Materials for HCCI Engines

G. Muralidharan (PI), Rick Battiste

Materials Science and Technology Division

Bruce Bunting

Engineering Science and Technology Division

Oak Ridge National Laboratory

Oak Ridge, TN

Project ID # PM018

U.S. DEPARTMENT OF ENERGY

OAK RIDGE NATIONAL LABORATORY

MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY

Overview

Timeline

- Project start: March 2005
- Project end: September 2011
- Percent complete: 95%

Budget

- Total project funding Received
  - DOE 100%
- Funding Received in FY10: $225k
- Funding for FY11: $225k

Barriers

Barriers Addressed

- Changing internal combustion engine regimes
- Long lead-times for materials commercialization
- Cost

Targets

- Improve passenger vehicle fuel economy by 25%
- Improve commercial vehicle engine efficiency at least 20%

Partners

- Lead: ORNL

Collaborators/Interactions

- Eaton – Manufacturer of valves
- Carpenter Technologies- Materials Supplier

Relevance and Objectives

- *Improvements in engine efficiency* alone have the potential to increase passenger vehicle fuel economy by 25 to 40 percent and commercial vehicle fuel economy by 30 percent with a concomitant reduction in greenhouse gas emissions, more specifically, carbon dioxide emissions
- *New engine regimes* and *higher performance engines* are required to reach engine efficiency goals while reducing pollutant formation
  - Certain higher performance engines need higher temperature-capable valve materials due to increased exhaust gas temperatures, higher exhaust flow rates, higher cylinder pressures, and/or modified valve timings
- There is a critical need to develop materials that meet projected operational performance parameters but meet *cost constraints*
- **Develop cost-effective exhaust valve materials suitable for operating at higher temperatures (870°C vs. current 760°C) for use in advanced engine concepts**
  - Test current exhaust valve material for fatigue performance at higher temperatures and compare performance with other suitable candidate materials
  - Develop new materials with high temperature stability and fatigue properties appropriate for operation at the higher temperatures based on fatigue data obtained earlier

Milestones

FY 2010

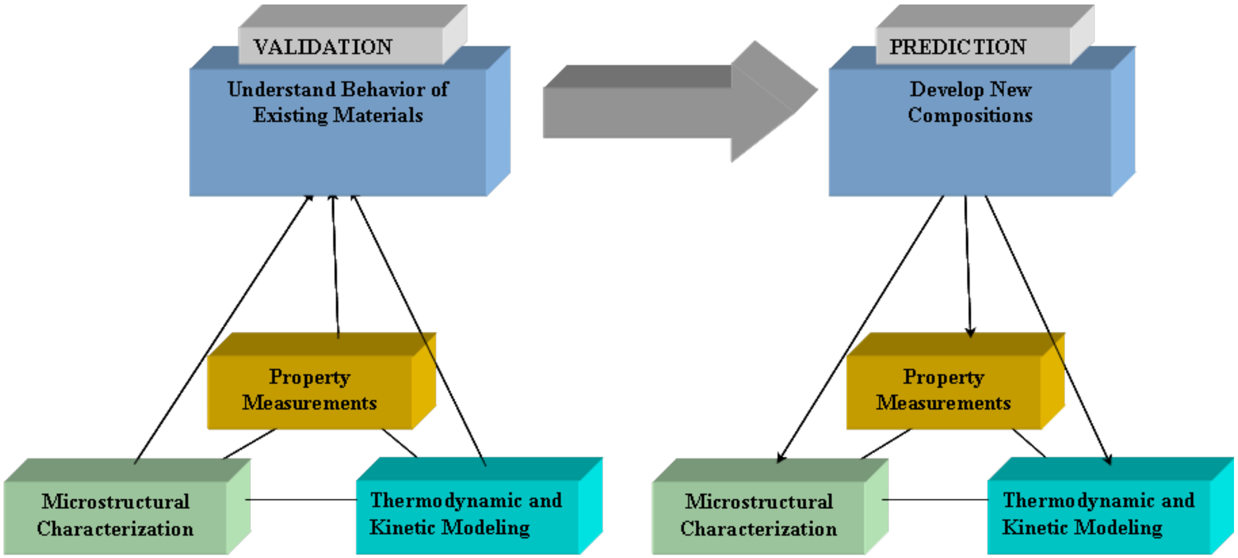
- Complete selection of one commercial alloy and develop one new alloy for high temperature valve application (9/10)
  - Accomplished on time

