Atomistic study on the generation and gliding properties of pyramidal dislocations in magnesium

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Atomistic study on the generation and gliding properties of pyramidal dislocations in magnesium

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Background and Objectives

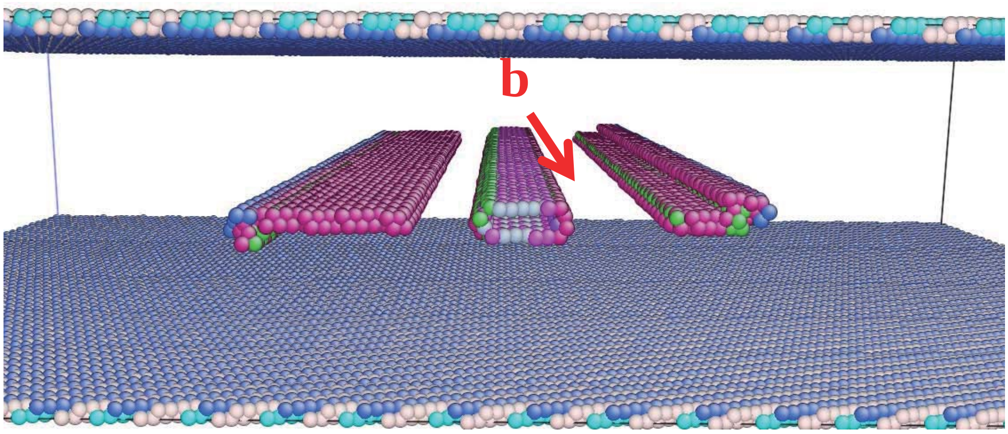
-molecular dynamics method
mechanisms of plasticity
in highly anisotropic hcp Mg
→ enhancement of ductility
for developing Mg alloys
-activation of non-basal dislocations
to accommodate strains
along the c-axis direction

-the understanding of the core structure and
and gliding properties of non-basal pyramidal
dislocations by generating them from the crack
in the basic configurations (mode III)

Emission of dislocations from the crack tip

Generation of pyramidal screw dislocations is observed from the crack tip oriented along the Burgers vector on the pyramidal type I (1st order) and type II (2nd order) plane

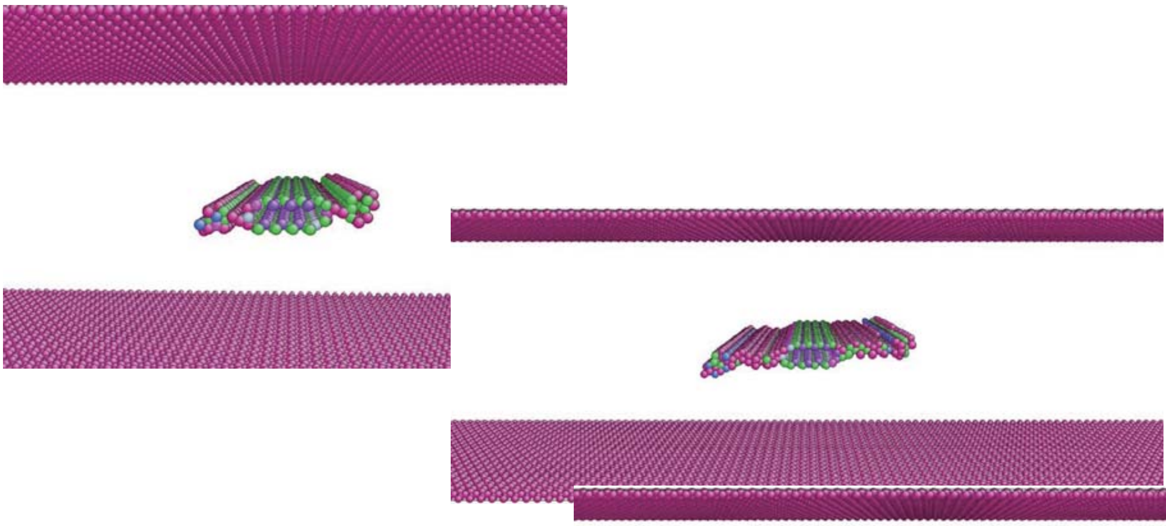
Mode III fracture

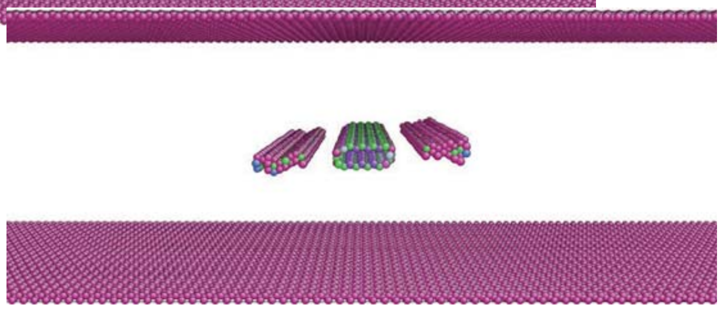


Pyramidal type I (1st order)

Two opposite type screw dislocations are created on both sides of the crack by displacing the upper and lower walls.

