Award No. DE-FEOO08719

Synergistic Computational and Microstructural Design of Next-Generation High-Temperature Austenitic Stainless Steels

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Students: T. Jozaghi, N. Chaudhary, Dr. Shujuan Wang

Department of Material Science and Engineering
Texas A&M University
Design new austenitic stainless steels (ASS) for advanced ultra supercritical combustion coal-fired power systems
- High temperature strength
- High ductility
- Good creep resistance
- Good high temperature oxidation/corrosion resistance

Design of micro-alloying additions, heat treatment schedules, and microstructure
- Cost-effective alternatives to Ni-base superalloys
- Higher-temperature alternatives to ferritic steels

Develop a robust ICME design/optimization framework for high temperature ASS.
Approach

Alloy + Microstructure Design

- Austenitic structure
- High density of low energy nano-twin boundaries
- Nano-scale precipitates, intermetallics, laves phases stable at high temperature
- Formation of alumina surface oxide

Nano-precipitates (carbides, intermetallics)

Laves phase

Deformation twinning with fine thickness
1. **The Study of Deformation Twinning**
   - Evolution with applied strain
   - Thermal stability
   - Interactions of twins
   - Effect of deformation twins on mechanical response

2. **Novel AFASS Alloy Design**
   - Initial characterization and evaluation of first-generation alloys
   - Processing of candidates from first-generation alloys
   - Introducing the second-generation alloys
   - Characterization, evaluation, and processing of second generation alloys
### Overview

**Single crystals**

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<th>Ni</th>
<th>Cr</th>
<th>Mn</th>
<th>Nb</th>
<th>Si</th>
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<th>Mo</th>
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#### First-Generation Alloys

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- **Alloy 1:** Need to validate the predictive power of thermodynamic databases and models developed (oxidation, twinning ability). Selected based on the literature material developed by Yamamoto et al., at ORNL
- **Alloy 2:** lower expensive Ni, V to form precipitate at high temp., N to improve twin-ability. Nb is for carbides and Laves phases
- **Alloy 3:** higher Ni than alloy 2 for FCC stability
- **Alloy 4:** between Alloy 1 (AFA) and 316 SS (twin)

#### Second-Generation Alloys

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<tr>
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<td>x</td>
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THE STUDY OF DEFORMATION TWINNING

- Evolution with applied strain
- Thermal stability
- Interactions of twins
- Effect of deformation twins on mechanical response

QUESTIONS AND CHALLENGES

- Fundamental study of recovery and recrystallization (ReX) of deformation twins in low SFE steels in the presence of various densities of dislocations
- The optimum thermo-mechanical processing path for high volume fraction of deformation twins
- Role of in-situ carbides and nitrides during recovery and ReX in the presence of deformation twins?
- Role of deformation twins and nano-particles on creep and stress rupture behavior of designed steels.
316 Stainless Steel, 40% Tension at RT

High density twins. Twins intersect with each other. Some twin bands include bunch of fine twins.
The twin density increases with increasing strain.

Twin width stays similar.
The nano twins are stable under 900 °C, no coarsening and detwinning were discerned. Dislocations were recovered by annealing.
NOVEL AFASS ALLOY DESIGN

- Initial characterization and evaluation of first-generation alloys
- Processing of candidates from first-generation alloys
- Introducing the second-generation alloys
- Characterization, evaluation, and processing of second generation alloys

First-Generation Alloys

<table>
<thead>
<tr>
<th>All in wt%</th>
<th>Fe</th>
<th>Ni</th>
<th>Cr</th>
<th>Mn</th>
<th>Nb</th>
<th>Si</th>
<th>Al</th>
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- Alloy 3: Higher Ni than alloy 2 for FCC stability.
- Alloy 4: Between Alloy 1 (AFA) and 316 SS (twin).
First-Generation Alloys

Alloy 1
- ✓ Fully austenite
- × Uncontrollable NbC precipitation
- × No Twinning
- ✓ Alumina scale formation

Alloy 2
- × Second phase formation
- × Uncontrollable Ti-rich NbC

Alloy 3
- ✓ Austenite, intra-granular second phase
- × Uncontrollable Ti-Nb carbo-nitrides and AlN precipitation

Alloy 4
- × Second phase formation

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What is Materials Design?