FY 2011

- Present progress detailing results on the high temperature tensile testing and fatigue testing of new ORNL-developed alloys at the Annual Merit Review
- Identify a path for the further development of exhaust valve alloys (7/2011)

Approach: Materials-By-Design

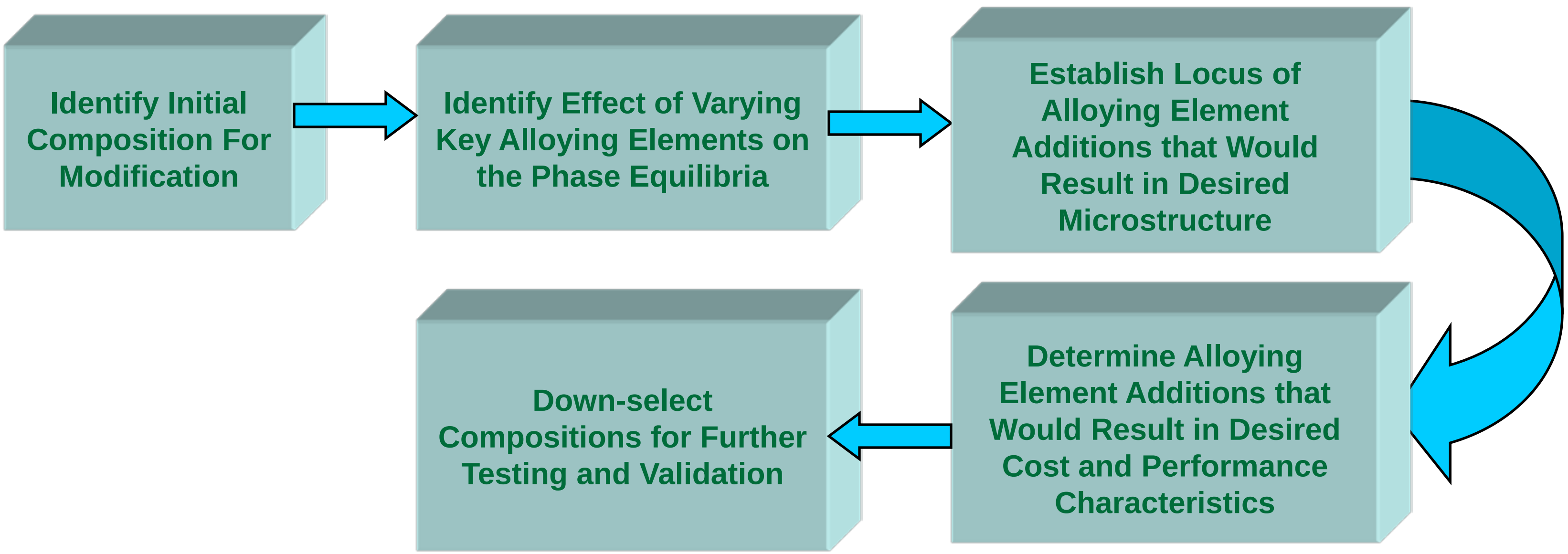
- Identify key material properties of interest for critical components
- Establish correlation between properties of interest and microstructural characteristics using existing alloys to identify desired microstructures
- Search composition space for alloys with desired microstructure and alloying element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



Why are New Alloys Necessary?

