Materials for HCCI Engines

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Outline of Talk

- Purpose of work
- Barriers
- Approach
- Technical Accomplishments: Valve Materials
  – Performance Measures and Goals
- Future Work
- Technology Transfer
- Summary
- Publications and Presentations

Purpose of Work

- Advanced combustion engine concepts such as HCCI are essential to achieve DOE energy-efficiency goals of 45% by 2012
- Higher pressures and higher flow rates in such operating modes result in higher component temperatures and stresses
- Existing materials used in such components may be inadequate to withstand temperature/stress conditions
- Need to evaluate the materials requirements and provide appropriate advanced materials solutions

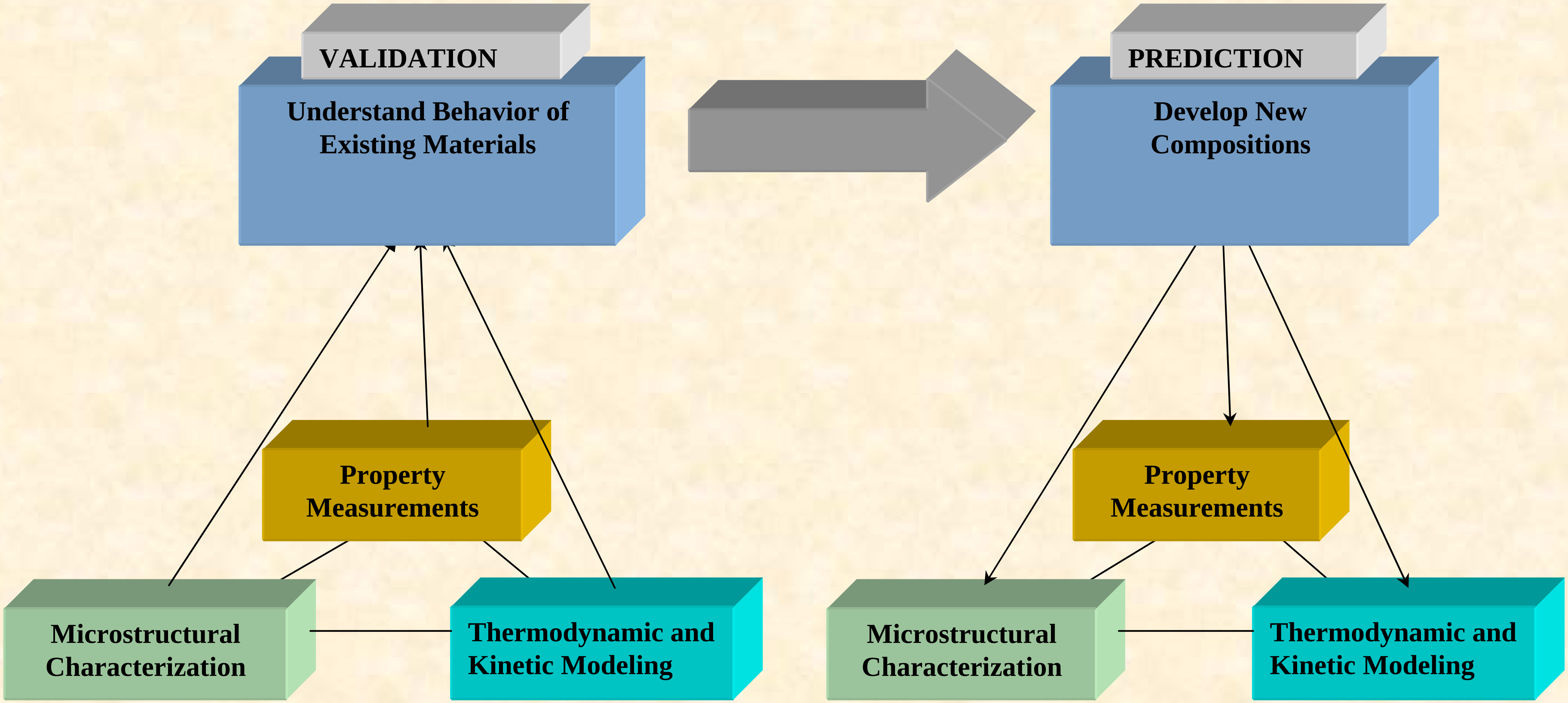
Barriers

- Critical properties for a wide range of alloy compositions of interest may not be available to enable materials selection
- Available materials may not satisfy the property requirements or may be cost prohibitive
- Path to develop alloy compositions with improved properties may not be apparent in complex, multi-component alloy systems
- Conventional trial-and-error methods used for alloy development are expensive and time-consuming

