Deformation of Single Crystal NiAl and Ni$_3$Al

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JULY 26, 2017
SuperAlloys

• Properties
  • High ductility, even at high temperatures
  • Oxidation Resistant
  • Low Density

• Applications
  • Advanced aerospace structures and propulsion systems
  • Electronic metallization for use in semiconductors


D.B. Miracel (1993)
Mechanical Properties

• Defect analysis is essential to the creation of sturdy and long-lasting alloys
• Introduce spherical voids at the center of a simulation cell
• Measure mechanical properties:
  • Stress-strain curve/Yield point
  • Elastic Constants
Methods: Molecular Dynamics

- LAMMPS was used to integrate Newton’s equation of motion (using Verlet’s method)
  - NPT Ensemble Conditions
- Collected a timeseries of configurations at various values of strain.
- Dislocations occur along highest-density planes

Ni$_3$Al – Perfect Lattice

Color Coding:  Blue/Red – Ni/Al atoms
Green – Volumetric Strain depicting slip planes in the fcc lattice
Spherical Voids

- We define a periodic box of volume \((La_o)^3\), where \(a_o\) is the lattice spacing of the material and \(L\) is an integer.

- We explored the parameter space:
  - Simulation Cell Size \(L\)
  - Void volume fraction \(\phi\)

<table>
<thead>
<tr>
<th>Material</th>
<th>(a_o) (Exp.)</th>
<th>(a_o) (EAM Results)</th>
<th>Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>NiAl</td>
<td>2.88 Å</td>
<td>2.83 Å</td>
<td>1.73 %</td>
</tr>
<tr>
<td>Ni$_2$Al</td>
<td>3.57 Å</td>
<td>3.53 Å</td>
<td>1.12 %</td>
</tr>
</tbody>
</table>

\(L = \{5, 10, 15, 30, 45, 60, 75, 90, 100, 125\}\)
\(\phi = \{0, 0.01, 0.02, 0.04, 0.05, 0.06, 0.08, 0.10\}\)

Mishen et Al. (2009)
Perfect Lattice with Varying Cell Sizes

Ni$_3$Al

NiAl

Stress (GPa) vs. Strain
Ni$_3$Al : $\phi = 1\%$

- We investigated the stress structure at the yield point of the stress-strain curve.
- Confirmed the nucleation of shear loops due to the decomposition of the Burger’s vectors along the slip planes.
- As the system size increases, the dislocation density increases, causing stacking faults to appear sooner due to the greater interaction of dislocations.

Ariza et al. (2013, 2015), Tschopp et al. (2010, 2013)
NiAl : $\phi = 1\%$
Ni$_3$Al Yield Stress at the Thermodynamic Limit

Yield = $a + \frac{b}{La_0}$

<table>
<thead>
<tr>
<th>$\phi$ (%)</th>
<th>a (GPa)</th>
<th>b</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>13.72</td>
<td>-0.0012</td>
</tr>
<tr>
<td>1</td>
<td>9.78</td>
<td>43.06</td>
</tr>
<tr>
<td>2</td>
<td>9.60</td>
<td>30.83</td>
</tr>
<tr>
<td>4</td>
<td>9.07</td>
<td>28.60</td>
</tr>
<tr>
<td>6</td>
<td>8.75</td>
<td>24.93</td>
</tr>
<tr>
<td>8</td>
<td>8.20</td>
<td>29.09</td>
</tr>
</tbody>
</table>
NiAl Yield Stress at the Thermodynamic Limit

Yield = \( a + \frac{b}{La_0} \)

<table>
<thead>
<tr>
<th>( \phi ) (%)</th>
<th>( a )</th>
<th>( b )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>20.12</td>
<td>0.014</td>
</tr>
<tr>
<td>1</td>
<td>9.76</td>
<td>12.79</td>
</tr>
<tr>
<td>2</td>
<td>9.90</td>
<td>0.111</td>
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<tr>
<td>4</td>
<td>9.34</td>
<td>11.57</td>
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<tr>
<td>6</td>
<td>9.39</td>
<td>0.0085</td>
</tr>
<tr>
<td>8</td>
<td>9.15</td>
<td>0.51</td>
</tr>
</tbody>
</table>
Further Work

• Collect strain rates of $10^7$ to $10^{11}$ (s$^{-1}$) to test for convergence

• Collect more extreme temperature variation data
  • Melting point of the materials $\sim$1700 K
  • Near 0 K (for MD, we choose 1 K as a benchmark)

• Further analyze the geometries of the dislocation networks and examine the mechanisms that cause them to interact
References


• LAMMPS. http://lammps.sandia.gov/

• Ovito. https://ovito.org/

References Cont.


Centrosymmetric Parameter

\[ CS = \sum_{i=1}^{N/2} |\vec{R}_i + \vec{R}_{i+N/2}|^2 \]

- Measures local disorder in a crystal on a per-atom level
- For FCC and BCC structures, N is set to 12 and 8, respectively
- For perturbations on the order of \( k_bT \), CS is near 0.
Dislocation Analysis

• In the FCC lattice:
  • Slip Plane: \{111\}
  • Burger’s Vector (Direction of Dislocation): \( \mathbf{B} = \frac{a_o}{2} <110> \)

• In the BCC lattice: (More Complicated)
  • Slip Plane: \{110\}, \{112\}, and \{123\}
  • Burger’s Vector: \( \mathbf{B} = \frac{a_o}{2} <111> \)

http://www.eng.fsu.edu/~kalu/ema4225/lec_notes/Web%20Class_13a_final.ppt
Ariza et al. (2013, 2015)
Partial Dislocations

- Burger’s Vector (length and direction of lattice distortion) will decompose due to energy minimization
  - \( \mathbf{b}_1 = \mathbf{b}_2 + \mathbf{b}_3 \), where the criterion for decomposition is “Frank’s Energy Criterion”:
    - \( |\mathbf{b}_1|^2 > |\mathbf{b}_2|^2 + |\mathbf{b}_3|^2 \)
- This decomposition creates loops around (instead of lines away from) the void due to vector addition
- “Perfect” Dislocation: \( \mathbf{b}_1 \)
- “Partial” Dislocation: \( \mathbf{b}_2 + \mathbf{b}_3 \)

https://www.tf.uni-kiel.de/matwis/amat/def_en/kap_5/backbone/r5_4_2.html