Materials Design is ultimately the solution to an inverse problem. Ideally, MD should be materials-agnostic (not realistic at this time).
Design Criteria

- Alumina Formation
- Low SFE – Twinnability
- Large stability region for FCC
- Low Ms

- Competing factors:
  - Al necessary for alumina formation
  - Al increases SFE, decreases twinnability
  - Al stabilizes BCC against FCC
  - Optimization is necessary
Today: Formation of Stable Alumina Layer

Necessary Conditions:

Kinetics:
- Low O diffusion
- High Al diffusion

Thermodynamics:
- Large Alumina Formation Driving Force
Testing the ‘Effective Growth Constant Criterion’

Effective Valence ($V_{eff}$) vs. Free Energy ($\Delta G$)

K Value

- Good oxidation resistance
- Bad oxidation resistance

Formula:

Fe - 20Ni - 14Cr - 2.5Al - 0.15Si - 2Mn - 2.5Mo - 0.86Nb - 0.08C - 0.01B

K = 700
Third Element Effect Predominance Maps

- Unstable Oxide Layer
  - Gas
  - AO
  - AO + BO + CO Dispersion
  - Alloy

- Mixed Stable Layer
  - Gas
  - BO + CO
  - Alloy

- Stable Layer
  - Gas
  - CO
  - Alloy

Minimum Chromium Needed for Third Element Effect
Minimum Aluminium Needed to form Alumina Scale
No Alumina Scale Formation
Al-rich oxide
Stable Mixed Layer
Testing Third Element Effect Predominance Maps

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<tr>
<th></th>
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<th>C</th>
<th>Mn</th>
<th>Si</th>
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- **HTUPS 4**: Al-rich oxide
- **AFA Alloy 4**: AFA Oxide
- **AFA Alloy 13**: AFA Alloy 13
- **1.5 Al Trip As**: HTUPS 2

- **Fe-Cr oxide**: Internal Al₂O₃
- **Fe, Cr-rich oxide**: Al-rich internal oxide
### Comparison of two Criteria

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</tr>
<tr>
<td>AFA Alloy 12</td>
<td>32.06</td>
<td>18.69</td>
<td>3.10</td>
<td>0.13</td>
<td>6.06</td>
<td>0.15</td>
<td>3.32</td>
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<td>0.1110</td>
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<td>AFA Alloy 13</td>
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<td>0.15</td>
<td>3.12</td>
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<td>0.15</td>
<td>0.15</td>
<td>3.27</td>
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<td>0.0160</td>
<td>0.0018</td>
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<td>0.14</td>
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<td>3.08</td>
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<td>2.50</td>
<td>0.00</td>
<td>0.00</td>
<td>0.0900</td>
<td>0.0100</td>
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<td>HTUPS 2</td>
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<td>14.20</td>
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<td>2.46</td>
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<td>0.50</td>
<td>0.0760</td>
<td>0.0150</td>
<td>0.00</td>
<td>0.00</td>
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<td>Pass</td>
<td>Fail</td>
<td>[6, 15]</td>
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<td>HTUPS 3</td>
<td>19.98</td>
<td>14.21</td>
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<td>1.92</td>
<td>2.46</td>
<td>0.14</td>
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<td>0.49</td>
<td>0.0790</td>
<td>0.0110</td>
<td>0.00</td>
<td>0.00</td>
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<td>Pass</td>
<td>Fail</td>
<td>[6, 15]</td>
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<tr>
<td>HTUPS 4</td>
<td>19.95</td>
<td>14.19</td>
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<td>Pass</td>
<td>Pass</td>
<td>[6, 15]</td>
</tr>
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</table>
Prediction of Stacking Fault Energy as a Function of Alloying Additions

Models:

Experimental Measurements
- (A. Dumay 2006)
- (Schramm 1975)
- (Xing Tian 2008)
- Many more

Theoretical Predictions
- (Cohen 1976)
- (Mullner 1998)
- (Jacques 2010)
- (Vitos 2011)
- (Q. Lu 2013)
- (K. Ishida 1976)
- Many more

Effects on SFE:
- 1. Alloyning elements
- 2. Temperature
- 3. Interstitials

Prediction:
- High
- Low

Effects on SFE: Relevant to creep, strain deformation, annealing twins, formation of dislocations, stress corrosion cracking, phase transformation stability, and electron/vacancy density, but we want to optimize SFE to ensure formation of deformation twins
The problem: Unpredictability!

- Significant inconsistencies (computational and experimental)

“...same alloying element cause totally opposite changes....no universal composition equations for SFE can be established....”

Vitos et al., 2006

Yet many linear regression equations relating SFE to composition in the literature.

**AISI 310**

94 +/- 14 mJ/m²  
(Xray profile analysis)  
*Schramm and Reed, 1975*

40 +/- 5 mJ/m²  
(TEM extended nodes)  
*Rhodes and Thompson, 1977*

**AISI 316**

44 mJ/m²  
*Yonezawa et al., 2013*

78 +/- 6 mJ/m²  
(Xray profile analysis)  
*Schramm and Reed, 1975*
From Prediction to Classification

- 20 mJ/m² Sato et al.
- 18 mJ/m² Allain et al.
- 25 mJ/m² Hamada Vecammen
- 50 mJ/m² Park et al.
- 60 mJ/m² Hamada
- 35 mJ/m² Allain et al.
- 80 mJ/m² Vecammen

- Martensitic Transformation (TRIP behavior)
- Mechanical Twinning (TWIP behavior)
- Dislocation glide
Neural Network-based Classifiers

