Towards a Unified Framework for Interatomic Potential Development: Application to the Fe-He System

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Outline

• Introduction

• Simulation Methodology
  • Global Approach (GA) & Local Approach (LA)

• Simulation Results
  • GA Potential Space Evaluation & Sensitivity Analysis
  • LA Potential Space Evaluation and Sampling, and Analytical Model Generation
  • Interatomic Potential Design Map Development and Validation
  • Uncertainty in Potentials…

• Conclusions
Nanoscale simulations play an important role in identifying mechanisms and quantifying relationships pertaining to radiation damage, which can provide valuable insight for macroscale material models.

However, the validity of the interatomic potential often limits the accuracy of nanoscale simulations for describing specific mechanisms or behavior.
Introduction

The interatomic potential fitting process plays a crucial role in the results of nanoscale simulations since critical properties are fixed during this process.

As nanoscale simulations steadily increase for material systems, often an interatomic potential formulated for one purpose is used for simulations outside of the intended purpose (which can affect the physics being studied).

In many cases, a researcher is restricted to evaluating existing potentials from the literature for their purpose. In part, OpenKIM (Knowledgebase of Interatomic Models) is motivated by this need.

Clearly, there is also a need for an alternative framework for developing potentials that will allow researchers to easily tailor potentials.

February 27-March 3, 2011 – San Diego, California
Simulation Methodology

Schematic of the generalized framework for interatomic potential development showing the Global and Local Approach stages.

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Simulation Results
 Initialization

Ab initio values

<table>
<thead>
<tr>
<th>Defect</th>
<th>VASP (17, 15)</th>
<th>VASP corrected</th>
<th>MEAM</th>
<th>Percent Difference</th>
</tr>
</thead>
<tbody>
<tr>
<td>(E_{He,sub})</td>
<td>4.08 eV</td>
<td>3.86 eV</td>
<td>3.88 eV</td>
<td>+0.5%</td>
</tr>
<tr>
<td>(E_{He,tetra})</td>
<td>4.37 eV</td>
<td>4.37 eV</td>
<td>4.32 eV</td>
<td>-1.1%</td>
</tr>
<tr>
<td>(E_{He,octa})</td>
<td>4.60 eV</td>
<td>4.60 eV</td>
<td>4.66 eV</td>
<td>+1.3%</td>
</tr>
<tr>
<td>(E_{He2})</td>
<td>8.72 eV</td>
<td>8.72 eV</td>
<td>8.29 eV</td>
<td>-4.9%</td>
</tr>
<tr>
<td>(E_{He2V,(100)})</td>
<td>N/A</td>
<td>6.58 eV</td>
<td>6.68 eV</td>
<td>+1.5%</td>
</tr>
<tr>
<td>(E_{He2V,(110)})</td>
<td>6.63 eV</td>
<td>6.41 eV</td>
<td>6.36 eV</td>
<td>-0.8%</td>
</tr>
<tr>
<td>(E_{He2V,(111)})</td>
<td>N/A</td>
<td>6.43 eV</td>
<td>6.62 eV</td>
<td>+3.6%</td>
</tr>
<tr>
<td>(E_{He3V})</td>
<td>9.44 eV</td>
<td>9.22 eV</td>
<td>9.33 eV</td>
<td>+1.2%</td>
</tr>
</tbody>
</table>

Scripts for assessing properties

\[ E^f(He_nVM) = E_{tot}(He_nVM) - [nE_{He} + (N - n)E_{Fe}] \]

