Advanced Materials Development Through Computational Design

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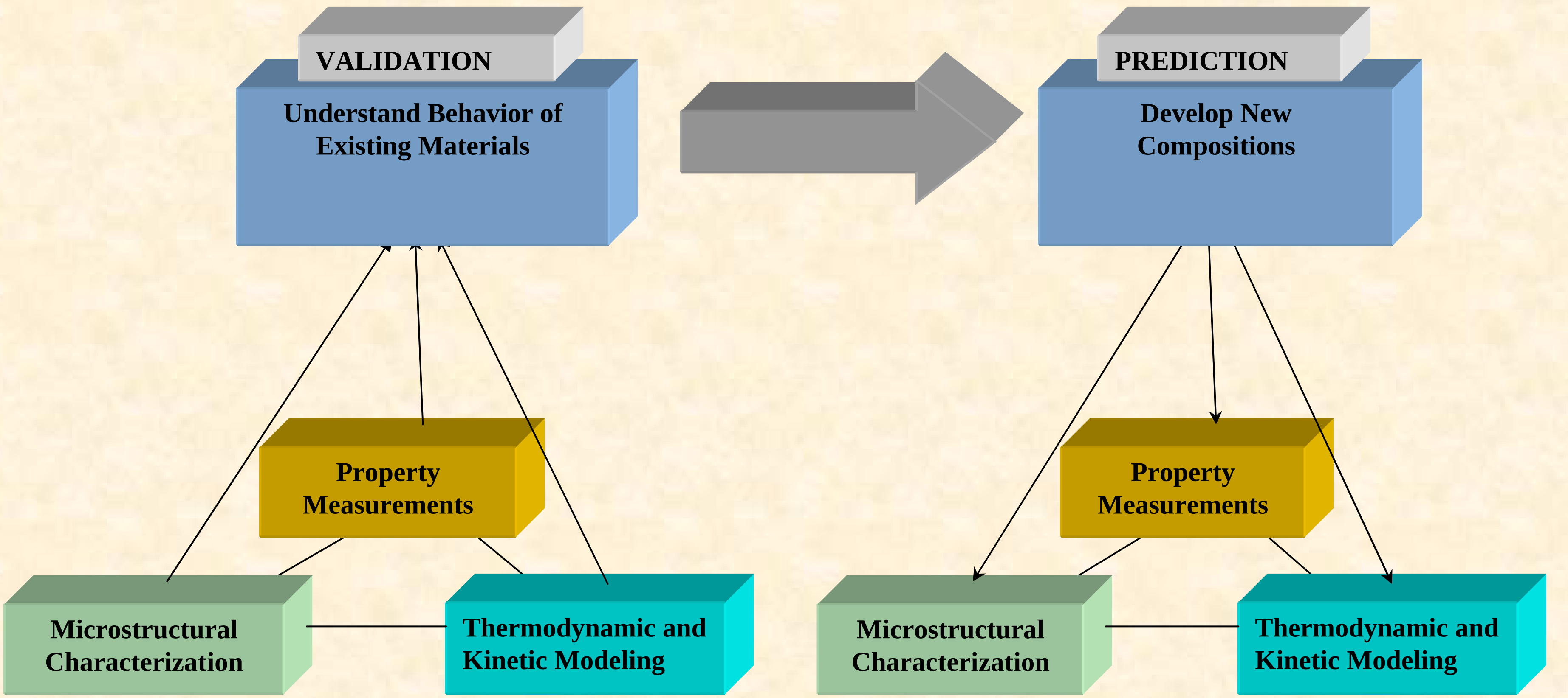
Advances in Computational Modeling Facilitate Rapid Alloy Development

- **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
      - Thermoydnamic modeling
      - Kinetic Modeling
- Combined Approach

