Dual Degree Project
Monte Carlo simulation of interfacial energy calculation in solid-solid systems

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August 29, 2016

Problem Description

- System and Modeling

Current Progress

- Code Base
- Repository

System

- What system we are trying to study?
  - Solid-solid binary systems.
- What properties are we interested in?
  - Equilibrium state of the system
  - Interfacial energy between an intermetallic phase and matrix.
  - Interfacial energy as a function of relative orientation
  - possibly other things as well

Modeling the system

- Crystal Structure.
  - Current code base implements FCC crystal
  - Possible to extend it to a more general system
- Bond Energy
  - Embedded atom method used to calculate bond energies.
  - Currently using Ni-Al system for proof of concept.
  - Possible to extend it to n-atom potential.

Code base

- Functionality currently implemented
  - Creating and reading various data
    - Crystal structure
    - Simulation parameters
    - EAM data
  - 3D coordinate manipulation
  - Analysis on crystal files
    - Counting ordered phase sites
    - Counting anti-order phase sites

Code Base issues

- Old code base unable to process large structures
  - Reason: Too much searching time in EAM table.
  - $\mathcal{O}(\log N)$ complexity binary search implemented.
- New code base issues
  - Too many memory leaks.
  - Must be made more modular for further development
  - No documentation written as of now.

On GitHub

- Link to repository