Approach

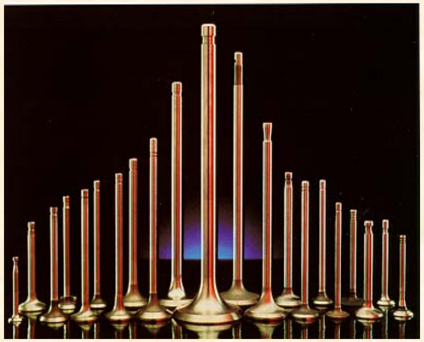
- Identify key material properties of interest for critical components
- Establish correlation between properties of interest and microstructural characteristics using existing alloys and identify desired microstructures
- Search composition space for alloys with optimum microstructure using validated computational models
- Reduce development time by selective testing of promising alloys with desired microstructure and cost

Schematic of Overall Technical Approach



Technical Accomplishments: Valve Materials For High Temperature Applications

- Several components and corresponding materials issues were identified with help from industrial partners
  - Exhaust valves, exhaust manifolds, fuel injectors, air coolers



- Design/identification of advanced materials for exhaust valves was suggested as an area of high priority
- Property of interest is improved fatigue life at 870^{o}C (from current 760^{o}C)
  - Desired: 10^{8} cycles to failure in rotating beam fatigue tests at 35 Ksi

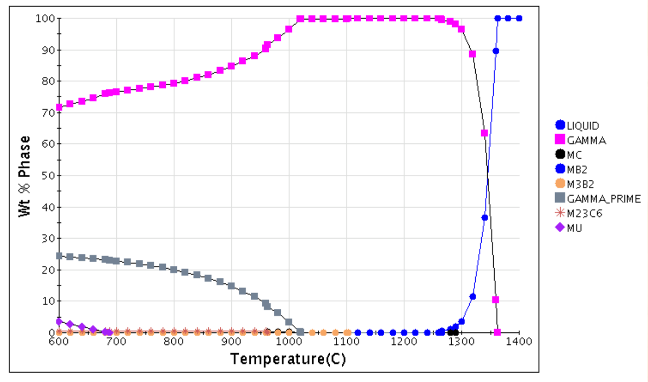
Correlations Between Fatigue Properties and Alloy Compositions Have Been Established

- Thermodynamic and kinetic modeling have been performed to correlate compositions with microstructure in selected alloys
- Microstructural characterization have been carried out to verify specific computational predictions
- High temperature fatigue properties have been obtained from alloys with well-defined compositions, heat-treatments, and microstructure
- Fatigue property variations with alloy composition have been characterized

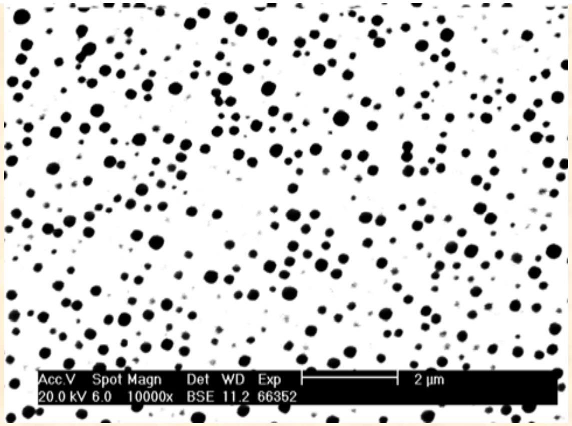
Selected Ni-based Alloys are Primarily Strengthened by γ' Precipitates