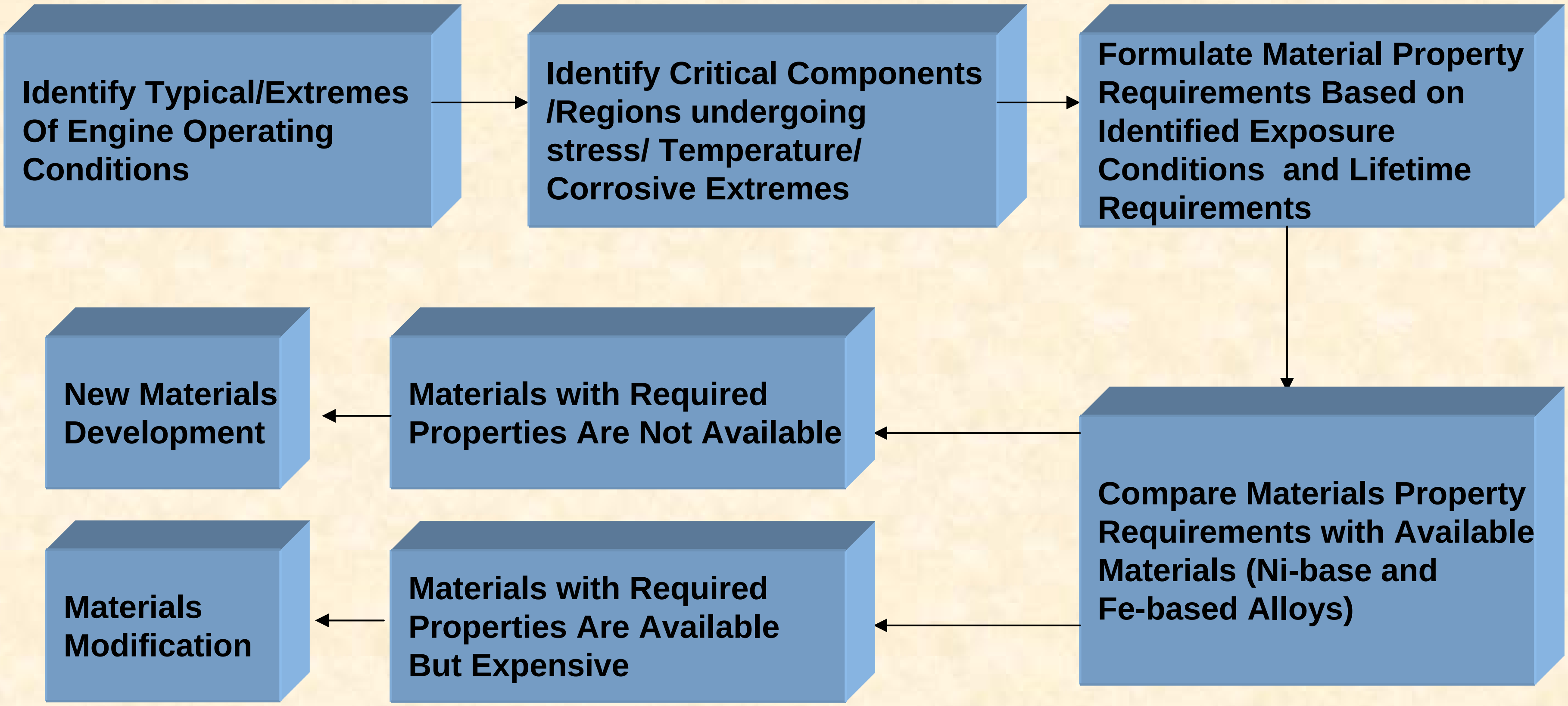
Overall Technical Approach for Computer-Aided Alloy Design



