High Temperature Materials for High Efficiency Engines

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U.S. DEPARTMENT OF ENERGY

OAK RIDGE NATIONAL LABORATORY
MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY

Overview

Timeline

- Project start: September 2013
- Project end: August 2016
- Percent complete: 15.0%

Budget

- Total project funding Received
  - DOE 100%
- Funding Received in FY14: $200k (anticipated)

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

Interactions/Discussions with:

- Carpenter Technologies- Materials Supplier
- Caterpillar

Oak Ridge National Laboratory

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 carbon dioxide emissions
- Exhaust gas temperatures are expected to increase in future high efficiency engines
  - **Temperatures are expected to increase from 870°C to 950°C in 2025 and to 1000°C by 2050* in light-duty vehicles and from 700°C to 900°C by 2050 in heavy duty vehicles****
  - Discussions with OEMs show that temperature limitations of current valve materials may already be limiting engine efficiencies in some designs
- There is a critical need to develop materials that meet projected operational performance parameters but meet ***cost constraints***
- **Objectives: Develop cost-effective exhaust valve materials suitable for operating at temperatures up to 950°C for use in advanced future engine concepts**
  - Develop new materials with high temperature stability, oxidation resistance, and fatigue properties appropriate for operation at the higher temperatures using a computationally guided approach

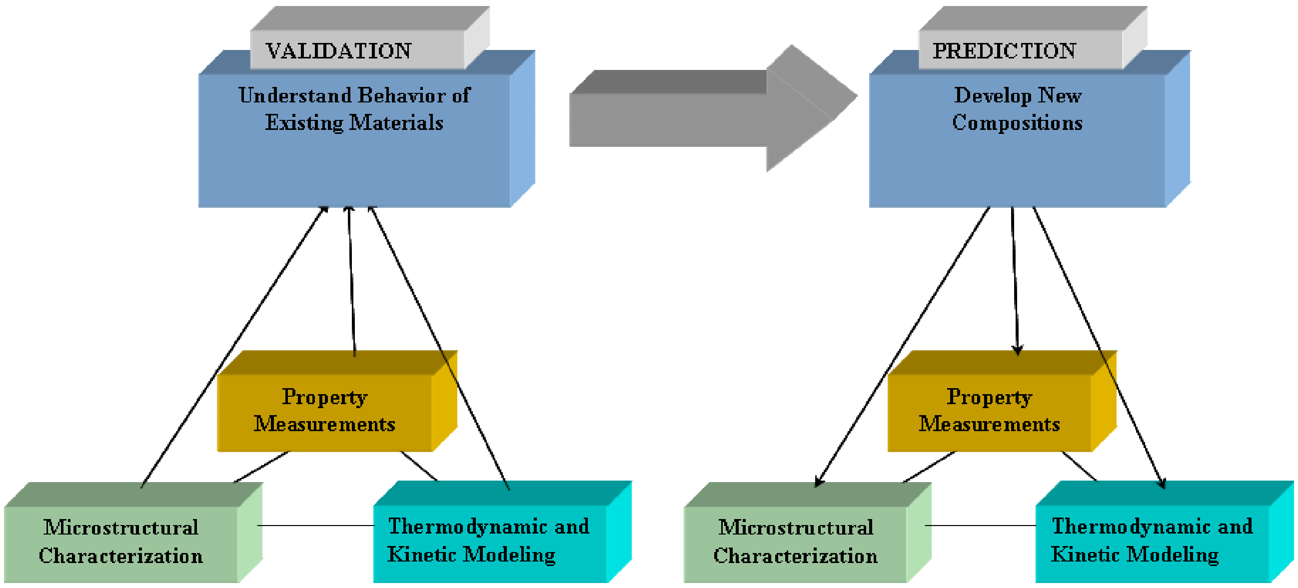
FY14 Milestones

Month/ Year	Milestone/ Go-No Go Decision	Description	Status
Dec. 2013	Milestone	Complete an initial evaluation of effect of composition on oxidation resistance at 800ºC	Complete
March 2014	Milestone	Identify initial target composition range of new alloys for desired oxidation resistance	Complete
June 2014	Milestone	Evaluate the effect of increasing temperatures on strength of selected alloys up to 900ºC	On Track
Sept. 2014	Milestone	Identify initial target microstructural constituents (strengthening phases) for new Ni-based alloys up to 900ºC	On Track

