First Principles Modeling of Phase Transformations in Materials

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Background

  – Michigan State University

M.S.E. Aerospace Engineering (1999)
  – The University of Michigan

M.S. Mathematics (2002)
  – The University of Michigan

  – The University of Michigan

Assistant Professor, Aerospace Engineering and Mechanics (2005)
  – The University of Minnesota
Solid-to-Solid Phase Transformations (PTs)

- Phase Transformations: crystal structures on the cusp of an *instability*

Chu & James (CuAlNi)  
Arlt (BaTiO\textsubscript{3})

Shape Memory Alloys (SMAs)

- *shape memory effect*
- *pseudo-elasticity*

Materials Research Science and Engineering Center, at the University of Wisconsin - Madison,  
www.mrsec.wisc.edu/Edetc/background/memmetal/
Scientific & Engineering Questions of Interest

• Why do these transformations exist and can we predict them from first principles?

I: First principles material model development (Dan Karls, Venkata Guthikonda)

II: Techniques for finding stable phases predicted by a model (Vincent Jusuf)

III: Techniques to solve engineering Boundary Value Problems (BVPs) based on these models (Slava Sorkin, with Prof. Tadmor)

IV: Study the possibility of finding phase transformations in biological- and nano-structures (Kaushik Dayal, with Prof. James)
I: First Principles Materials Modeling

- Effective Interaction Potentials (EIP)
  \[ \phi(r; \theta) \] — temperature-dependent
  - “effective” change in behavior with temperature
  - fit to known material properties
  - predict other properties

- Captures the temperature dependent properties of phase transformations in shape memory alloys

- Molecular Dynamics (MD) studies
  - Understand nonlinear dynamics of phase transformations (time consuming)
  - Build statistical models that capture correct physics (efficient)
II: Finding Predicted Stable Material Phases

Suppose we have an excellent material model. How do we know what it predicts?

- Branch-Following and Bifurcation (BFB) techniques

Develop efficient and automatic methods to perform BFB investigations
- Automatic branch-following
- Automatic bifurcation point detection and identification of bifurcating branches
- Challenging issues in both applied math and computational science
II: Finding Predicted Stable Material Phases

- EIP models with BFB techniques
  - stress-induced transformations

*Identification of stress induced transformation*

*Identification of other stable structures*

*Vast amount of information about the material’s energy function*
II: Finding Predicted Stable Material Phases

- Example: motion of atoms in unit cell for one equilibrium path

### Diagram:

- **Atom 1**
  - Motion in the $x$, $y$, and $z$ directions

- **Atom 2**
  - Motion in the $x$, $y$, and $z$ directions

- **Atom 3**
  - Motion in the $x$, $y$, and $z$ directions
III: BVPs with First Principles Material Models

- Quasi-Continuum methods for phase transforming materials
  - Cascading Cauchy-Born kinematics (CCB)
  - Modeling and simulation issues for first-order PTs
IV: PTs in Biological- & Nano-Structures

- Objective Structures (Prof. James)
  - Generalization of the idea of a crystal
  - "each atom sees identically the same environment"

- Find formulas to generate *all* possible objective structures
- Develop numerical BFB techniques for objective structures and look for phase transformations