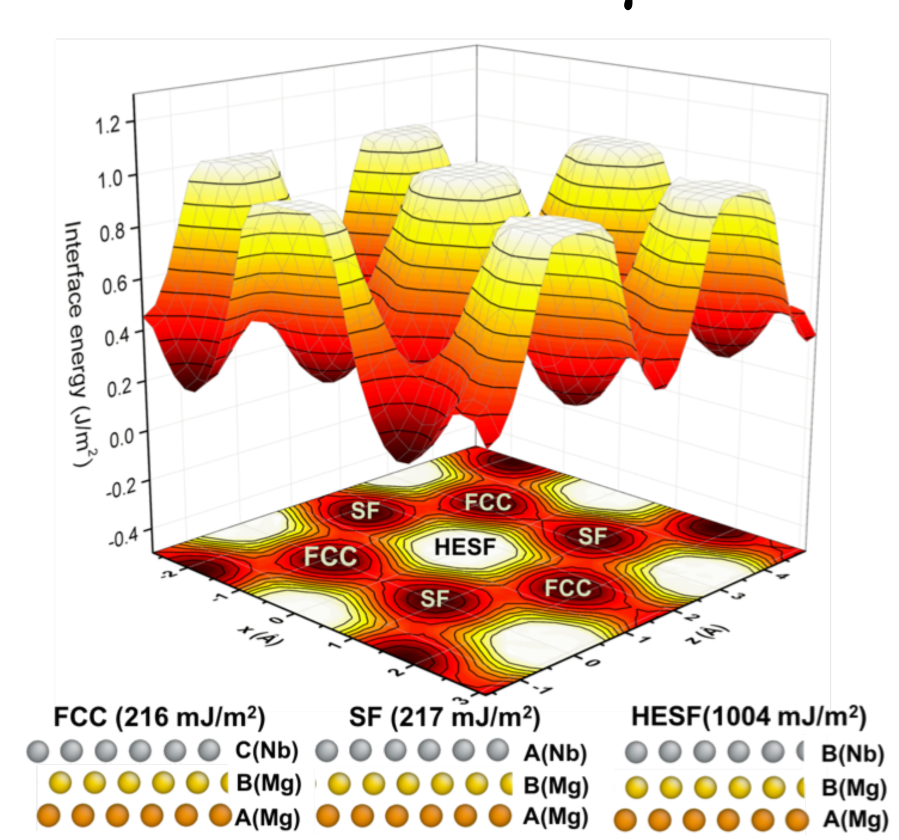
❖ **KS Orientation:**
- $(110)_{Nb}||(0002)_{Mg}$
- $[111]_{Nb}||[2\bar{1}\bar{1}0]_{Mg}$