Approach: Integrated Computational Materials Engineering (ICME) -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 for ICME
- Search composition space for alloys with desired microstructure and alloying element additions using validated ICME models

Validated ICME Models are Used to Predict New Alloy Compositions



Approach has been successfully used to develop cost-effective valve alloys for use at temperatures up to 870°C

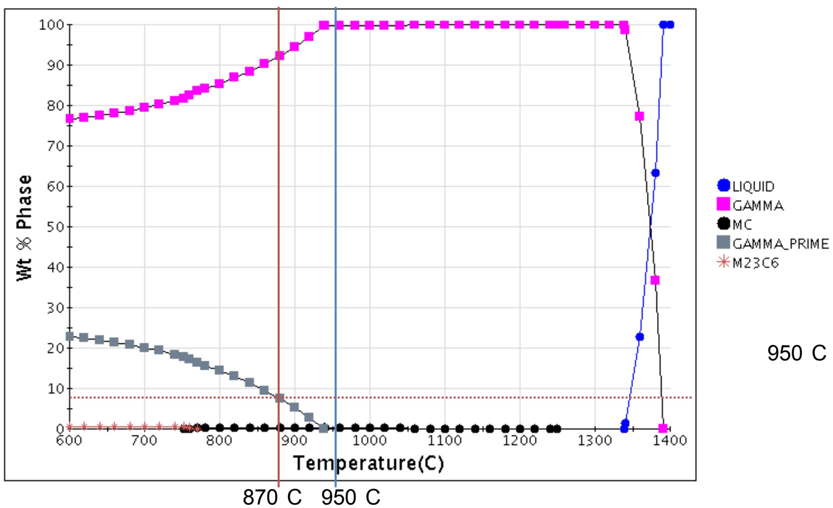
Why are New Alloys Necessary?

- **Current baseline commercial valve alloy 751 is** a high-Ni superalloy (71%Ni, 16 % Cr, 8 %Fe, 1.2%Al, 2.56%Ti, 0.86%Nb, 0.03%C) all in wt. %
  - Primarily strengthened by coherent, intermetallic precipitates- γ' ($Ni_3(Al,Ti,Nb)$)
  - Does not have significant strength at 950°C due to potential dissolution of strengthening phase
- Other traditional Ni-based alloys used in aerospace applications are very expensive due to high Ni and other expensive alloying element contents
- Reliability requirements for Ni-based alloys in automotive valve applications are lower compared to aerospace applications due to lower life expectations
  - Challenge is to achieve desired performance while reducing expensive alloying element additions such as Ni and Co
- **Target is to achieve high cycle fatigue life comparable to a target high Ni alloy at a temperature of 950°C, while maintaining at least 15% lower cost (lower Ni levels)**
  - **At 950°C, oxidation resistance is also anticipated to play an important role in a water-vapor containing environment such as exhaust gases**

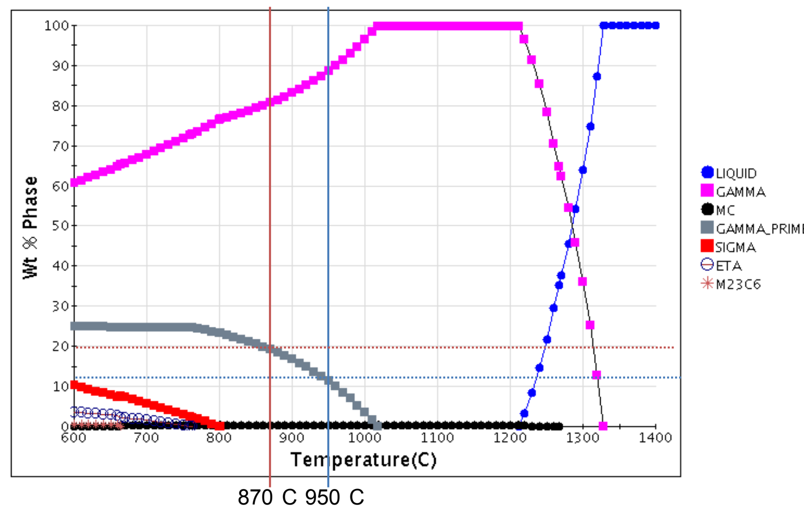
Computational Thermodynamics Predictions are Used to Guide Alloy Development