Principal Advantages of Computational Design

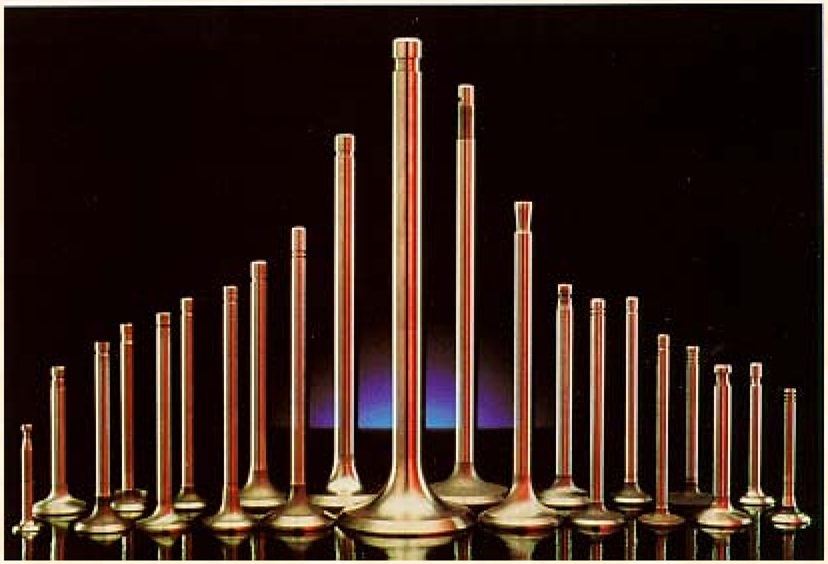
- **Effectively search composition space and guide alloy development**
  - Search multi-component composition space for preferred microstructure
  - Minimize experimental work
  - Reduce development time
- **Convenient to enact “what-if-scenarios” in minimum time according to customer needs**
  - Cost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

Typical Flow Chart for the Accelerated Development of Materials for Automotive Applications



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 1600ºF
- 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

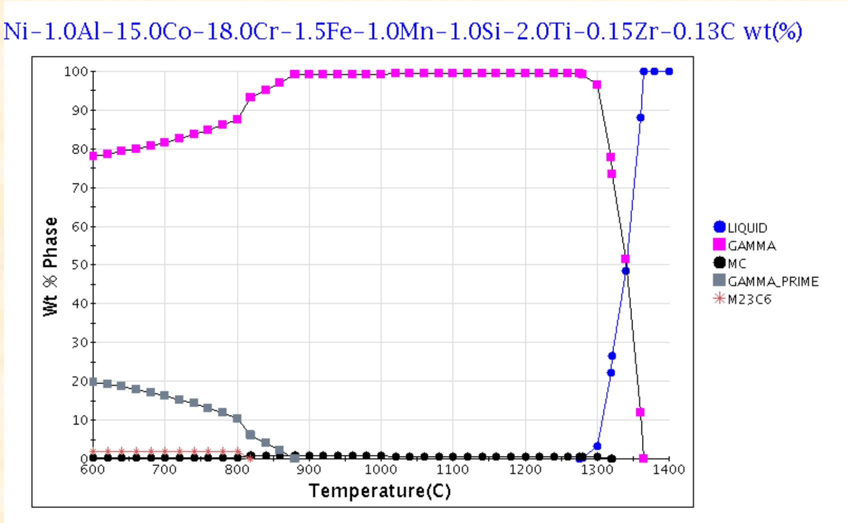
- **Issues:**
  - **Lack of reliable data on relationship between high temperature fatigue property and specific alloy composition (only nominal composition or composition range information available)**
  - **Lack of detailed microstructural information to enable development of quantitative correlations 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