- Eight commercially available Ni-based alloys were 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



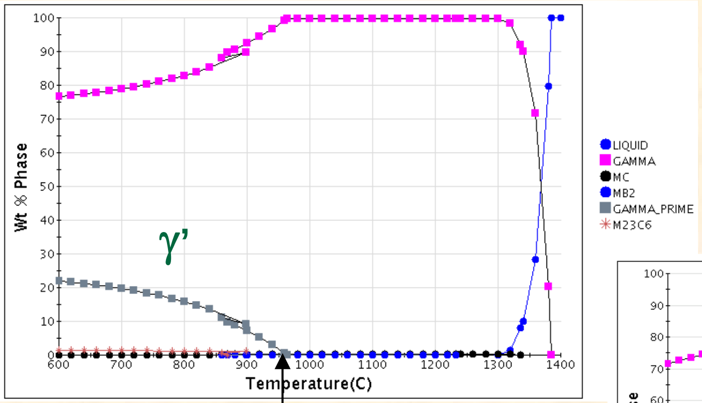
Waspaloy ®



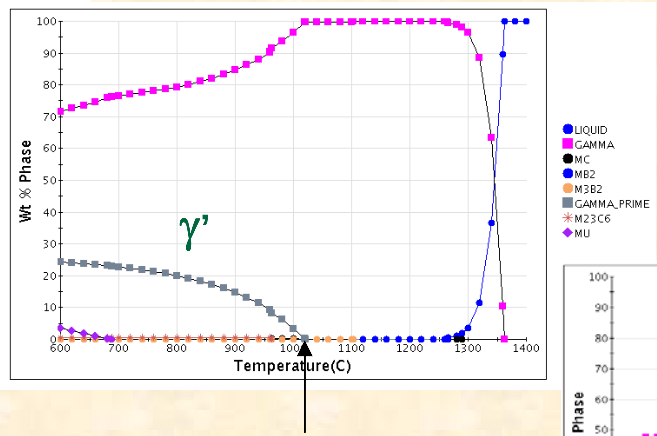
Back-scattered SEM Image showing γ' Precipitates

Computational Thermodynamic Modeling Predicts Correlation Between Composition and γ’ Contents