Two major steps are anticipated in new alloy development:

- Oxidation testing will be performed to identify alloying element additions required for desirable oxidation resistance at temperatures up to 950°C
- Computational modeling will be used to identify alloy compositions with lower Ni levels but with high enough γ' content for required strength

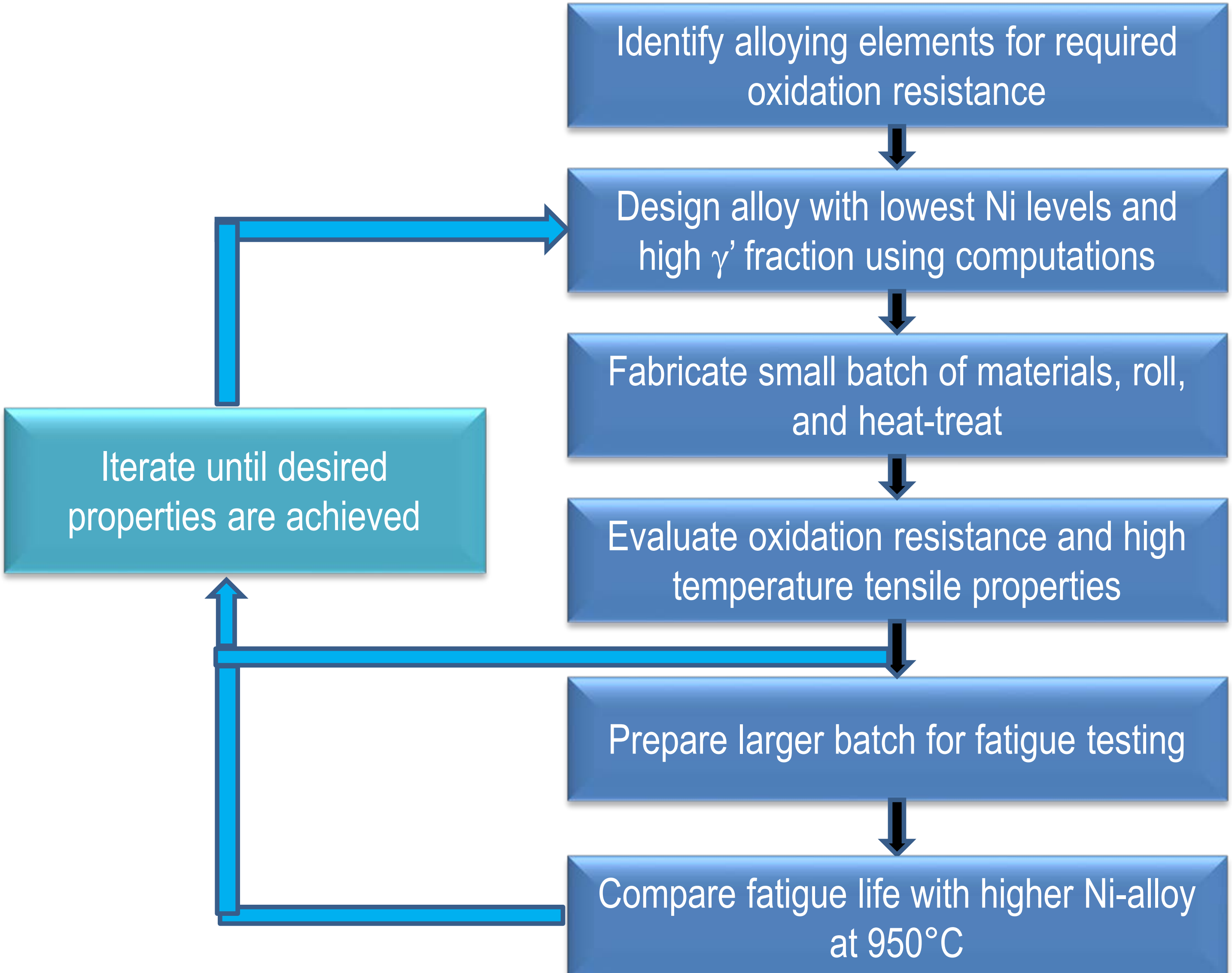


Phase Equilibria Predicted in Existing Commercial Alloy 751 Shows Dissolution of Strengthening Phase at 950°C