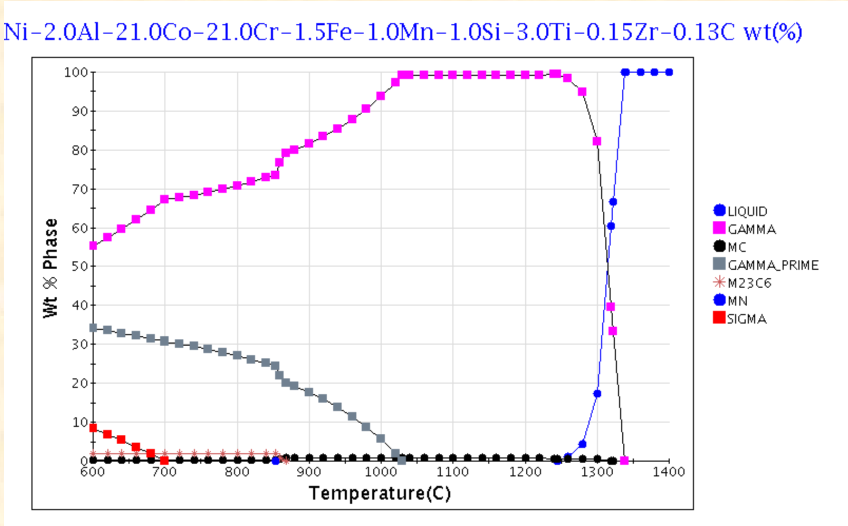
Composition, %

Carbon	0.13 max.
Silicon	1.0 max.
Copper	0.2 max.
Iron	1.5 max.
Manganese	1.0 max.
Chromium	18.0-21.0
Titanium	2.0-3.0
Aluminum	1.0-2.0
Cobalt	15.0-21.0
Boron	0.02 max.
Sulfur	0.015 max.
Lead	0.0020 max.
Zirconium	0.15 max.
Nickel	Balance

Lower Limit



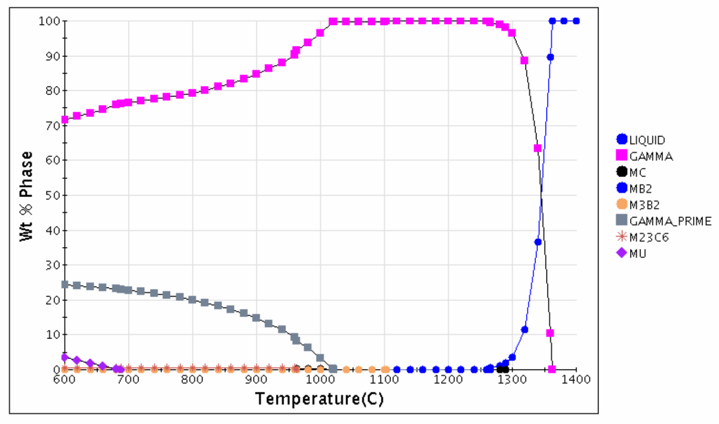
Upper Limit



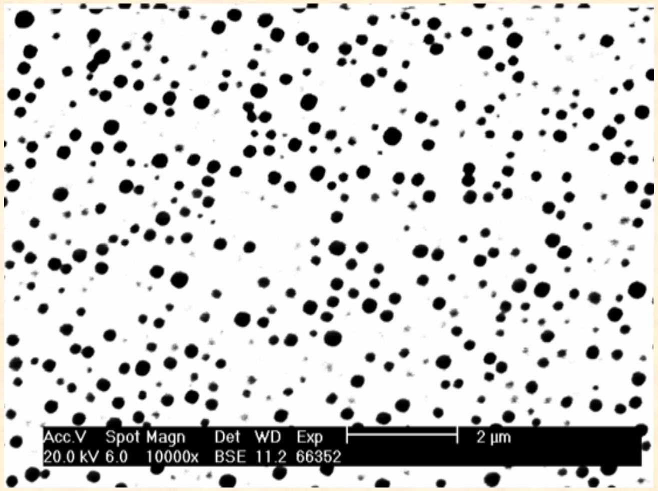
Compositions allowed within the specifications show a wide range in phase fractions and hence differences are anticipated in mechanical properties

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: γ'**
  - **Carbides (MC, $M_{23}C_6$) can also be present in alloys**
  - **Undesirable topological close packed phases (sigma, mu etc) may precipitate at certain temperatures**



