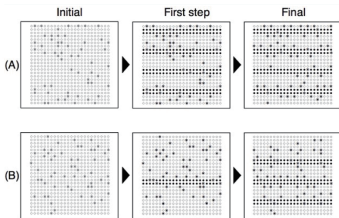# First principles calculations for LPSO formation scenarios

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Illustrations of LPSO formation scenarios

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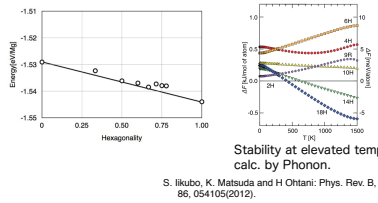

Initial | First step | Final

(A)

(B)

LPSO form scenarios

- Stacking Fault initiate
  - Stacking faults are introduced periodically in hcp-Mg.
  - Solute atoms are then trapped.
- Solute Ordering initiate
  - A SF traps the solution atoms.

- Solutions are condensed at four layers off from the initial SF.
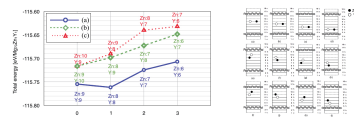- Condensed solutions initiate the stacking fault.

First principles calcs.

- Stacking Fault initiate
  - ☐ Long period stackings are stable in Mg?
  - ☐ Solute atoms are stable in SF?
- Solute Ordering initiate
  - ☐ Really does SF trap the solutions?
  - ☐ Does a SF with solutions stabilize the middle range ordering of solutions?
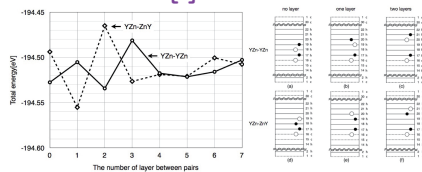 - ☐ Does condensed solutions really initiate the stacking fault?
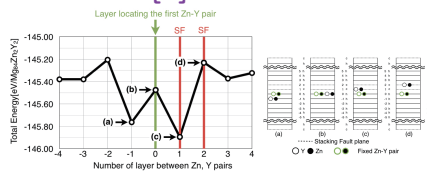
Periodic Stacking Fault?

Stability at elevated temps. calc. by Phonon.

S. Iikubo, K. Matsuda and H Ohtani: Phys. Rev. B, 86, 054105(2012).
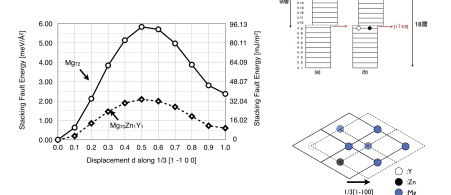
Does SF trap solutions?

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Middle range ordering of solutions[I]

Middle range ordering of solutions[II]

Does condensed solutions initiate SF?

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List checked by first principles calcs.

- Stacking Fault initiate
  - ☐ Long period stackings are stable in Mg?
  - ☐ Solute atoms are stable in or around SF?
- Solute Ordering initiate
  - ☐ Really does SF trap the solutions?
  - ☐ Does a SF with solutions stabilize the middle range ordering of solutions?
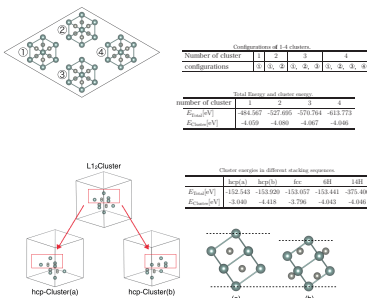 - ☐ Does condensed solutions really initiate the stacking fault?

Cluster?

- ☐ Cluster stability in hcp, fcc, SF Mg.
- ☐ Interactions btw clusters.
- ☐ SF in cluster
- ☐ Interactions btw cluster and solutions.

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Modified scenario

1. Zn and Y pairs stayed in the same stacking layer.
2. Zn and Y condensed layer induces SF easily.
3. SF traps Zn and Y.
4. Clusters are formed there.
5. Further Zn and Y are swept out or step away from SF with clusters.
6. Repeat 2-5 processes.

Cluster stability

Interaction btw cluster and solutions

Zn

Y