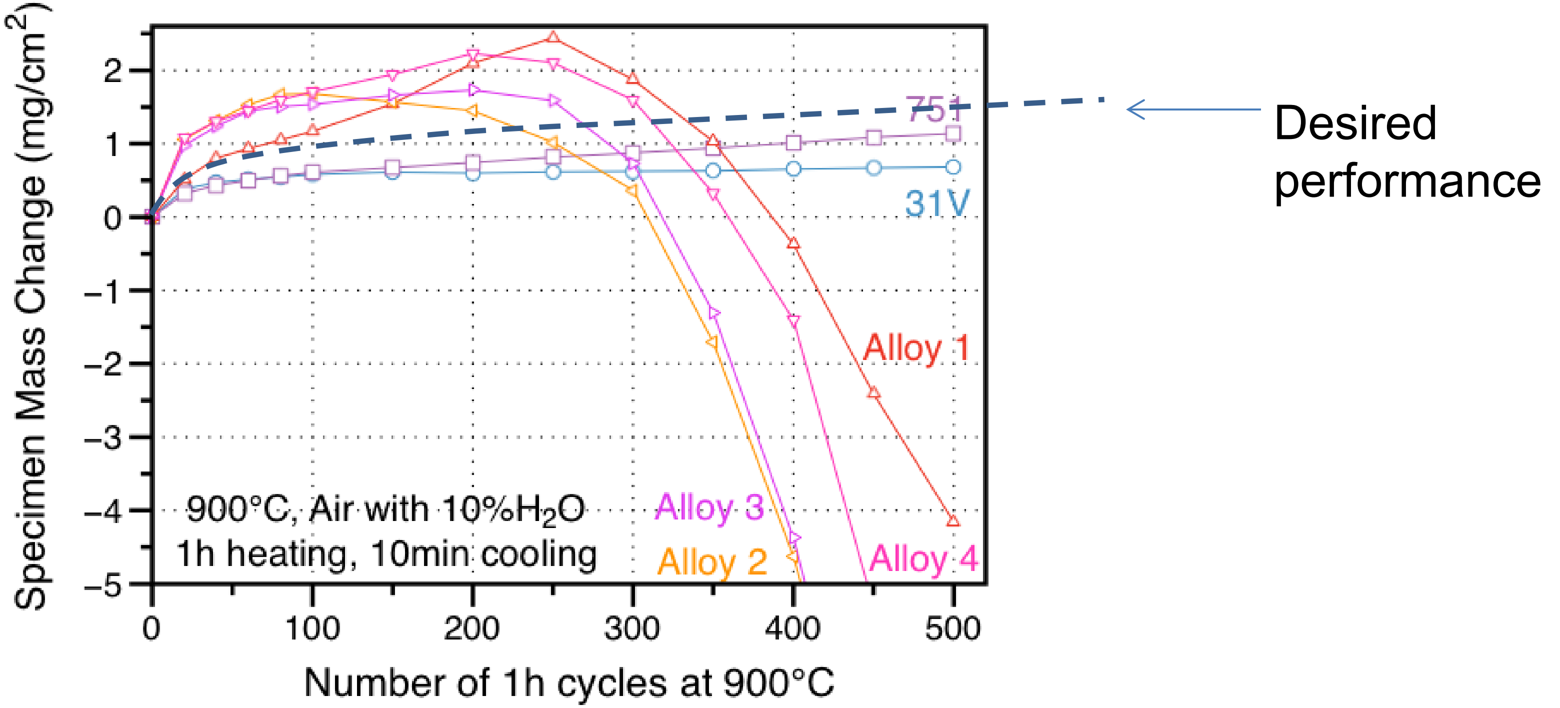
Phase Equilibria Predicted in an ORNL Alloy Shows Presence of Strengthening Phase at 950°C