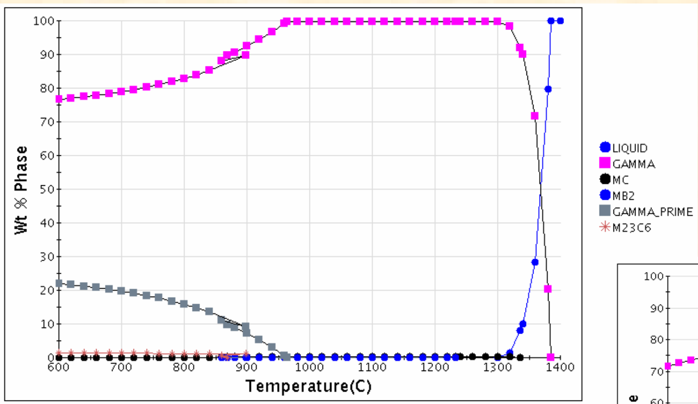
Waspaloy ®



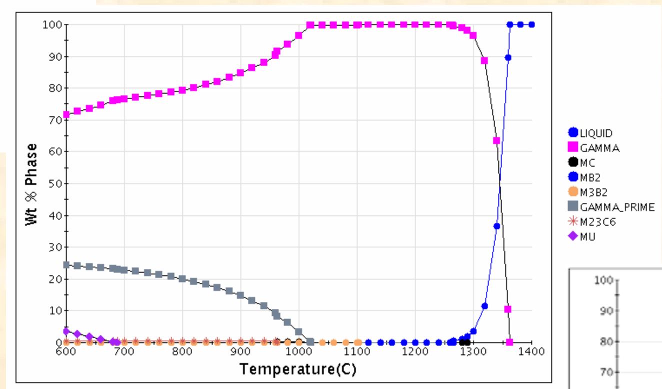
Back-scattered SEM Image showing γ' Precipitates

Computational Thermodynamic Modeling Shows Differences in Amount and Stability of Strengthening Phases

