Advanced Materials Development Through Computational Design

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Advances in Computational Modeling Facilitate Rapid Alloy Development

- There is a recurring need for modification or development of improved alloys and may be
  - Performance driven (example: increased operating temperature of exhaust valves)
  - Cost driven (example: lowering cost of cast irons)
- Conventional trial-and-error alloy development methodology is expensive and time consuming
- Path to improved alloy composition may not be obvious in complex, multi-component systems
- Significant advances have been made in computational thermodynamic and kinetic modeling tools
  - Improved models for multi-component systems are available
  - Large experimental database of phase equilibria available for comparison and verification
Various Computation-Aided Approaches to Development of New Alloys

- **Empirical approaches for interpolation/extrapolation**
  - **Database driven**
    - Uses existing database of relationship between material composition and its properties
    - Relationships are used to identify new composition with required properties
    - Curve fitting, neural networks, etc
  - **Disadvantages**
    - Need Access to a large database relating inputs (composition/microstructure) to outputs (microstructure/properties)
    - Extrapolation beyond available parameter space is difficult
- **Phenomenological approaches**
  - Driven by understanding of physical phenomena
    - Alloy properties controlled by microstructural design
      - Thermodynamic modeling
      - Kinetic Modeling
- **Combined Approach**
Overall Technical Approach for Computer-Aided Alloy Design

VALIDATION
Understand Behavior of Existing Materials

PROPERTY MEASUREMENTS
Microstructural Characterization
Thermodynamic and Kinetic Modeling

PREDICTION
Develop New Compositions

PROPERTY MEASUREMENTS
Microstructural Characterization
Thermodynamic and Kinetic Modeling
Principal Advantages of Computational Design

- Effectively search composition space and guide alloy development
  - Search multi-component composition space for preferred microstructure
  - Minimize experimental work
  - Reduce development time
- Convenient to enact “what-if-scenarios” in minimum time according to customer needs
  - Cost of an alloying element increases
  - Processing limitations etc.
Typical Flow Chart for the Accelerated Development of Materials for Automotive Applications

1. Identify Typical/Extremes Of Engine Operating Conditions
2. Identify Critical Components /Regions undergoing stress/ Temperature/ Corrosive Extremes
3. Formulate Material Property Requirements Based on Identified Exposure Conditions and Lifetime Requirements
4. Compare Materials Property Requirements with Available Materials (Ni-base and Fe-based Alloys)
   - Materials with Required Properties are Not Available
   - Materials with Required Properties are Available But Expensive
   - New Materials Development
   - Materials Modification
Valve Materials For High Temperature Applications

• In consultation with various industrial collaborators, design/identification of advanced materials for exhaust valves was identified as an area of interest

• Property of significant interest is high temperature fatigue life at 1600°F

• A few target alloys were down-selected and correlation was attempted between composition, high temperature fatigue properties, and microstructure
Progress in Correlating Mechanical Property Data with Composition

• Issues:
  – Lack of reliable data on relationship between high temperature fatigue property and specific alloy composition (only nominal composition or composition range information available)
  – Lack of detailed microstructural information to enable development of quantitative correlations between microstructure and property of interest
  – Kinetic factors are important but may not be available

• Solutions and Methodology
  – Mechanical property measurement in alloys with well-defined compositions and microstructure needs to be carried out
  – Microstructure evaluation and correlation with thermodynamic and kinetic modeling
Effect of Variation in Compositions of Commercial Nimonic 90 on Phase Fractions