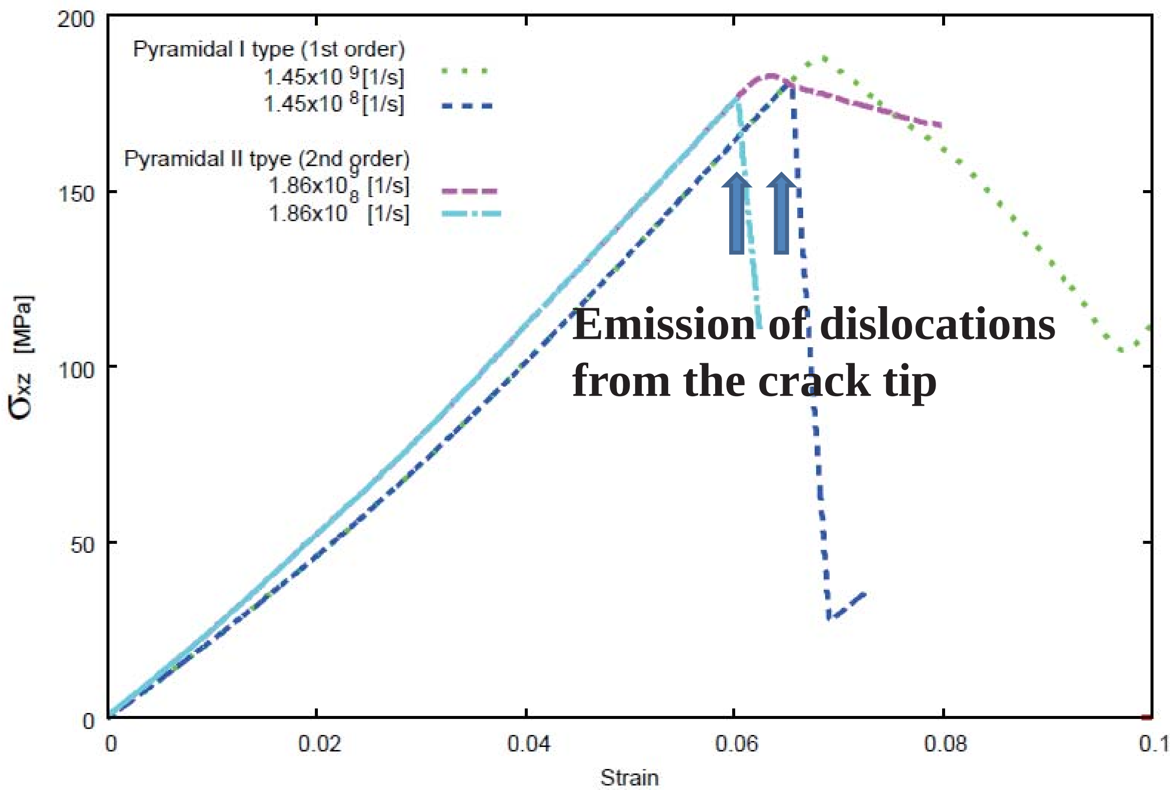
Pyramidal type II (2nd order)





The stacking faults of the emitted screw dislocations on the pyramidal II plane have a corrugated structure.

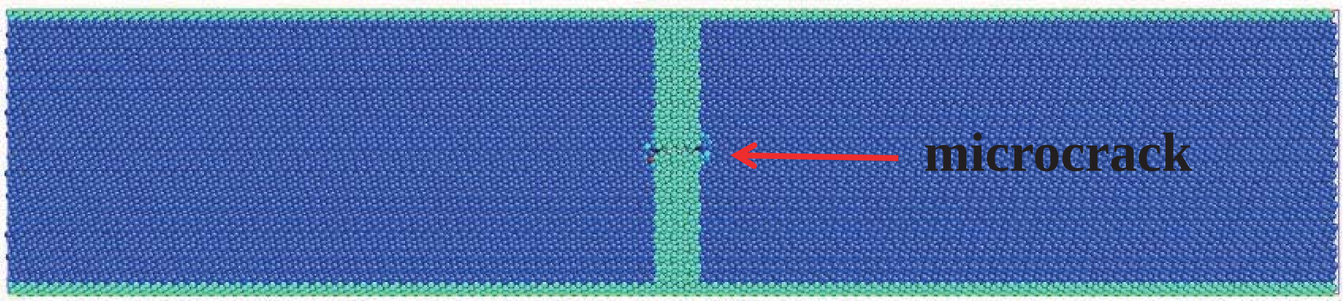
Stress-strain relation for the emission of pyramidal dislocations from the crack tip