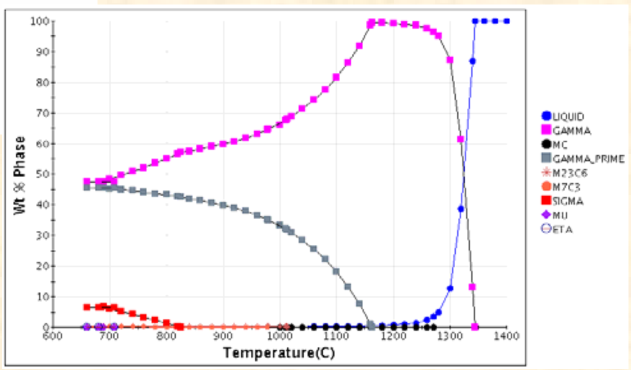
Nimonic ® 90



Waspaloy ®

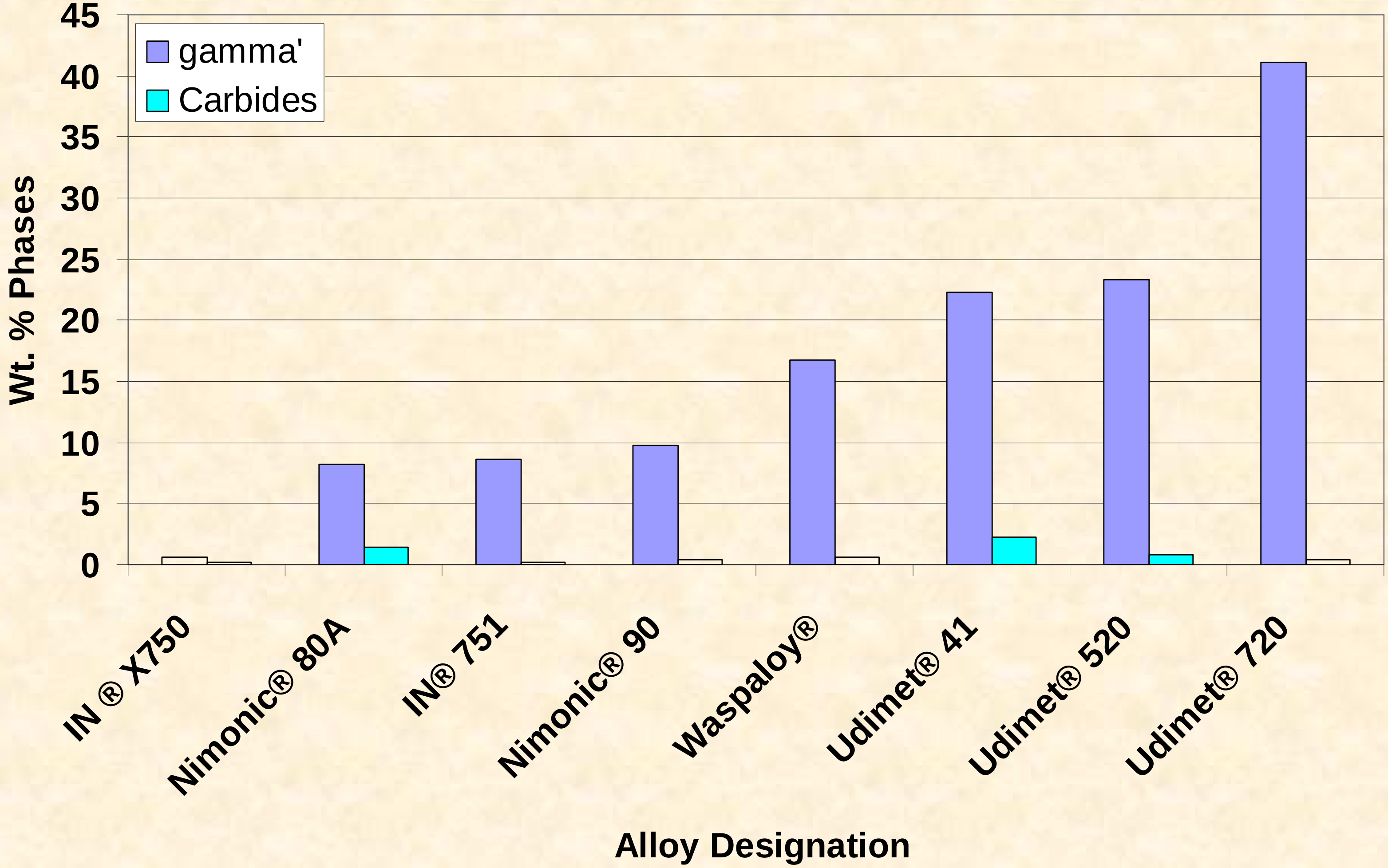


Udimet ® 720

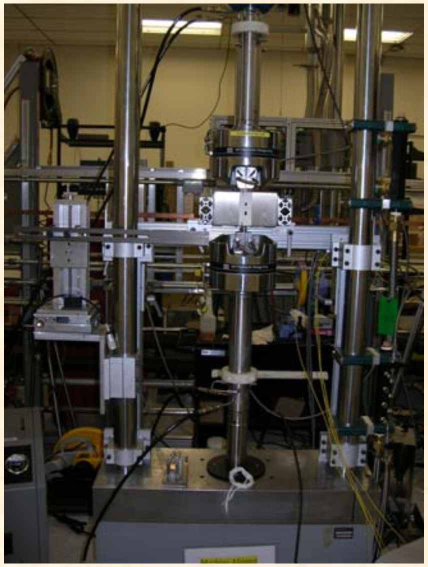


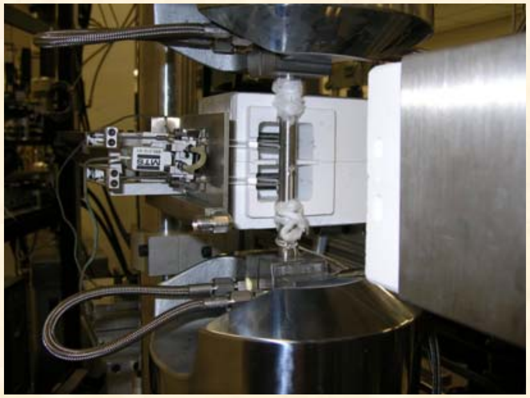
Amount of γ' and highest temperature of stability of γ' are affected by alloying element additions

