Computational Framework for Assessing Grain Boundary Structure-Property Relationships at Nanoscale

M.A. Tschopp, M.F. Horstemeyer

Center for Advanced Vehicular Systems (CAVS), Mississippi State University
Introduction

CAVS: Multiscale Models of Mechanical Behavior

Where do grain boundaries enter into multiscale models?
Outline
Grain boundary structure-property relationships

Electronic Principles (DFT)

Interatomic Potential Development

Molecular dynamics

GB structure database

GB properties database

Mesoscale models

Phase Field

Dislocation Dynamics

Potts Model

Continuum models

Molecular

Continuum
Toolboxes

- MATLAB
- Optimization
- Parallel Processing
- Image Processing
- Genetic Algorithm
- Neural Network
- Spline Fitting
- External Programs
  - DYNAMO
  - LAMMPS
  - GNUPLOT
  - VASP
  - ABAQUS
  - VPSC
- GUI
- Data Management
  - *.mat datafiles
  - Write to Excel
  - Generate LaTeX reports
  - Output images
  - Write to *.ppt
- *.fig graphs

Integration Driver

Tschopp et al. MSMSE (2009), Wilks et al. MSEA (2010)

Tschopp et al. ScrMater (2010)
CAVS - Interatomic Potential Development

- Aluminum
  - Al-Mg, Al-Si, Al-Cu, Al-Fe, etc.
- Magnesium
  - Mg-Al, etc.
- Steel
  - Fe-V, Fe-C, etc.

- Nuclear Applications
- Polymer/composites

New research areas

Still needs some work...
- Needs to be efficient!!!
- Optimization techniques – what methodology works best?
- Ease of transferability to new potentials
- Addition of new response variables (e.g., stacking fault energy)
Interatomic Potential Development
Simulation Methodology

Interatomic Potential Design Methodology

Global Approach
- Initialization
  - Design Space Evaluation
  - Sensitivity Analysis

Local Approach
- Design Space Evaluation
- Design Space Sampling
- Response Surface Generation
- Multi-Objective Optimization
- Potential Validation

Fe-He potential
Design Space Evaluation

- He in Octahedral Site
- He in Tetrahedral Site
- He in Substitutional Site

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Interatomic Potential Development
Fe-He Results

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<th>$E_{\text{octa}}$(eV)</th>
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<th>$E_{\text{He}_3\text{V}}$(eV)</th>
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<td>4.64</td>
<td>6.43</td>
<td>8.48</td>
<td>9.12</td>
</tr>
</tbody>
</table>

Ran for 1 starting point

Advantage of optimization on response surface is that 100’s of different starting points, weighting factors, can be ran quickly.

How well does the response surface model (RSM) capture the atomistic results?

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Molecular Continuum
Grain Boundary Structure Database
GB Energy Results

Symmetric Tilt Grain Boundary
\[ \Sigma = 3/(111)/109.47^\circ \text{ STGB} \]
Rotate (a) by -54.74°, +54.74°

Asymmetric Tilt Grain Boundary
\[ \Sigma = 3/(110)_{1}/(114)_{2} \text{ ATGB} \]
Rotate (b) by +35.26°

FCC Cu/Al

M. A. TSCHOPP† and D. L. MCDOWELL*†
Structures and energies of \( \Sigma 3 \) asymmetric tilt grain boundaries in copper and aluminium
*Philosophical Magazine*,
Vol. 87, No. 22, 1 August 2007, 3147–3173

Asymmetric tilt grain boundary structure and energy in copper and aluminium
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**BCC Fe**

<100> Fe Symmetric Tilt Grain Boundaries

<110> Fe Symmetric Tilt Grain Boundaries
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HCP Mg
Grain Boundary Structure Database
GB Structure Results

<100> Symmetric Tilt Grain Boundary Structure

Cu

Fe

Mg
The structure, energy and free volume of symmetric and asymmetric tilt grain boundaries can provide insight into interfacial properties, such as dislocation nucleation.

Grain boundary structures of a few $\Sigma 3$ asymmetric boundaries in Cu compared to HRTEM images in Ag (Ernst et al. 1992).

Grain Boundary Properties
Grain boundary dislocation nucleation

No apparent correlation with...
• GB ENERGY
• MISORIENTATION ANGLE
• SIGMA VALUE
• FREE VOLUME
Grain Boundary Properties
Point defect formation energy results

Normalized point defect formation energies

Interstitial formation energies vs GB energy

Site binding energies for vacancies & interstitials

Influence of grain boundary character on point defect formation energies
Grain boundary hierarchical strategy

Do correlations exist that allow us to predict the properties for a wide range of GB character?

Increasing GB size

Increasing CPUs needed

Mechanical Properties
Diffusivity
Elastic Properties
Segregation Energies
SIA Formation Energies
Vacancy Formation Energies
Free Volume
Energy

STGB
ATGB
STTwistGB
ATTwistGB
CAVS: Cyberinfrastructure

IT technologies (hidden from the engineer)

Conceptual design process (user-friendly interfaces)

Engineering tools (CAD, CAE, etc.)

CAVS: Cyberinfrastructure

ccg.hpc.msstate.edu
QUESTIONS?