Generation and gliding of pyramidal II screw dislocations from the microcrack under the multiaxial loading boundary condition

The microcrack is created on the pyramidal II plane.

upper boundary ◎ (displacing to the front)

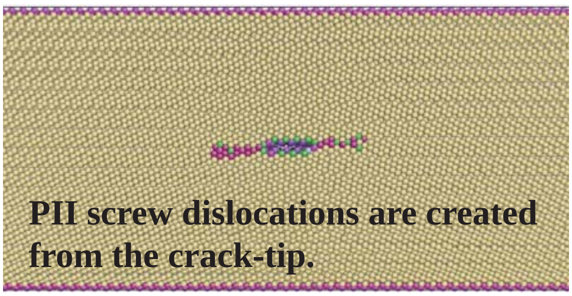


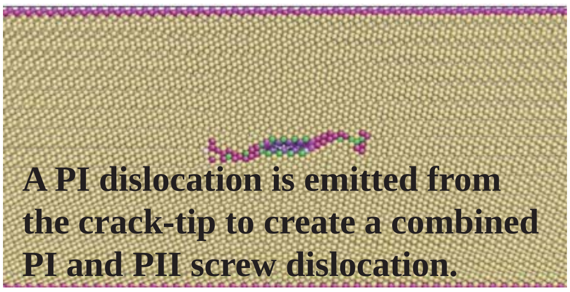
lower boundary ⊗ (displacing inward)

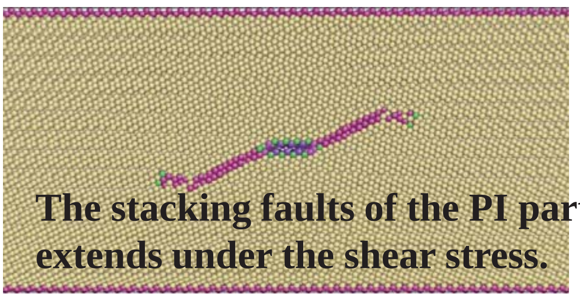
The upper and lower boundaries are displaced
in the opposite directions along the Burgers vector
Mode III fracture mode

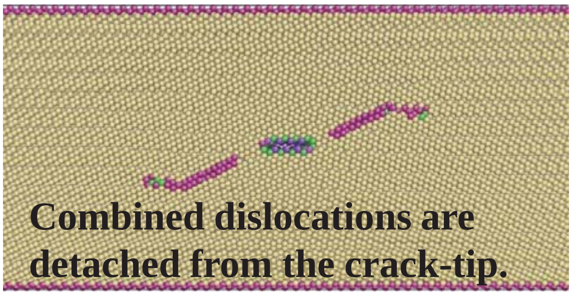
Pyramidal type II screw dislocation

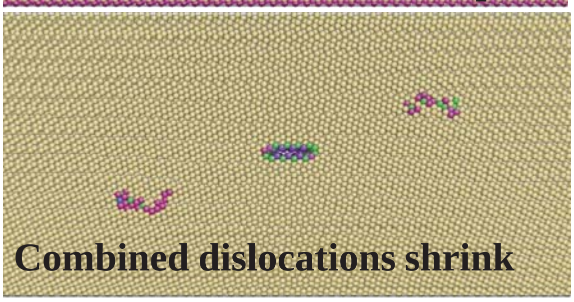
Shear displacement
20 m/sec

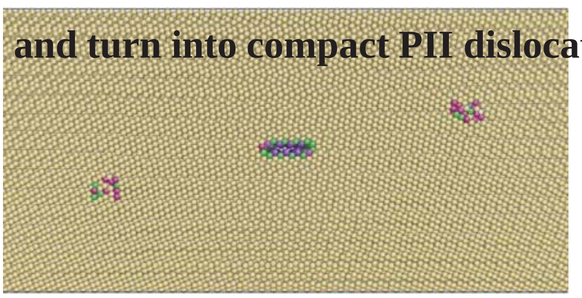

PII screw dislocations are created from the crack-tip.