Single element parameters

<table>
<thead>
<tr>
<th>(E_c)</th>
<th>(r_e)</th>
<th>(\alpha)</th>
<th>(A)</th>
<th>(\beta^{(0)})</th>
<th>(\beta^{(1)})</th>
<th>(\beta^{(2)})</th>
<th>(\beta^{(3)})</th>
<th>(t^{(0)})</th>
<th>(t^{(1)})</th>
<th>(t^{(2)})</th>
<th>(t^{(3)})</th>
<th>(\delta_3)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fe</td>
<td>4.280</td>
<td>2.851</td>
<td>5.027</td>
<td>0.585</td>
<td>3.8</td>
<td>2</td>
<td>0</td>
<td>1</td>
<td>-0.8</td>
<td>12.3</td>
<td>2</td>
<td>0.3</td>
</tr>
<tr>
<td>He</td>
<td>0.032</td>
<td>4.100</td>
<td>8.050</td>
<td>1.000</td>
<td>6.0873</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0.0</td>
</tr>
</tbody>
</table>
The **GA Potential Space Evaluation** step calibrates the interatomic potential while comparing properties with *ab initio*/experimental values.
The **GA Sensitivity Analysis** step evaluates the relative influence of each potential parameter on the potential properties.
The **LA Potential Space Evaluation** step uses the sensitive potential parameters to evaluate the bounds for sampling the potential space.
The **LA Potential Space Sampling** step calculates the potential properties for the interatomic potential design map by varying potential parameters to accurately sample the potential design space.
The LA Potential Space Sampling step calculates the potential properties for the interatomic potential design map by varying potential parameters to accurately sample the potential design space.

Simulation Results
Potential Space Evaluation

- Latin Hypercube
- Stratified Random Sampling
- 2000 Fe-He MEAM potentials

Roadmap
Simulation Results
Analytical Model Generation

The **LA Analytical Model Generation** step fits a higher order polynomial regression model that provides an analytical representation of the relationship between potential parameters and properties.

<table>
<thead>
<tr>
<th>Defect Energy</th>
<th>$R^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_{He,sub}$</td>
<td>1.000</td>
</tr>
<tr>
<td>$E_{He,tetra}$</td>
<td>0.999</td>
</tr>
<tr>
<td>$E_{He,octa}$</td>
<td>0.973</td>
</tr>
<tr>
<td>$E_{He_2}$</td>
<td>0.982</td>
</tr>
<tr>
<td>$E_{He_2V,(100)}$</td>
<td>0.679</td>
</tr>
<tr>
<td>$E_{He_2V,(110)}$</td>
<td>0.978</td>
</tr>
<tr>
<td>$E_{He_2V,(111)}$</td>
<td>0.999</td>
</tr>
<tr>
<td>$E_{He_3V}$</td>
<td>0.988</td>
</tr>
</tbody>
</table>

$R^2 > 0.95$ for most responses

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**Roadmap**

- Initialization
- Potential Space Evaluation
- Sensitivity Analysis
- Potential Space Evaluation
- Potential Space Sampling
- Analytical Model Generation
- Potential Design Map Development
- Potential Design Map Validation

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A global analytical expression, or objective function, for optimization is easily formulated from the individual analytical expressions. Potential optimization takes minutes…
The **LA Potential Design Map Development** step formulates the interatomic potential design map and then uses optimization techniques to generate an optimal interatomic potential for a specific application.
Simulation Results
Interatomic Potential Design Map

An example of an interatomic potential design map for Fe-He.
Simulation Results
Interatomic Potential Design Map

An example of an interatomic potential design map for Fe-He, where only one potential parameter is modified.
Simulation Results
Application: Uncertainty Analysis

1000 optimal Fe potentials were generated using a +/- 2% uncertainty in \textit{ab initio} values.

Variation in potential parameters
Simulation Results
Application: Uncertainty Analysis

1000 optimal Fe potentials were generated using a +/- 2% uncertainty in \textit{ab initio} values.

Variation in He formation energies
Why MD?

Energetic driving force for preferential binding of self-interstitial atoms to Fe grain boundaries over vacancies

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GB Site Preference

Prefers SIA

Prefers Vacancy

Vac SIA

$E_f \begin{array}{c}
\Sigma 5(310) \\
\theta = 36.87^\circ
\end{array}$

$\begin{array}{c}
1.72 \\
3.52
\end{array}$

<100> Symmetric Tilt Grain Boundaries

Vacancy Formation Energy (eV)

Distance from GB (Ångstroms)

Vacancy Binding Energy (eV)

<100> Fe Symmetric Tilt Grain Boundaries

Grain boundary energy (mJ/m²)

Misorientation angle (degrees)
Summary

1. Formulated a generalized framework for interatomic potential development and have applied this to the Fe-He system

2. Introduced the concept of an interatomic potential design map as a tool that contains multiple potentials and is capable of exploring nanoscale phenomena

3. Analyzed how uncertainty in the interatomic potential design process affects potential parameters and properties

Thank you for your time! Questions...

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