Machine Learning - Artificial Neural Networks for Classification

Our Model

<table>
<thead>
<tr>
<th>Input Layer</th>
<th>Hidden Layer</th>
<th>Output Layer</th>
</tr>
</thead>
<tbody>
<tr>
<td>9 units representing wt.% of different elements</td>
<td>40 units to capture complex relationships between elements</td>
<td>3 units representing 3 different SFE regimes</td>
</tr>
</tbody>
</table>

Training Set: 60 alloy compositions
Accuracy: 97%
The data collected was broken into training and testing sets.
- The ANN has trained well as evident ( ~97% accuracy )
- The ANN has generalized well which is shown from good predictions on Test set.
Genetic Algorithm-based Optimization

- Computational Genetic Algorithms are a necessity to:
  - Streamline Alloy Design Process
  - Decrease Time and Cost of Alloy Discovery
  - Decrease Time and Cost of Alloy Refinement

- GA will be used to find a heat treatment process for:
  - Maximizing FCC Phase
  - Minimize BCC and Unwanted Phases
  - Ensure Twinning through control of Stacking Fault Energy
  - Austenite Stability
  - Alumina Formation
  - Critical Stress for Creep
Proposed Genetic Algorithm Alloys

<table>
<thead>
<tr>
<th>PGAA</th>
<th>Fe</th>
<th>C</th>
<th>Mn</th>
<th>Ni</th>
<th>Mo</th>
<th>Al</th>
<th>Cr</th>
<th>Si</th>
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</thead>
<tbody>
<tr>
<td>1</td>
<td>Bal.</td>
<td>0.073</td>
<td>3.893</td>
<td>11.000</td>
<td>2.026</td>
<td>2.994</td>
<td>19.820</td>
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<tr>
<td>2</td>
<td>Bal.</td>
<td>0.088</td>
<td>8.993</td>
<td>17.140</td>
<td>2.242</td>
<td>3.112</td>
<td>15.300</td>
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<td>3</td>
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<td>0.050</td>
<td>10.000</td>
<td>10.000</td>
<td>2.500</td>
<td>3.000</td>
<td>16.000</td>
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Computational Alloy Design

Second-Generation Alloys

<table>
<thead>
<tr>
<th>wt.%</th>
<th>C</th>
<th>Mn</th>
<th>Ni</th>
<th>Mo</th>
<th>Al</th>
<th>Cr</th>
<th>Si</th>
<th>Fe</th>
</tr>
</thead>
<tbody>
<tr>
<td>PGAA</td>
<td>0.08</td>
<td>9</td>
<td>17.1</td>
<td>2.24</td>
<td>3.11</td>
<td>15.3</td>
<td>0.19</td>
<td>bal.</td>
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</table>

As-received, etched

Cold rolled 80%
HT1080°C-23ht
HT1150°C-1hr
Can the second generation alloy

• Form alumina?

• Undergo deformation twinning?
PGAA2: Oxidation at 850°C

156hrs

Aluminum diffusion zone gets thicker with time
• Stress-strain curve suggests deformation by twinning. TEM in progress…
1. Work on twinning:
   - Single crystals of three austenitic steels have been grown.
   - High volume fractions and hierarchical structure of deformation nano-twins were confirmed in single and polycrystals.
   - Nano-twins are thermally stable up to 900°C. Deformation – annealing – deformation route can increase the twin density and the strength levels.

2. A new method has been developed to successfully predict the alumina formation in multicomponent alloys.

3. We have developed an extensive datasets for SFE of austenitic stainless steels.

4. We have developed a classifier to predict in a robust manner whether any alloy would have low, medium or high SFE.

5. A preliminary alloy design framework has been developed through the use of Genetic Algorithms.

6. Two generations of new alloys have been designed and characterized.

7. First generation of designed alloys suffers from lack of twinning, two phase formation, and AlN formation.

8. Second generation of designed alloys look more promising for alumina formation and twinning, more work is needed.
Computational Alloy Design

- ICME---Integrated Computational Materials Engineering
- Multi-objective optimization through Generic Algorithms

Material Selection, Processing

Genetic Algorithm

Thermodynamic & Kinetics Predictions

Mechanical Properties

Microstructure

Thermo-mechanical treatments

Chemistry, Thermodynamics, Kinetics

Processing

Microstructure

Properties

- Intensive deformation twinning / low energy GBs
- Carbides, intermetallics, Laves phases
- Creep resistance
- Oxidation resistance
- High temperature strength

<table>
<thead>
<tr>
<th>Ti</th>
<th>V</th>
<th>Cr</th>
<th>Mn</th>
<th>Co</th>
<th>Ni</th>
<th>Cu</th>
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<tbody>
<tr>
<td>Al</td>
<td>Si</td>
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</table>

<table>
<thead>
<tr>
<th>Zr</th>
<th>Nb</th>
<th>Mo</th>
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<tr>
<td>Ta</td>
<td>W</td>
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