Calculated Major Phase Contents of Various Alloys at 870°C



Fatigue Tests are Being Carried out *in-situ* at 870^{o}C



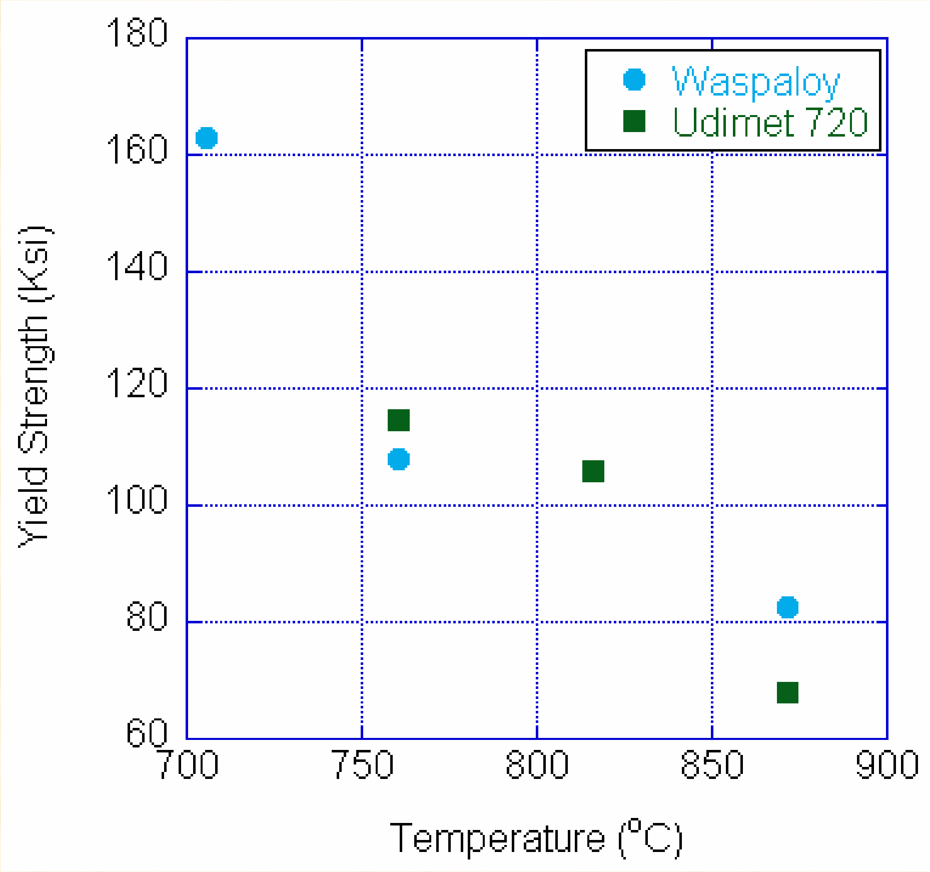


- **Fully reversed fatigue tests are being carried out at temperature of interest under load control**
- **Tests are carried out at frequency of about 30 Hz**
- **Stresses of**
  - **21.8 (150) Ksi (MPa),**
  - **29 (200),**
  - **39.9 (275),**
  - **43.5(300),**
  - **50.8(350),**
  - **54.4(375)**

  are used in the tests

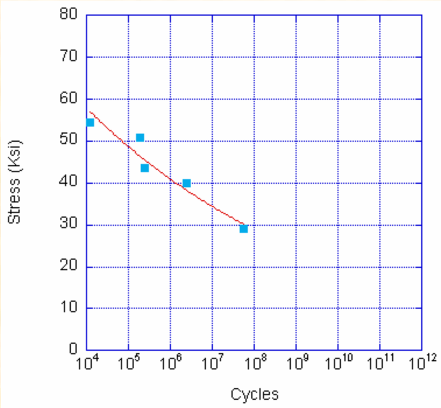
Correlating Fatigue Properties with Microstructure