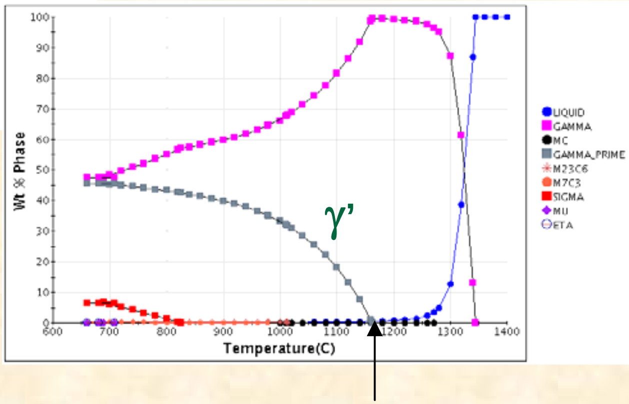
Nimonic ® 90



Waspaloy ®

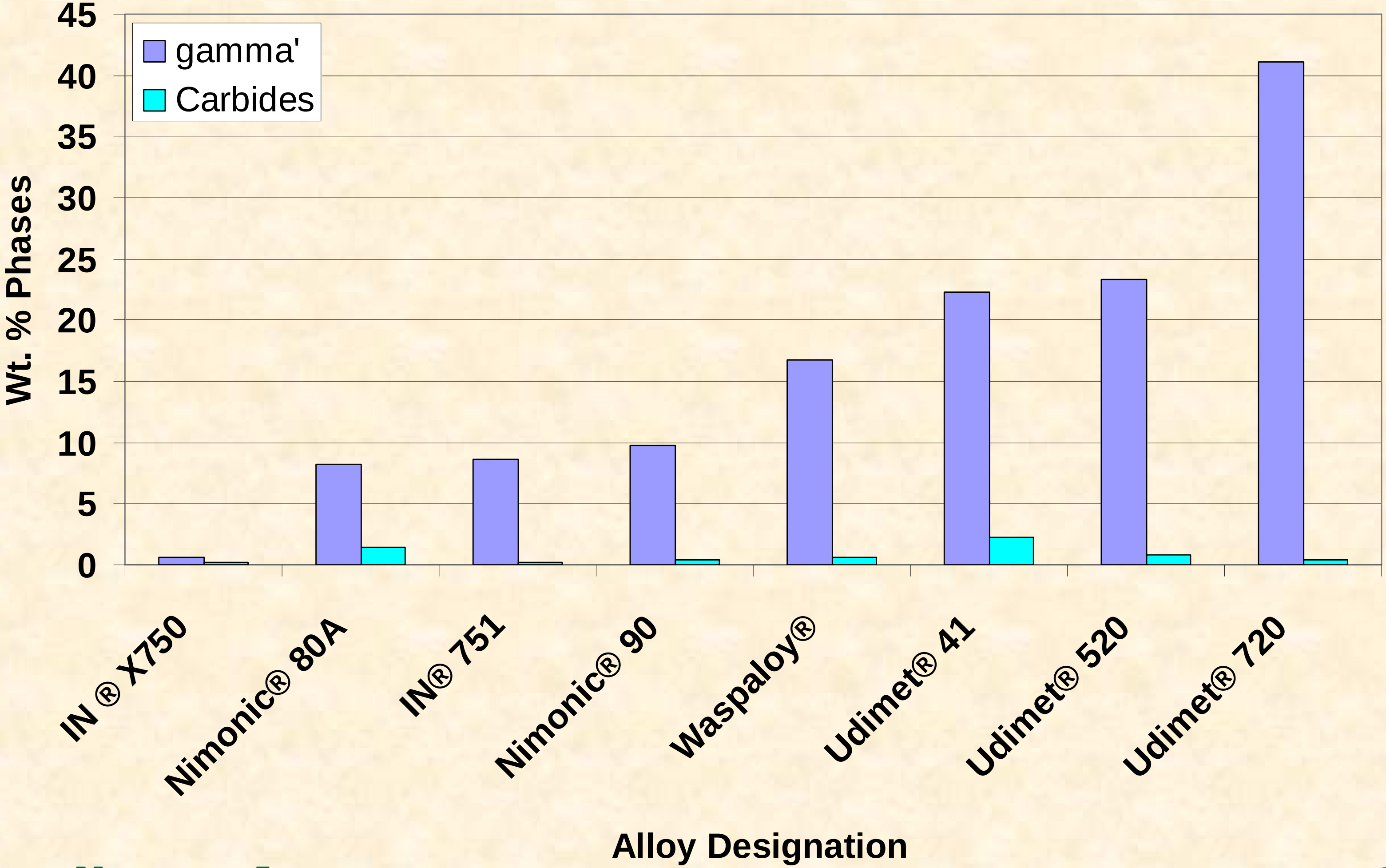


Udimet ® 720

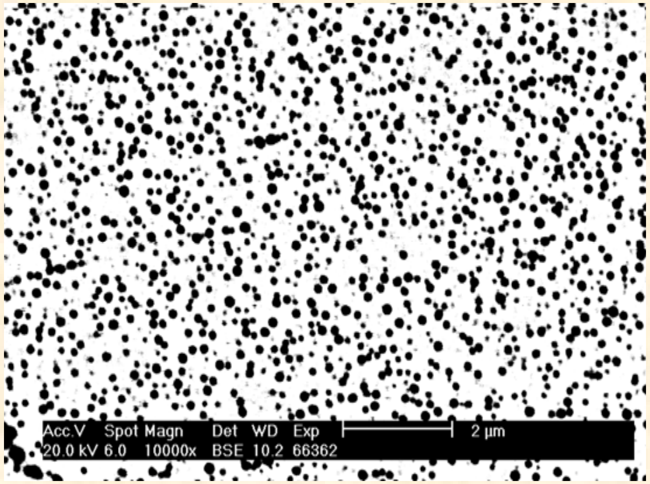


Amount of γ’ and highest temperature of stability of γ’ are affected by alloying element additions