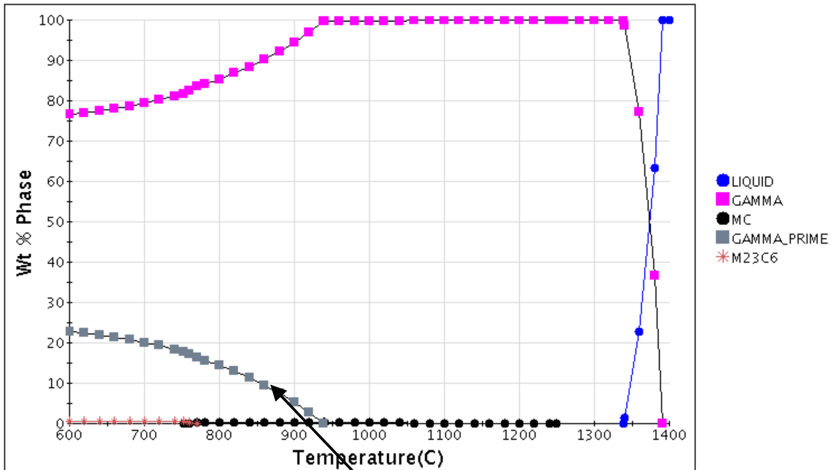
- New alloys are required to
  - Achieve improved performance when compared to existing alloys at same or reduced cost
  - Achieve desired performance while reducing expensive alloying element additions such as nickel and cobalt
  - Achieve manufacturability at low cost
- Alloys have been developed by emulating microstructure of existing desirable alloys
- Target is to improve fatigue life at a temperature of 870ºC, 35Ksi stress while maintaining the lowest possible cost (lowest Ni additions)
  - Commonly used exhaust valve alloy is Alloy 751 which has 71 wt.% Ni and a fatigue life of about 5*10^6 cycles under these conditions

Example Methodology For New Alloy Development

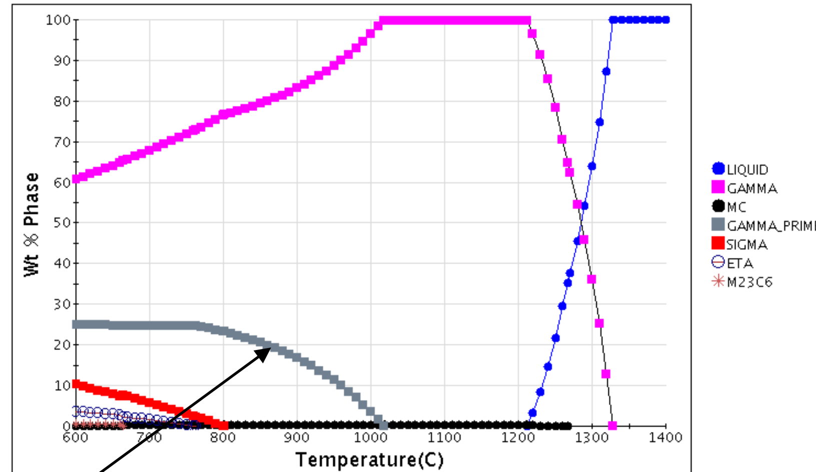


Computational thermodynamic/kinetic modeling allows for rapid identification of new alloys with desired microstructure, and alloying element characteristics

Computational Thermodynamics Predictions are Used to Guide Alloy Development



Phase Equilibria Predicted in Existing Commercial Alloy: X751 (Has 71 wt. % Ni)



Phase Equilibria Predicted in A New Alloy: HCCI-9 (Has 40.4 wt. % Ni)

Primary Strengthening Phase (γ') is Predicted to be Present in Larger Amounts in HCCI-9 at 870ºC

Phase equilibria predictions are used to estimate amount of strengthening phases (γ' and carbides(MC and $M_{23}C_6$)) as a function of alloying element additions

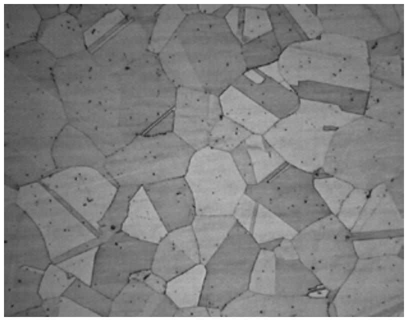
Technical Accomplishments and Progress: New Alloys with Potential to Perform at Higher Temperatures Have Been Developed

- Thermodynamic and kinetic modeling has been performed to correlate compositions with microstructure in selected commercial alloys
- Microstructural characterization has been carried out to verify specific computational predictions of microstructure
- High temperature fatigue properties using fully reversed fatigue tests have been obtained from alloys with well-defined compositions, heat-treatments, and microstructure
  - Relationship between rotating beam fatigue data (required by the industry) and fully reversed fatigue data has been developed
  - Desirable microstructures have been identified
- Several commercial alloys with the desired microstructure have been identified and performance has been verified using rotating beam fatigue tests
- Several new alloys with lower Ni+Co contents (reduced to ~40-50 wt.% from 70-85 wt.%) with desirable microstructures have been designed and fabricated