A PI dislocation is emitted from the crack-tip to create a combined PI and PII screw dislocation.


The stacking faults of the PI part extends under the shear stress.


Combined dislocations are detached from the crack-tip.

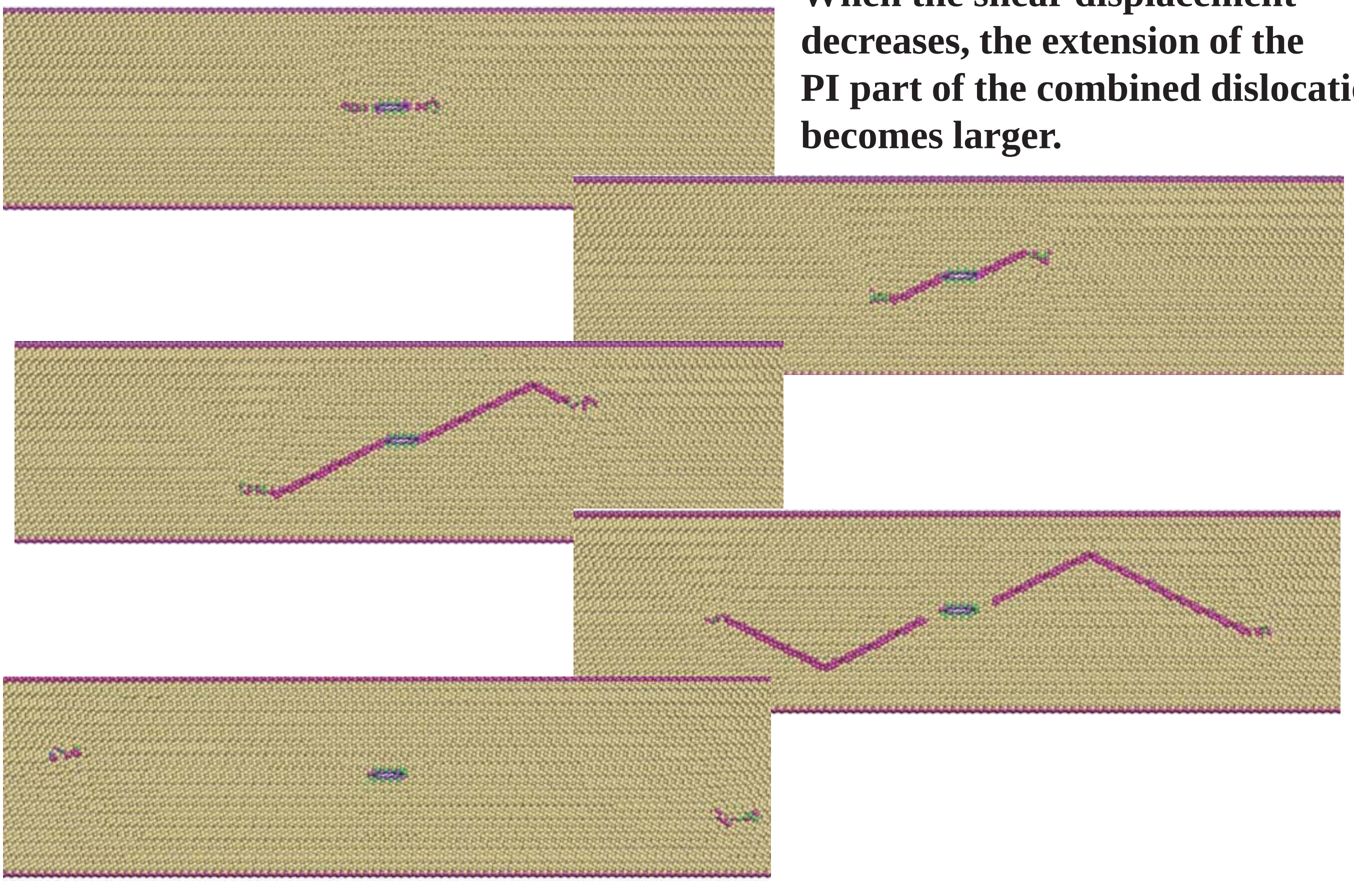

Combined dislocations shrink


and turn into compact PII dislocations.