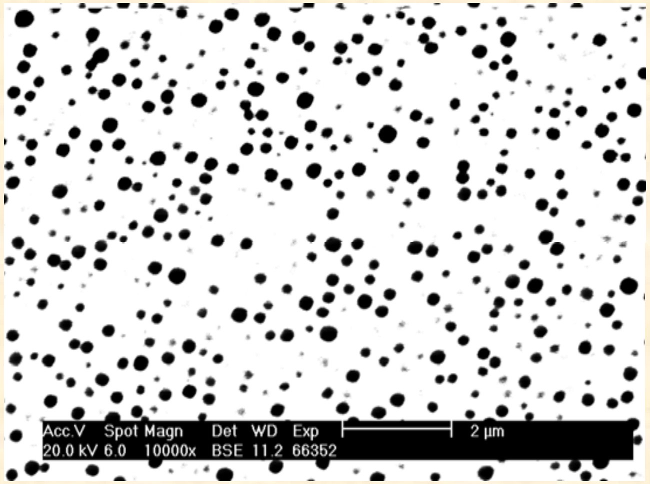
Calculated Major Phase Contents at 870°C Vary Significantly with Alloy Composition



Microstructure of Waspaloy® Shows Reasonable Agreement with Calculations



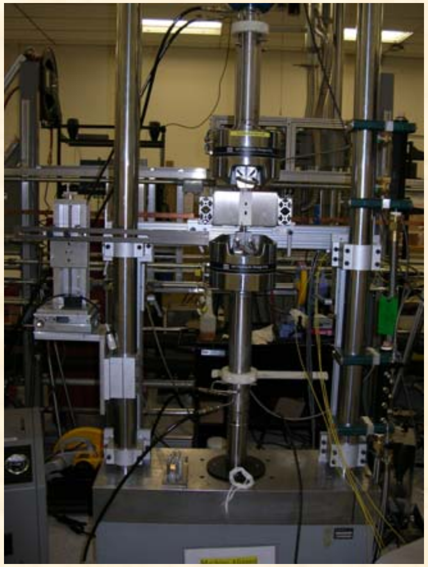
2.4 million cycles
Time: 22 hours
Average V_f=17.1%
D_{Ave}=130.0 nm



