Configuration Space:  
A Final Frontier of Nano-Scale Simulations

A Continuously Growing Web-Based Interface Structure Databank

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Configuration Space:
A large challenge at the small scale

Atomistic modeling challenges: *(mechanics perspective)*
1. Computationally feasible & accurate force calculations
2. Incorporation of long-range effects
3. Discrepancy of temporal scales
4. Vast, complex, and influential atomic configuration space
Motivating Example:
Mechanism-based material failure modeling

- Continuum polycrystal and defect models require input from atomic scale
  - Grain boundary (interface) properties
  - Defect interaction properties
- Huge parameter spaces to characterize
GB Parameter Space

Atomic structure is probabilistic quantity

Mechanical properties depend on loading rate and direction in GB plane

Multiple properties:
Decohesion and plasticity

<table>
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<tr>
<th>Parameters</th>
<th>Number</th>
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<tr>
<td>Impurities</td>
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Structure Matters

Example: Dislocation Nucleation from GB

<110> symmetric tilt Cu GBs


“E” structural unit
Temperature Matters

Example: GB sliding

- GB structure changes with temperature
- GB shear strength changes with temperature
- **Shear stress** can also initiate structural change
- **Impurities** can initiate structural change, Bishop et al. 1971
  - Suppression of faceting
Geometry Matters

Example: Grain Boundary Sliding

- Qualitative differences can exist
- Effect of normal stress on stress to initiate GB sliding
- Cu symmetric tilt <110> GBs

$\Sigma 9 \ (221) \ 38.9^\circ \ 833 \text{mJ/m}^2$

Warner and Molinari, MSMSE 2008
A Significant Problem

• Mechanical properties depend 12+ GB parameters
• Even simplified case is challenging
  – mode I GB fracture
  – pure elemental material
  – fixed temperature
  – 5 geometric parameters
  – Discretize parameter space by one degree increments
  – ~1 billion simulations
• Surveying this space is too expensive
  – 1 min simulations
    -> 1 week on 100,000 processors

• Comprehensive understanding via brute force will remain limited
• Targeted or on-the-fly investigations of interface properties will remain popular
2 Steps of Interface Characterization

1. Create structure
2. Perform characterization

- Often, same structures must be generated regardless of characterization goals
- Leads to an overlap of effort among researchers, i.e. wasted of time
- Generating a set of interface structures is not a quick task
Protein Structure Databank

Welcome to the RCSB PDB

The RCSB PDB provides a variety of tools and resources for studying the structures of biological macromolecules and their relationships to sequence, function, and disease.

The RCSB is a member of the wwPDB whose mission is to ensure that the PDB archive remains an international resource with uniform data.

This site offers tools for browsing, searching, and reporting that utilize the data resulting from ongoing efforts to create a more consistent and comprehensive archive.

Information about compatible browsers can be found here.

A narrated tutorial illustrates how to search, navigate, browse, generate reports and visualize structures using this new site. (This requires the Macromedia Flash player download.)

Comments? info@rcsb.org

Molecule of the Month: Selenocysteine Synthase

If you have visited your local health food store or looked closely at the ingredients in your daily multivitamin, you may have noticed that the element selenium is often listed as one of the beneficial supplements. Selenium is a double-edged sword, however. In general, selenium compounds are toxic and have an unpleasant garlic odor, but in trace amounts, selenium is essential for our health. Selenium atoms are similar to sulfur atoms, with similar properties, except that selenium compounds tend to be more reactive. In a few specialized proteins, this extra reactivity is just what is needed. For instance, by using a selenium atom instead of sulfur, thio-destoxin reductase improves its rate of catalysis by 100 times, and formate dehydrogenases act 300 times faster.

More ...

Previous Features
The Interface Structure Data Bank hosts interface atomic structures created from simulation. Use as both a starting point for your own research and as a forum for published structure material.

Follow tabs above to search the **Data Bank** for available GB structures, properties, and related research articles.

Updatable **Add Content** feature allows you to share your interface structure research on this centralized database.

The databank is intended to aid the broad effort of connecting atomistic scale mechanisms to macroscopic material behavior, whether mechanical, thermal, electrical, or optical. Visit the **About** link for an in-depth background.

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**ISDB created by Nathaniel Erwin; supervised by Dr. Derek Warner, Cornell University**

**E-Mail site problems or suggestions to: nae7@cornell.edu**
The default orientation options use up to 7 degrees of freedom (DOF) to characterize the interface; however, there are only 5 unique DOF.

Each rotational axis $[uvw]$ is chosen where $u>v>w$ are positive integers.

**note:** the "Extra Criteria" orientation options may be redundant.
Material
   Bi-Crystal

Orientation
   GB Plane 1
   Twist Angle
   Asymmetric
      GB Plane 2

More>
   \( \Sigma \) Number
   GB Energy
   Rotational Axis
   Tilt Angle

details
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<td>Reference Paper:</td>
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</table>
ALUMINUM --

Crystal Lattice  FCC
Structure

Orientation
Symmetry  Symmetric
Planes  \langle 1 1 1 \rangle
\langle 1 1 1 \rangle
Sigma Number  \Sigma 3
Tilt Angle  0.0000
Twist Angle  60.0000

Structure
Energy Density  75.6379 mJ/m²
Free Volume  11.0552
Inter-atomic Potential Model  Eam
Reference Paper
Outstanding Issues

• Downloads
  – Format
    • Automated builder

• Uploads
  – Format and procedure
    • Human intervention required

• Continued management strategy

• Motivating contributions
  – Critical mass is needed
  – Initial contributions less than anticipated
    • Sethna et al. and Sansoz et al.

• Build critical mass ourselves
A Continuously Growing ISDB

- Initially focus on EAM Al pure twist grain boundaries
- Recipe (balance accuracy and expense)
  - Boundary conditions
    - X & Z-directions: periodic
    - Y-direction: vacuum
  - Cell size
    - X & Z-directions: bulk lattice periodicity
    - Y-direction: 15nm (<1% error)
  - Crystal geometry
    - Grain boundary plane (Miller indicies)
      - Coincident site lattice number (twist angles)
        » Discrete lattice shift vectors (translations parallel to GB)
  - Equilibrate structure
    - Initial 3A separation between crystals
    - 50ps of NVT dynamics at 100K
    - Conjugate gradient minimization to 10meV/A force tolerance
  - Energy computation
    - Energy of atoms not within 7A of surfaces
  - Minimum energy structure taken to be structure with lowest energy over all discrete lattice shift vectors

Local von Mises strain
Current Status

- ~385 minimum energy structures obtained
- ~240,000 energy minimization computations
- Generation recipe validated against Spearot’s data
- Comparison against experimental EBSD data (Saylor et al.)
Harnessing Web-Based Grid Computing
utilize unused cycles on desktops across campus
Summary and Conclusions

1. Hard to generalize the mechanical behavior of material interfaces
2. Created web-based databank for easy sharing of interface structures
3. Ensure continuing growth of databank by using automated generation algorithm
4. Grid-based automated generation