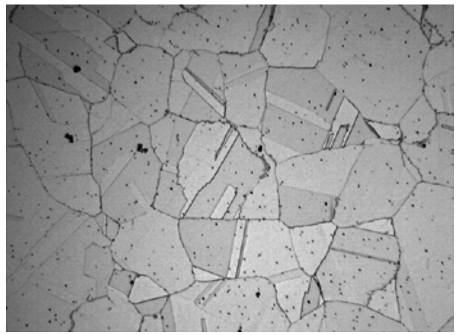
Technical Accomplishments: FY 11

- Computational modeling was carried out along several composition schemes to identify new alloy compositions with comparable/better properties with cost benefits
- Three revisions of alloy development have been accomplished so far in FY11
  - Air melt of three alloys (HCCI-9, HCCI-16, HCCI-17) computationally identified in FY10 were prepared; two alloys were rolled, and tensile and fatigue properties have been tested at 870^{o}C
  - A second batch of alloys (a total of three additional alloys) have been cast, rolled, tensile tests have been completed, and fatigue tests have been initiated
  - A third batch of alloys (a total of an additional three alloys) have been cast, rolled, and are being prepared for testing
- Fatigue tests have shown that the alloys with the lowest Ni + Co (about 40 wt.%) do not have much ductility, and do not have required fatigue properties at 870^{o}C although their tensile strengths are high
- Second batch of alloys show promising characteristics- high yields strengths, and improved ductility at 870^{o}C and better fatigue properties at 870^{o}C
- Further refinement of alloy compositions will be accomplished in remainder of FY11

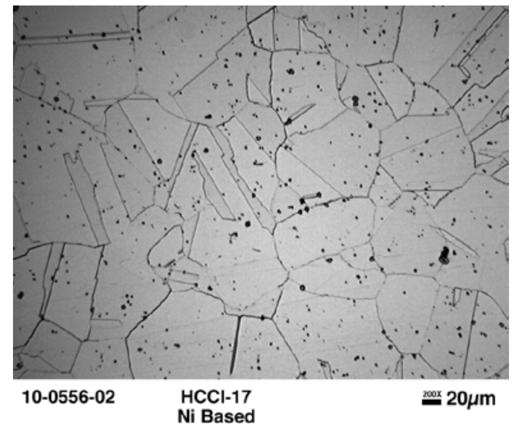
Technical Accomplishments: An Initial Set of Three Alloys were Selected for Preparation of Larger Heats for Fatigue Testing



HCCI-9
0.2% YS at 870^{o}C= 63.4 Ksi
Plastic Strain at Break= 0.35%
Ni+Co~41.9 wt. %



HCCI-16
0.2% YS at 870^{o}C= 71.5 Ksi
Plastic Strain at Break= 2.26%
Ni+Co ~ 41.3 wt. %



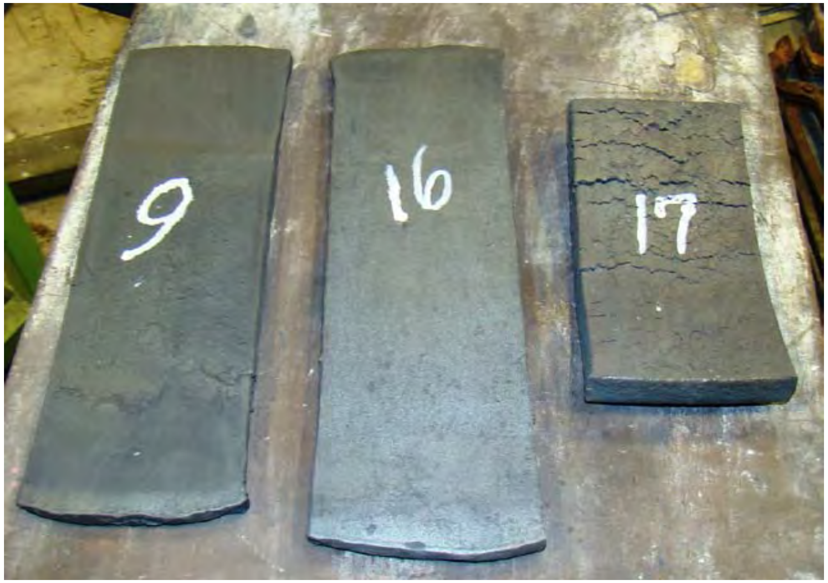
HCCI-17
0.2% YS at 870^{o}C= 63.1 Ksi
Plastic Strain at Break= 14.42%
Ni+Co ~ 36.7 wt. %