- **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**

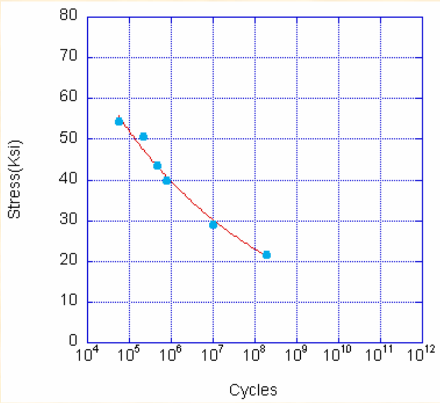


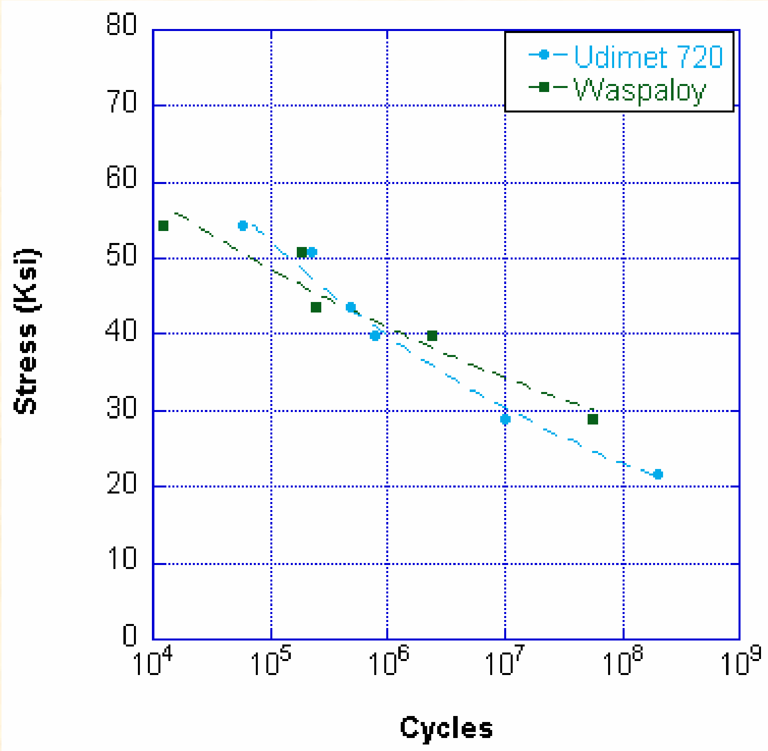
Fatigue Tests Show Differences in High Temperature Fatigue Properties

Waspaloy ®



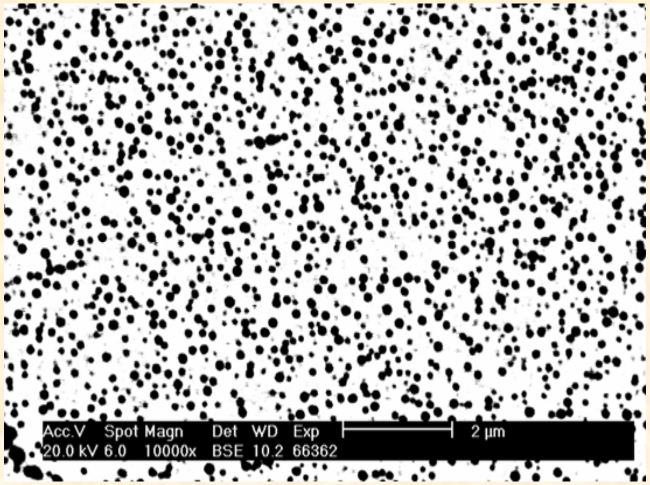
Udimet ® 720



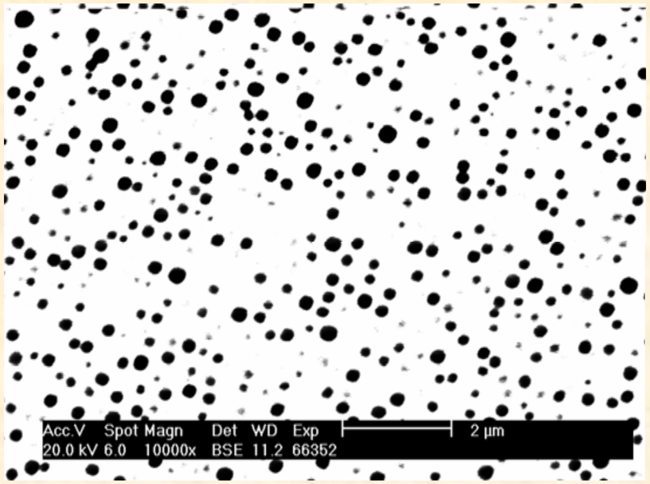


- **Results from fatigue tests are consistent with results from high temperature tensile tests but not consistent with calculated wt. % γ'**
- **Actual microstructure of sample needs to be characterized with particular reference to γ' content**

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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