Example ICME-Based Methodology For New Alloy Development



Accomplishments and Progress: Initial Oxidation Testing Has Been Performed on Several Alloys at 900°C to Identify Composition Effects (Milestone 1)

- **Oxidation tests have been performed in a Air + 10% water vapor environment**
  - **Environment may be harsher than actual exhaust gas but is expected to indicate correct trends with alloy composition**



- Alloys 1 – 4 are high strength ORNL alloys, arc cast in inert gas
- Alloy 751, and 31V are commercial alloys typically processed using triple vacuum processing with low impurity levels

Accomplishments and Progress: Initial Effect of Composition Has Been Evaluated and New Alloys Have Been Identified

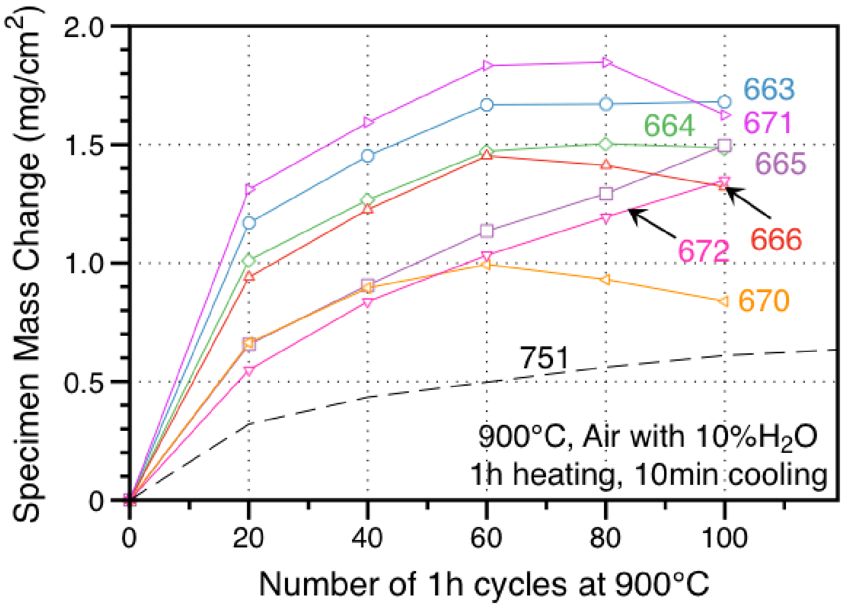
- Two potential causes have been identified for poorer oxidation performance of ORNL alloys at longer times
  - Low Cr/(Fe+Ni) ratio
  - Excessive impurity levels in starting material
- Three parallel paths are being evaluated to improve oxidation resistance
  - Seven new alloys with higher Cr/Ni ratios have been identified, cast and processed at ORNL (Milestone 2)
  - Improved purity feedstock is being procured for future heats
  - Two alloy compositions are being processed by Carpenter Technologies, adopting processing techniques designed for manufacture of higher purity Ni-based superalloys