Alloys show very limited ductility at 870^{o}C but yield strengths comparable to commercial Ni-based alloys YS at 870^{o}C= 40-80Ksi*

*L. M. Pike, Superalloys 2008, pp.191-200

Technical Accomplishments: Two Large Heats of Alloys Were Cast and Successfully Fabricated into Plates For Specimen Machining

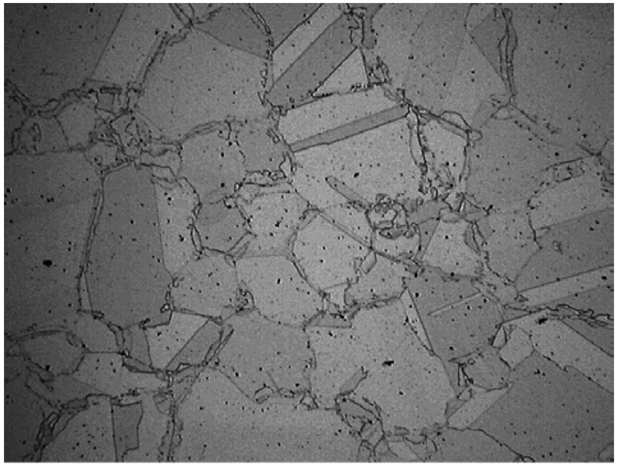
Cast



Rolled

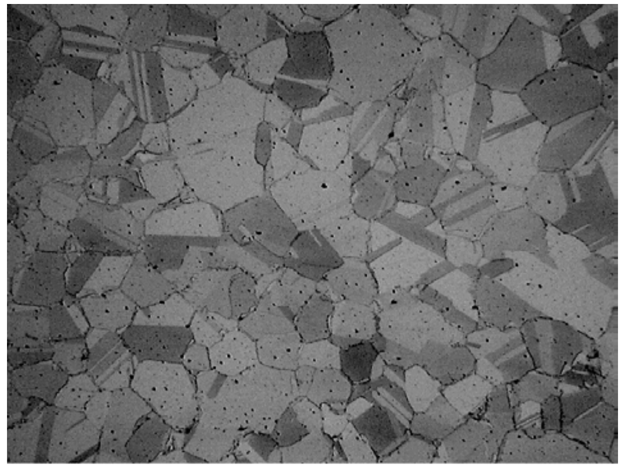
Alloys 9 and 16 were effectively rolled at high temperatures while 17 cracked during rolling

Technical Accomplishments: Three New Alloys Have Been Designed with Higher Nickel Contents



