

Tutorial 3: Constructing Atomic Models for DFT calculations

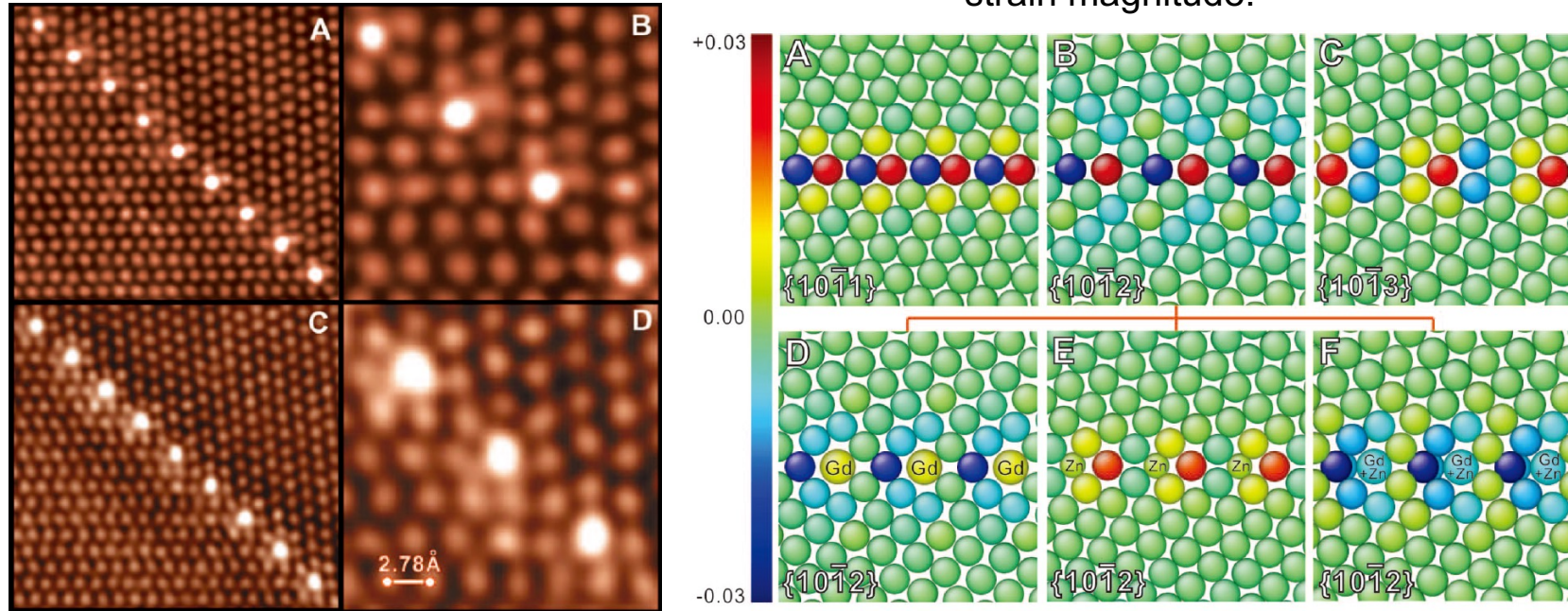
Y. Yin



Atomic Models

- A reasonable simplification of actual material structure.