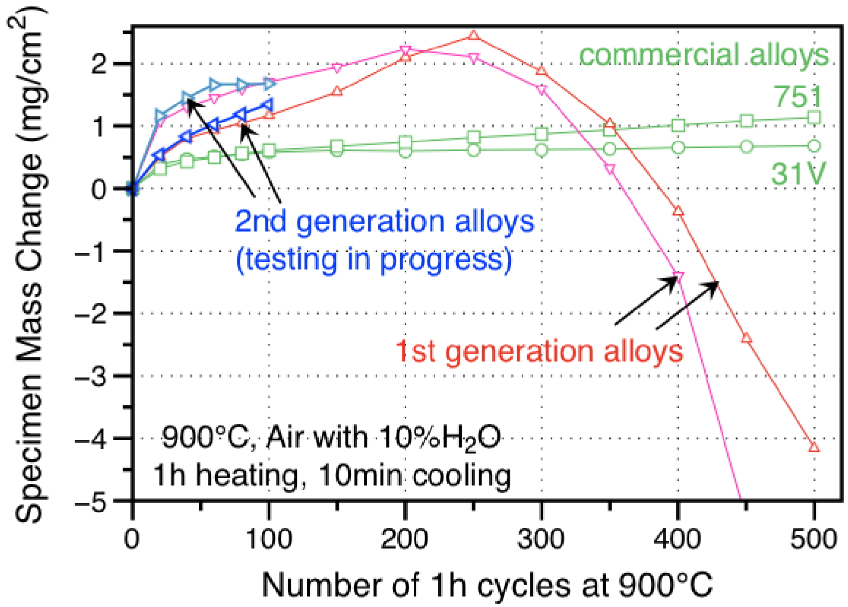
Accomplishments and Progress: New Alloys Have Been Processed using Arc-Casting, and Rolling

Arc cast

Rolled

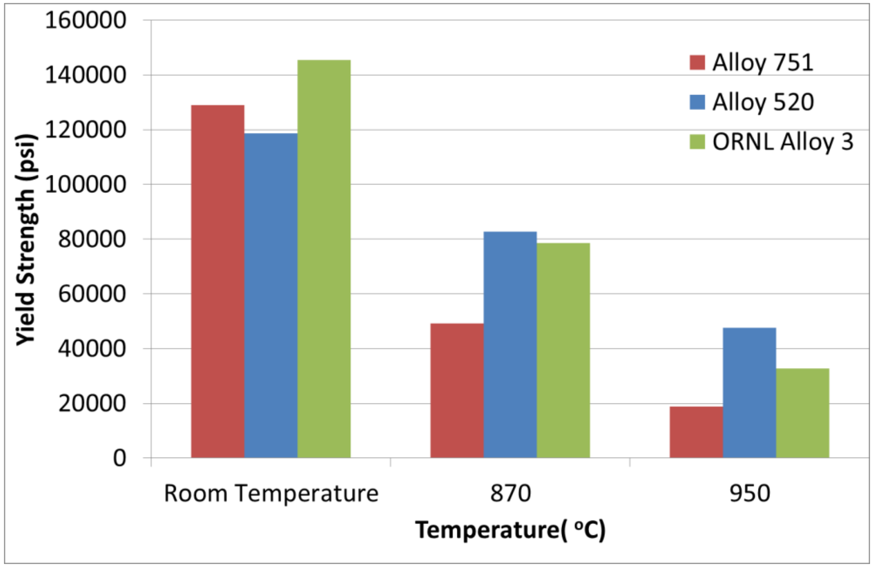
Accomplishments and Progress: Oxidation Tests on New Alloys are On-going in Air + 10% water vapor environment at 900°C

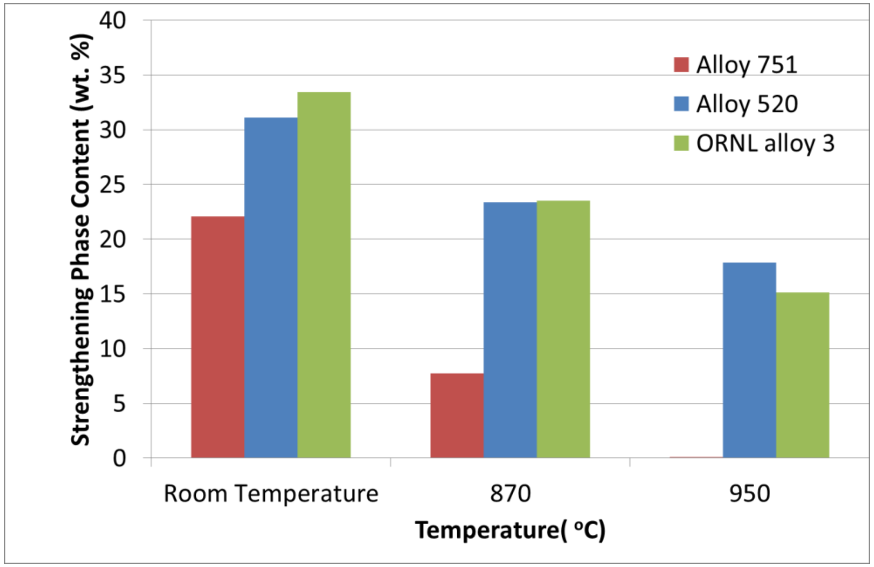




- Early stage data shows that some new alloys may perform better than ORNL alloys 1-4
- Further improvements are required to achieve oxidation resistance levels of higher Ni alloys