55 million cycles
Time: 509 Hours
Average V_f=17.1%
D_{Ave}=189.0 nm

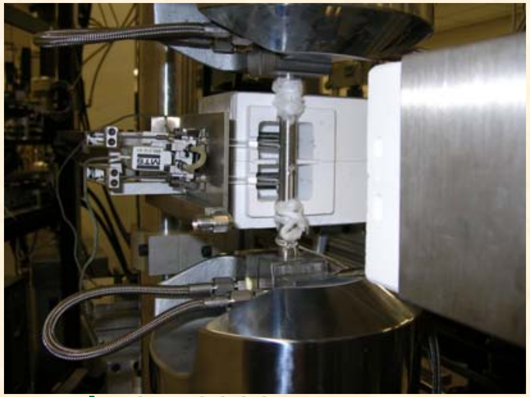
Predicted γ'= 16.7 wt.%

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



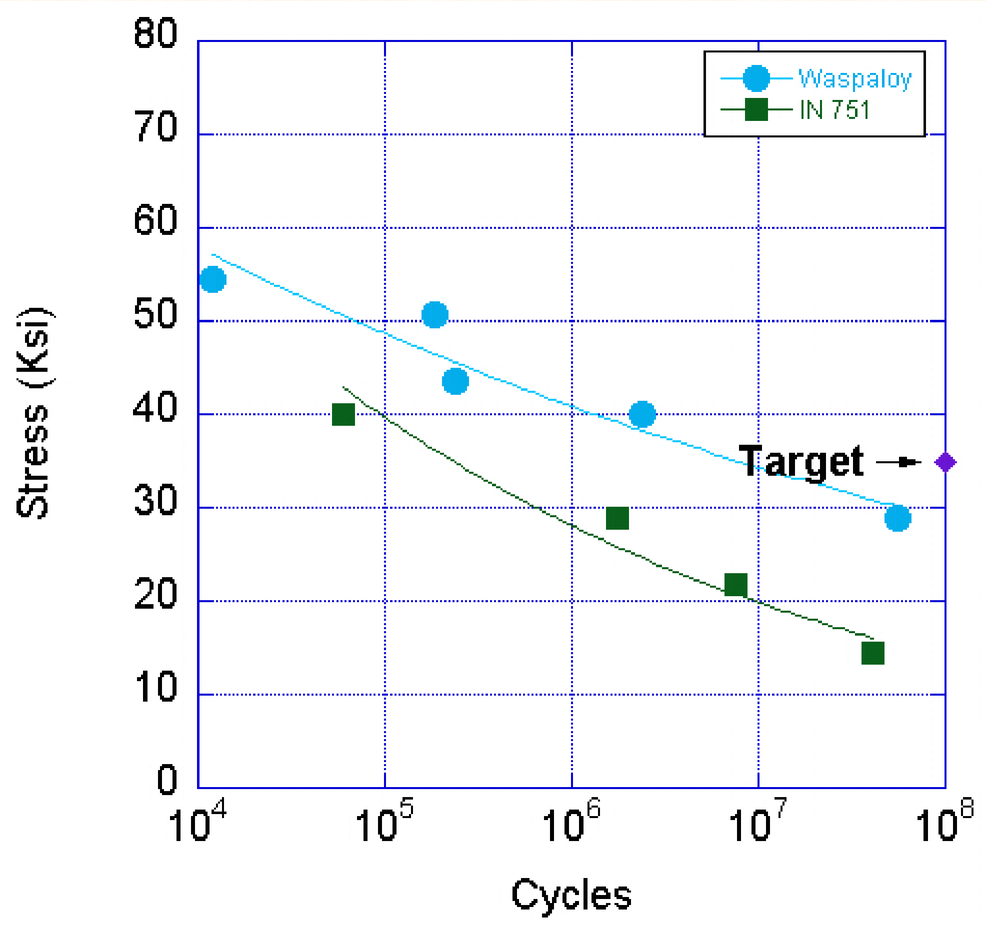
- **Fully reversed fatigue tests are being carried out at temperature of interest under load control**
- **Tests are carried out at frequency of about 30 Hz**
- **Stresses of**
  - **21.8 (150) Ksi (MPa),**
  - **29 (200),**
  - **39.9 (275),**
  - **43.5(300),**
  - **50.8(350),**
  - **54.4(375)**