Pyramidal type II screw dislocation

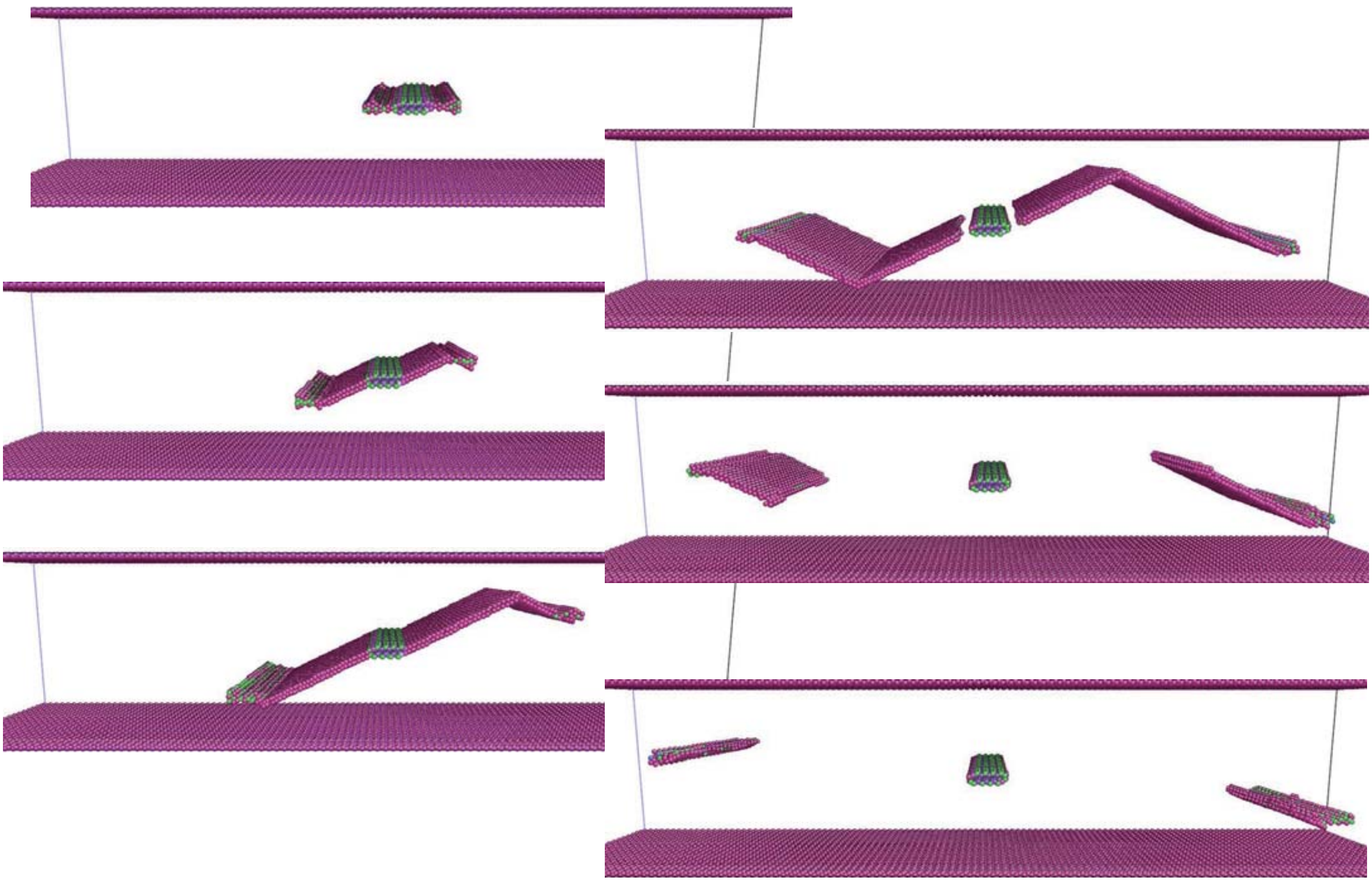
Shear displacement
2 m/sec

When the shear displacement decreases, the extension of the PI part of the combined dislocation becomes larger.



Pyramidal type II screw dislocation

Shear displacement
2 m/sec



Conclusions

- Non-basal pyramidal screw dislocations have been created from the crack tip under the external shear stress.

- Core structures of both pyramidal type I and type II screw dislocations are elucidated by the visualization of the molecular dynamics simulation.
  The core of the pyramidal type II screw dislocation is found to have a corrugated structure, while that of pyramidal type I screw dislocation has a smooth stacking fault. Both dislocations are able to cross-slip to other pyramidal planes.

- It is observed that a combined screw dislocation, consisting of PI and PII dislocation cores, is created under the multiaxial loading boundary condition. It is found that PI and PII screw dislocations can easily cross-slip to each other's slip plane to form a combined screw dislocation.