Accomplishments and Progress: TemperaturemDependence of Strengths Has Been Measured for Selected Commercial and ORNL Alloys to Evaluate Effect of Strengthening Phases





Alloy 751: 71 wt. %(Ni +Co), Alloy 520 : 68.3 wt. % (Ni+Co), ORNL alloy 3: < 60 wt. % Ni+Co

- ORNL alloy has a higher yield strength than alloy 751 at high temperatures
- Yield strength of ORNL alloy developed for use at 870°C shows a more rapid decrease between 870°C and 950°C when compared to Alloy 520
- Increase in amount of strengthening phase is required to achieve yield strength of alloy 520 and other higher Ni alloys at temperatures greater than 870°C

Response to Reviewer’s Comments

- This is a new project

Collaborations and Coordination with Other Institutions

- Collaborations are on-going with Carpenter Technologies (industry)
  - Two heats are being produced for property evaluation
- Conversations have been held with Caterpillar (industry) about needs and potential future collaborations for valve manufacture and testing
- Discussions have also been held with Cummins on potential collaborations
- Several discussions were held with OEMs at the 2014 SAE World Congress about potential collaborations (industries)

Remaining Challenges and Barriers

- Oxidation resistance at temperatures up to 950°C has to be improved to be comparable to alloy 751 and other higher Ni alloys
- Strength levels at temperatures up to 950°C have to be improved by increasing strengthening phase content without degrading oxidation resistance
- Microstructural stability must be evaluated and optimized to achieve desired fatigue life at temperatures up to 950°C
- Material production should be scaled up after properties are achieved

Proposed Future Work

FY14

- Complete evaluation of oxidation resistance of new alloys at 900°C up to 500 hours
- Complete tensile tests of additional baseline alloys to establish microstructure desirable for achieving yield strength target of high-Ni alloy at 900°C
- Evaluate microstructural stability and degradation of strength at 900°C of high-Ni alloy and establish fatigue life target

FY15

- Design, fabricate, and test a revised batch of alloys that have the potential to meet oxidation resistance targets at temperatures up to 900°C
- Design, fabricate and test new alloys that have the potential to meet yield strength targets at temperatures up to 900°C
- Identify and downselect alloys that have the potential to meet fatigue life targets at 900°C

Summary

- **Relevance:**
  - Temperatures are expected to increase from 870°C to 950°C in 2025 and to 1000°C by 2050* in light-duty vehicles and from 700°C to 900°C by 2050 in heavy duty vehicles. Current valve alloy cannot meet strength requirements and new cost-effect materials are needed for use at these temperatures
- **Approach/Strategy:**
  - A computationally guided approach will be used to develop new lower Ni-alloys with high temperature stability, oxidation resistance, and fatigue properties required for operation at temperatures up to 950°C. Similar approach has been used previously to develop new cost-effective alloys for use at temperatures up to 870°C
- **Accomplishments:**
  - Initial oxidation tests at 900°C have been completed for several high strength alloys developed by ORNL and the need for improved oxidation resistance was identified. New alloys with the potential to have improved oxidation resistance have been designed, fabricated, and oxidation tests are on-going. Initial results are promising. Tensile tests have been completed on selected baseline and ORNL alloys at temperatures up to 950°C and relationships between strength and microstructure of alloys will be used to design improved alloys
- **Collaborations:**
  - Collaborations are on-going with Carpenter Technologies
- **Proposed Future Work:**
  - Results from oxidation and tensile tests will be used to related composition and microstructures of alloys to properties. New alloys with microstructures capable of achieving desired mechanical properties at temperatures up to 900°C will be designed