  are used in the tests



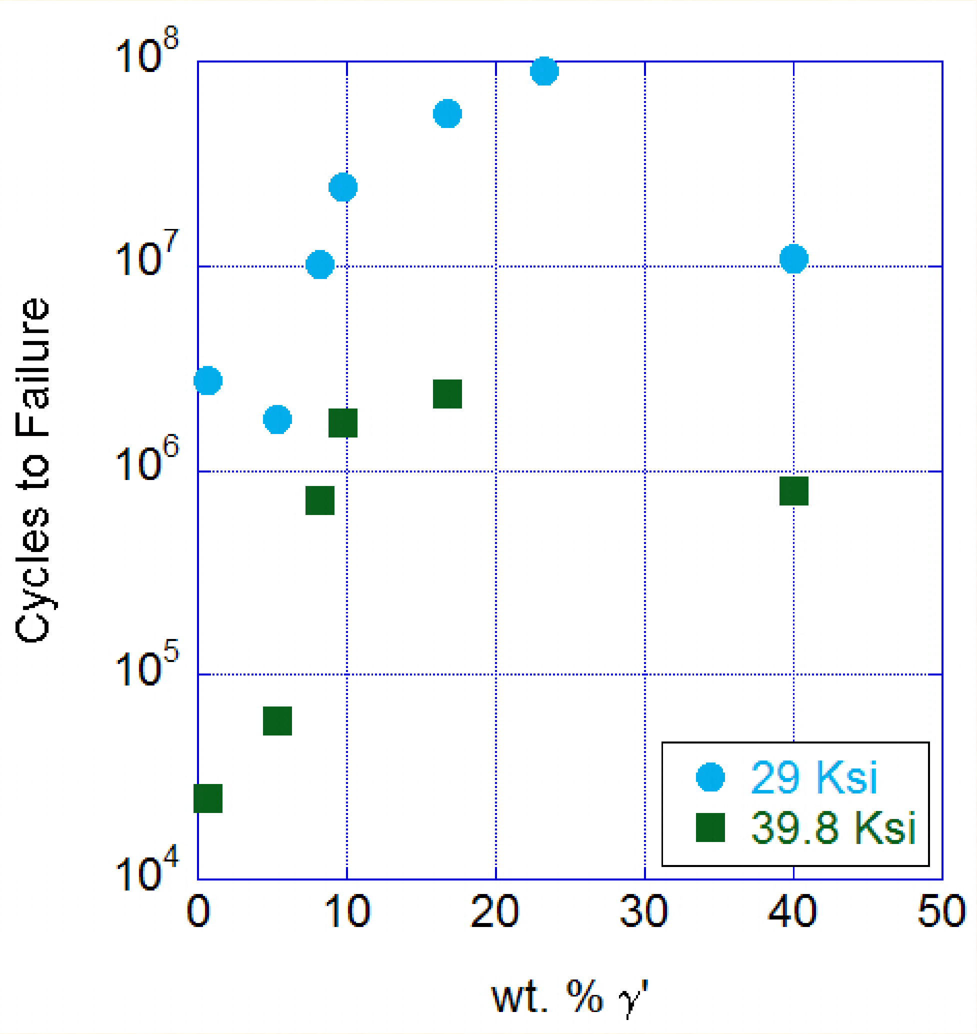
S-N Curves Show Compositions With Better Fatigue Properties

- *In-situ* long term tests (upto $5x10^8$ cycles~5000 hours) provide valuable materials property data for specific alloy compositions



Effect of Strengthening Phase on Fatigue Properties Has Been Established

Fatigue life (cycles to failure) generally increases with calculated strengthening phase contents



Future Work

- Validation of computational models for microstructure prediction will be completed
- Using the correlation established between fatigue property and γ' contents, composition space will be searched with computational thermodynamic models for desirable alloy compositions
  - Milestone for FY '08 is to identify alloy composition/s that have the potential for appropriate performance in valve application
- Anomalous behavior at higher γ' contents will be studied
- Newly identified alloy compositions will be fabricated and high temperature fatigue properties will be evaluated

Technology Transfer

- Discussions on property requirements and property measurements are currently being carried out with
  - Valve manufacturer (Eaton Corporation)
  - Materials supplier (Carpenter Technologies)
- New materials identified/developed will be
  - Tested using alternate techniques appropriate such as rotating beam fatigue
  - Fabricated into prototype valve components and field-tested
- Collaborative effort with GM resulted in development of novel cast iron compositions for exhaust manifolds (patent pending)

Summary

- Improvement in high temperature capability of exhaust valve materials is an enabler for future advanced engine concepts
- Target for improvement are the fatigue properties of exhaust valve materials at 870^{o}C
- Correlations have been established between amount of strengthening phase and fatigue properties
- In the following year, compositions that could potentially meet the target fatigue properties will be identified, fabricated, and tested

Publications, Presentations, Patents

- R. Shah (General Motors), V. K. Sikka, and G. Muralidharan, “Cast irons for high temperature use,” U.S. Patent Application, Filed December 21, 2006
- G. Muralidharan, V. K. Sikka, Rick Battiste, and Bruce Bunting "Advanced Materials Development Through Computational Design," Diesel Engine-Efficiency and Emissions Research Conference 2007, Detroit, Michigan, Aug. 13- 16, 2007
- Santhana K. Eswaramoorthy, James M. Howe, and Govindarajan Muralidharan, “In Situ Determination of the Nanoscale Chemistry and Behavior of Solid-Liquid Systems,” Science, 2007, Vol. 318, p.1437.