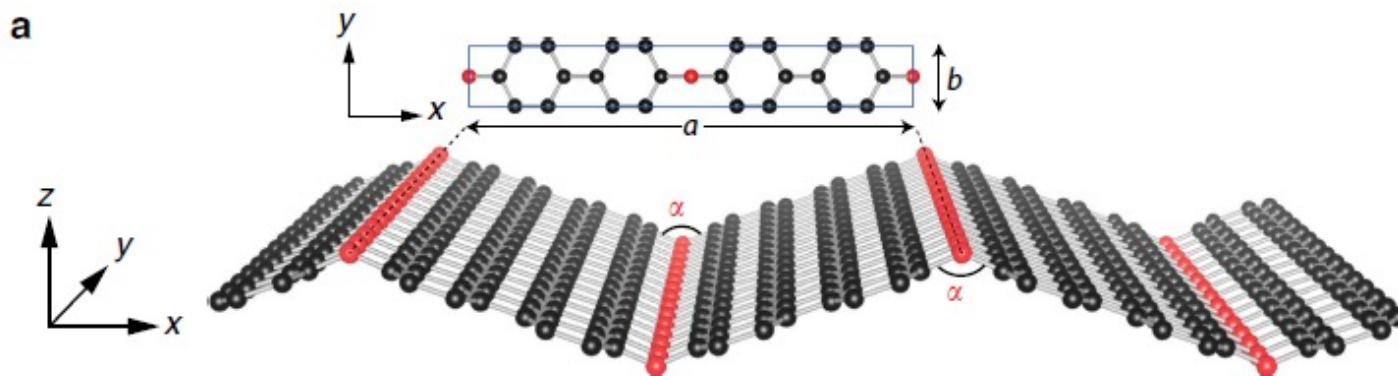
Corresponding DFT model showing strain distribution. The color strip shows the strain magnitude.



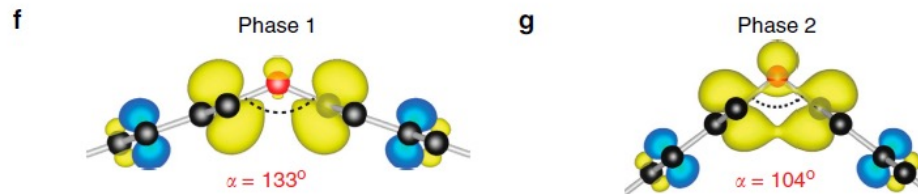
High-resolution TEM image of Mg-Zn and Mg-Zn-Gd alloy.
Solute atoms are highlighted at twin boundaries

Atomic Models

C_8O with ordered epoxy groups

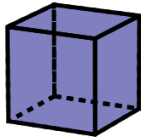


Phase transformation upon external electric field

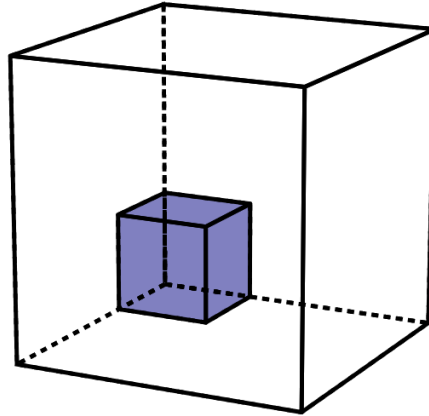


From Primitive Unit Cell to Supercell

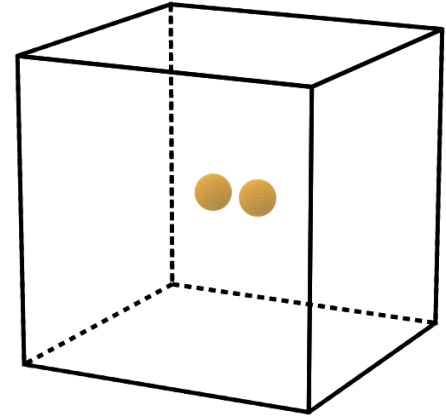
- A unit cell is the smallest unit of volume that contains all of the structural and symmetry information and that by translation can reproduce a pattern in all of space.
- Supercell is a repeating unit cell of the crystal that contains several primitive unit cells.



primitive unit cell



ideal supercell



defect supercell

Creating Atomic Structure with VESTA

DEMO



Resources

- List of visualization softwares:
- https://en.wikipedia.org/wiki/List_of_molecular_graphics_systems
- Materials database (lattice parameters, electronic structure etc.):
- <https://materialsproject.org>
- Answers to MC problems sent to me by the end of the week.