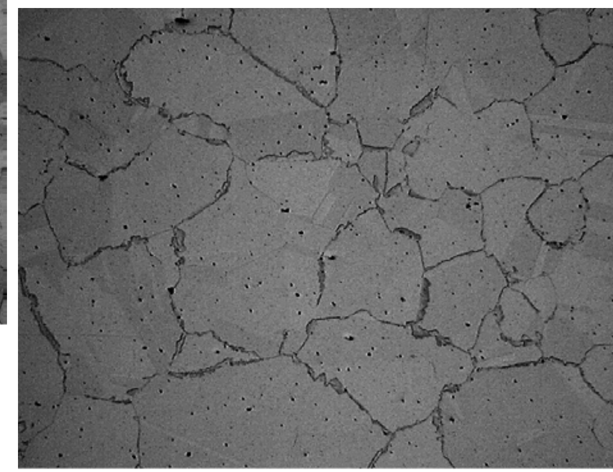
10-1935-01 HCCI-20 50X 100μm

HCCI-20
0.2% YS at 870°C= 54.5 Ksi
Plastic Strain at Break= 19.29%



10-1936-01 HCCI-34 50X 100μm

HCCI-34
0.2% YS at 870°C= 61.2 Ksi
Plastic Strain at Break= 11.85%

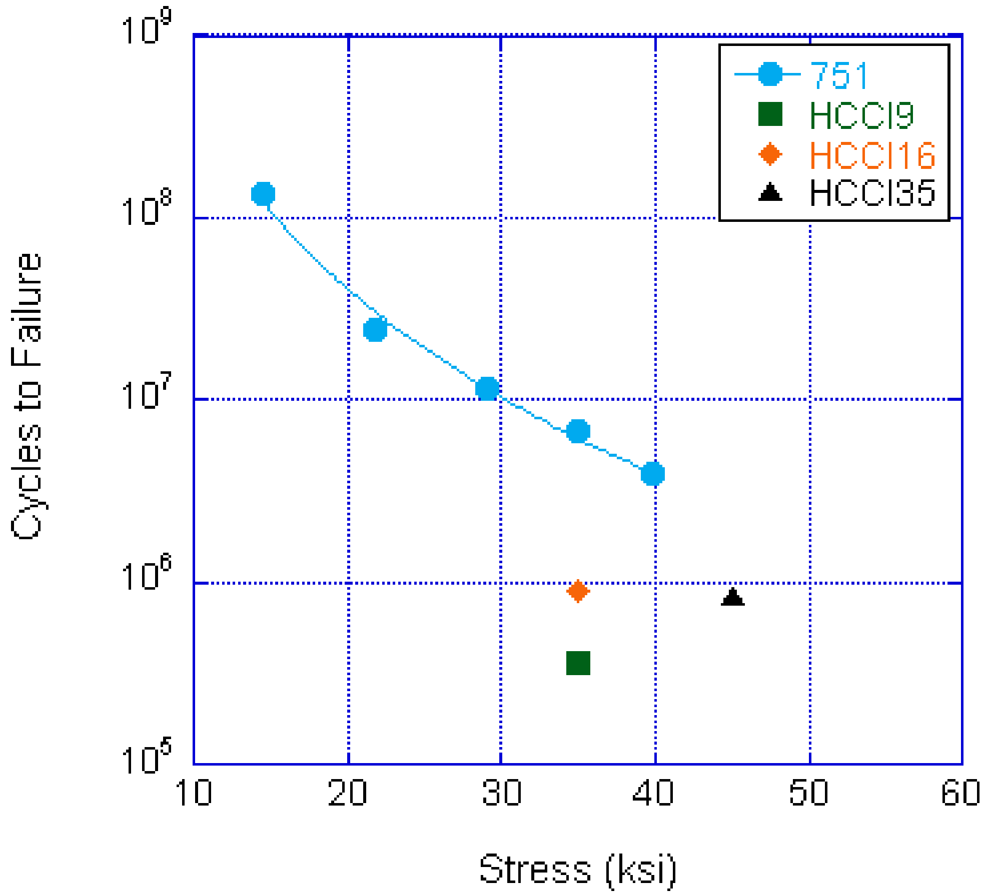


10-1937-01 HCCI-35 50X 100μm

HCCI-35
0.2% YS at 870°C= 60.5 Ksi
Plastic Strain at Break= 11.89%

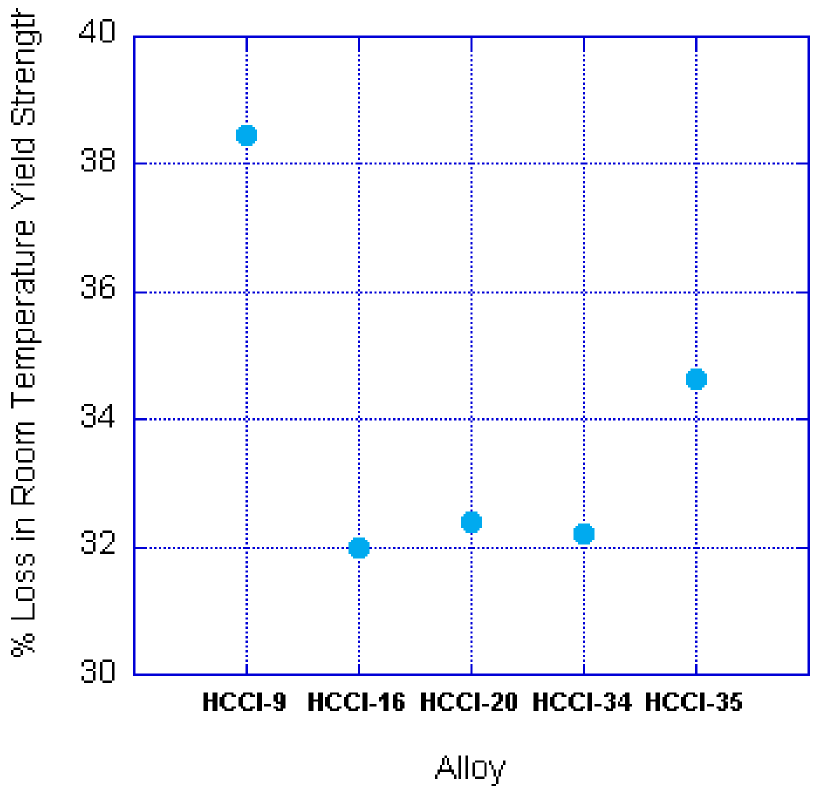
- Primary strengthening phase: γ’
- Alloys show greater ductility combined high yield strengths at 870°C

Rotating Beam Fatigue Tests Show Improved Properties of HCCI-35



Further improvements in alloy performance are required to surpass existing high-Ni alloys such as 751 which contains 71 wt.% Ni

Technical Accomplishments: Long-term Aging at 870ºC for 216 Hours Shows Evidence of Coarsening

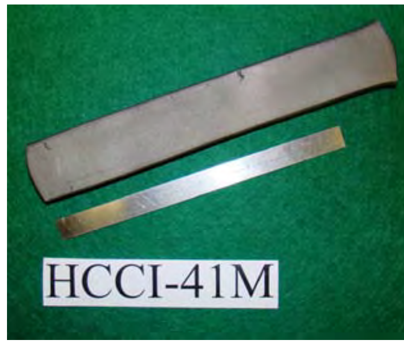


- Alloy HCCI-9 shows a greater loss than HCCI-16 consistent with observation on fatigue properties
- Achieving slower coarsening rates will improve alloy fatigue performance at 870ºC

Technical Accomplishments: A Third Batch of Alloys Has Been Prepared, Successfully Rolled and Specimens Will be Machined Shortly

Cast and Annealed

Rolled



~40.3 wt. % Ni

~44.8 wt. % Ni

~44.3 wt. % Ni

Alloys have higher Nickel levels (max of 44.8 wt. %) along with additional strengthening

Collaborations and Coordination with Other Institutions

- Suggestion have been sought from Carpenter on potential paths for alloy development
- Periodic discussions are carried out with Eaton Corporation regarding range of alloying elements that are desired (Ni Vs. Fe), formability characteristics, and along with mechanical property requirements as a function of temperature
- A follow-on project with 50% matching industrial cost share has been proposed with Eaton Corporation to improve alloys and commercialize the compositions in valve applications
  - Accelerates commercialization of new materials technologies

Future Work

FY11

- Complete rotating beam fatigue and fully reversed fatigue tests on the newly fabricated alloys
- Prepare atleast three additional alloys with modified compositions and complete tensile and fatigue tests
  - Nickel levels will be increased as needed
  - Amount of strengthening phases will be increased
- Recommend path for refining alloy compositions for follow-on CRADA work based on fatigue properties measured from the newly developed alloys to obtain target of fatigue life at 870^{o}C
- Complete initial microstructural characterization of selected alloy/s

Summary

- Improvement in high temperature capability of exhaust valve materials is an enabler for future advanced engine concepts with higher efficiencies
- Targets for improvement are the fatigue properties of exhaust valve materials at 870^{o}C with improved performance/cost ratio
- Several commercial alloys with potential for improved performance at the higher temperature have been identified based on microstructural characteristics and performances have been verified using rotating beam tests
- Based upon feedback from initial fatigue tests of experimental alloys and the "Materials-by-design approach", several new alloys with the potential for improved performance/cost ratio have been developed using computational modeling techniques