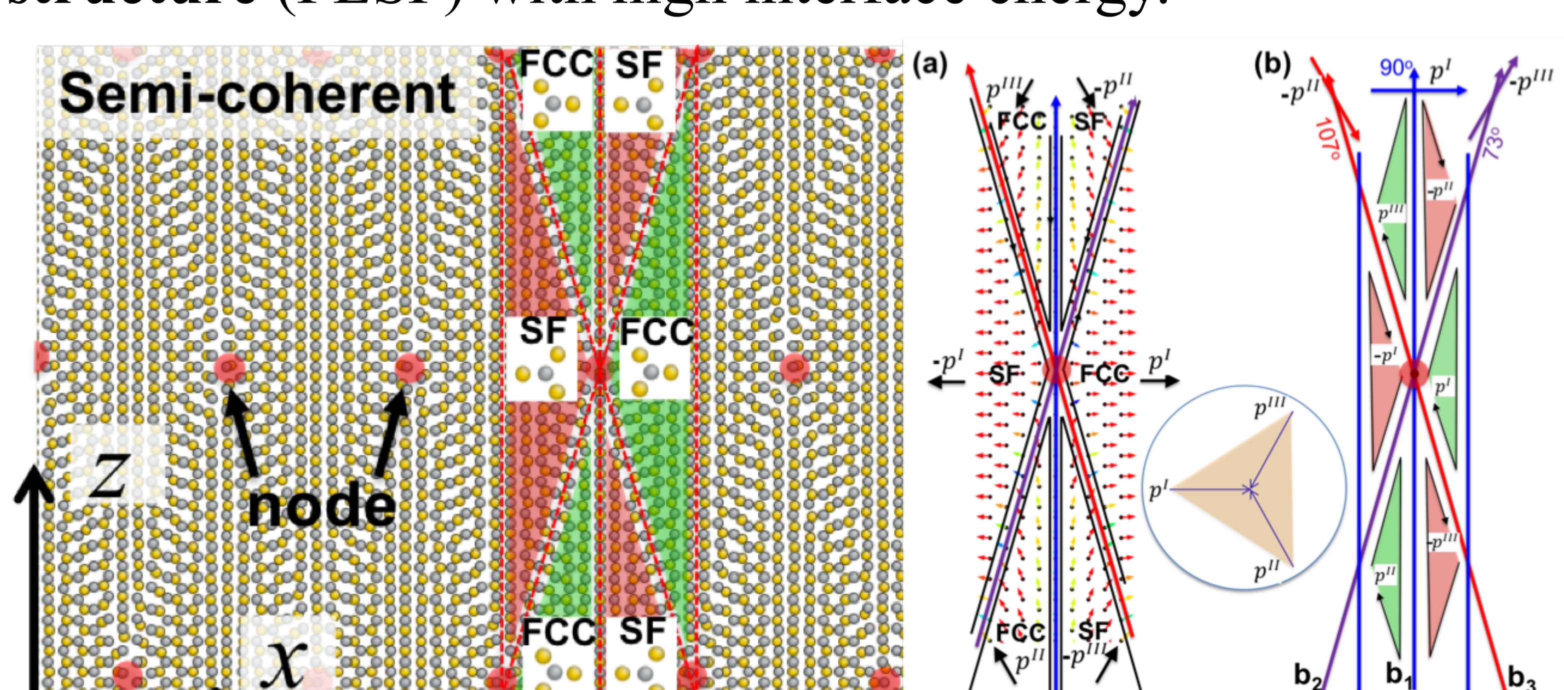
Interface Structures



Coherent interface: γ-surface

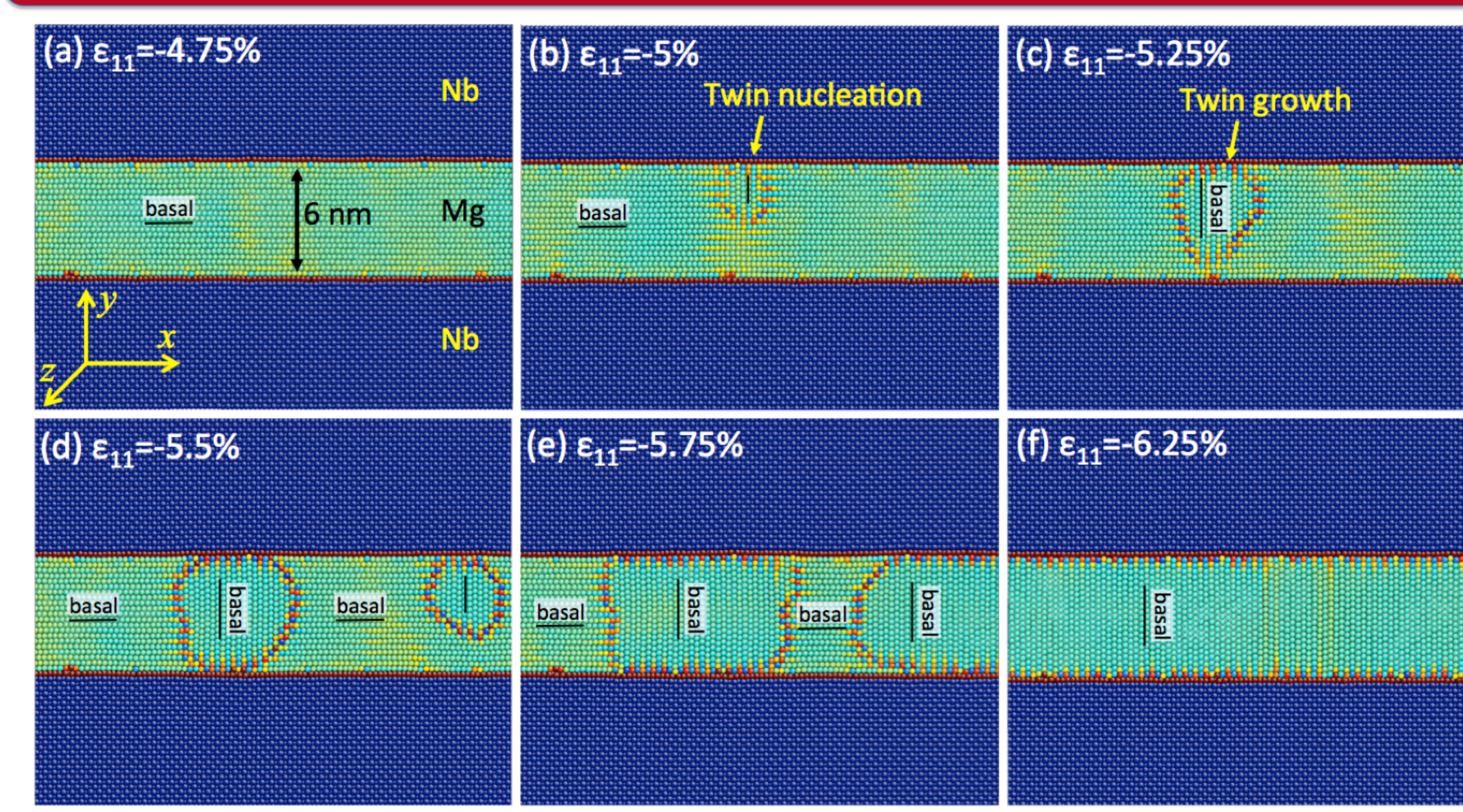


γ-surface shows two **stable coherent structures** (FCC and SF) with low interface energy and a **metastable coherent structure** (FESF) with high interface energy.



With atomically informed Frank-Bilby (AIFB) theory, misfit dislocations on Mg-Nb interfaces with NW orientation are characterized as three sets of **partial dislocations**, resulting six coherent regions around the node.

Deformation: twinning



Twinning of Mg involves three process: **nucleation**, **propagation** and **growth**. Twin nucleation via pure-shuffle takes place near interface dislocations at interface, where sources for a large number of partials exist. Twin propagation and growth is mainly accomplished by BP interface migration, producing tetragonal deformation instead of simple shear. The **critical stress** and **strain hardening rate** associated with the migration of BP interfaces are significantly higher than those associated with twinning shear mechanism.

Conclusion:
- Interface structure of Mg-Nb interface with NW orientation is characterized. It is composed of six coherent regions separated by **three sets of partial dislocations**.
- Interface dislocations facilitating **BP transformation** dominates the **twinning process**, which has higher **critical stress** and induces higher **strain hardening rate**. This partly explains how forming Mg-Nb multilayers improves the mechanical properties.

[1] Ham, B.,&Zhang, X., High strength Mg/Nb nanolayer composites. *Mater. Sci. Eng. A*, *528*(4-5), 2028-2033 (2011)