**Composition, %**

<table>
<thead>
<tr>
<th>Component</th>
<th>Lower Limit</th>
<th>Upper Limit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon</td>
<td>0.13 max.</td>
<td></td>
</tr>
<tr>
<td>Silicon</td>
<td>1.0 max.</td>
<td></td>
</tr>
<tr>
<td>Copper</td>
<td>0.2 max.</td>
<td></td>
</tr>
<tr>
<td>Iron</td>
<td>1.5 max.</td>
<td></td>
</tr>
<tr>
<td>Manganese</td>
<td>1.0 max.</td>
<td></td>
</tr>
<tr>
<td>Chromium</td>
<td>18.0-21.0</td>
<td></td>
</tr>
<tr>
<td>Titanium</td>
<td>2.0-3.0</td>
<td></td>
</tr>
<tr>
<td>Aluminum</td>
<td>1.0-2.0</td>
<td></td>
</tr>
<tr>
<td>Cobalt</td>
<td>15.0-21.0</td>
<td></td>
</tr>
<tr>
<td>Boron</td>
<td>0.02 max.</td>
<td></td>
</tr>
<tr>
<td>Sulfur</td>
<td>0.015 max.</td>
<td></td>
</tr>
<tr>
<td>Lead</td>
<td>0.0020 max.</td>
<td></td>
</tr>
<tr>
<td>Zirconium</td>
<td>0.15 max.</td>
<td></td>
</tr>
<tr>
<td>Nickel</td>
<td>Balance</td>
<td></td>
</tr>
</tbody>
</table>

Compositions allowed within the specifications show a wide range in phase fractions and hence differences are anticipated in mechanical properties.
Typical Microstructure of Selected Ni-based Alloys

- Eight commercially available Ni-based alloys with different levels of alloying elements have been down-selected.
- Selected Ni-base alloys are:
  - austenitic
  - primarily strengthened by the precipitation of coherent intermetallic precipitates: $\gamma'$
  - Carbides (MC, $M_2C_6$) can also be present in alloys
  - Undesirable topological close packed phases (sigma, mu etc) may precipitate at certain temperatures
Computational Thermodynamic Modeling Shows Differences in Amount and Stability of Strengthening Phases

Nimonic ® 90

Waspaloy ®

Udimet ® 720

Amount of $\gamma'$ and highest temperature of stability of $\gamma'$ are affected by alloying element additions

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Calculated Major Phase Contents of Various Alloys at 870°C

Alloy Designation:
- IN® X750
- Nimonic® 80A
- IN® 751
- Nimonic® 90
- Waspaloy®
- Udimet® 41
- Udimet® 520
- Udimet® 720

Phases:
- gamma'
- Carbides

Wt. % Phases
0 5 10 15 20 25 30 35 40 45

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Fatigue Tests are Being Carried out *in-situ* at 870°C

- Fully reversed fatigue tests are being carried out at temperature of interest under load control
- Tests are carried out at frequency of about 30 Hz
- Stresses of
  - 21.8 (150) Ksi (MPa),
  - 29 (200),
  - 39.9 (275),
  - 43.5(300),
  - 50.8(350),
  - 54.4(375)
are used in the tests
Correlating Fatigue Properties with Microstructure

- Microstructure of Ni-based alloys can change with heat-treatment
  - Fatigue testing is carried out in optimum aged condition
- Alloys are typically subject to a multi-step heat-treatment consisting of solution annealing and one or more aging steps
- Focus on results of two alloys: Udimet 720 and Waspaloy
Results from fatigue tests are consistent with results from high temperature tensile tests but not consistent with calculated wt. % $\gamma'$

Actual microstructure of sample needs to be characterized with particular reference to $\gamma'$ content
Microstructure of Waspaloy® Shows Coarsening of Particles During High Temperature Exposure

2.4 million cycles
Time: 22 hours
Average V_f=17.1%
D_Ave=130.0 nm

55 million cycles
Time: 509 Hours
Average V_f=17.1%
D_Ave=189.0 nm

Predicted γ'= 16.7 wt.%
Future Work

- High temperature fatigue tests will be continued on alloys of interest
- Correlation of high temperature fatigue properties with actual microstructural characteristics (including grain size) observed in the samples will be performed
- Kinetics of microstructural evolution will be modeled and incorporated into property correlation
- An integrated approach that includes modeling of environmental interactions would be a challenging goal for future work
Acknowledgments

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