High Temperature Materials for High Efficiency Engines

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Project ID # PM053

This presentation does not contain any proprietary or confidential information

Overview

Timeline

- Project start: September 2013
- Project end: August 2016
- Percent complete: 50%

Budget

- Total project funding Received
  - DOE 100%
- Funding Received in FY14: $330K

  FY15: $ 0K (pending)
- Funding anticipated

  FY15: $ 190K

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

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 affordable new materials with high temperature strength, oxidation resistance, and fatigue properties appropriate for operation at the higher temperatures using a computationally guided approach

*DOE Vehicle Technologies Workshop report: Light-Duty Vehicles Technical Requirements and Gaps for Lightweight and Propulsion materials, Feb. 2013
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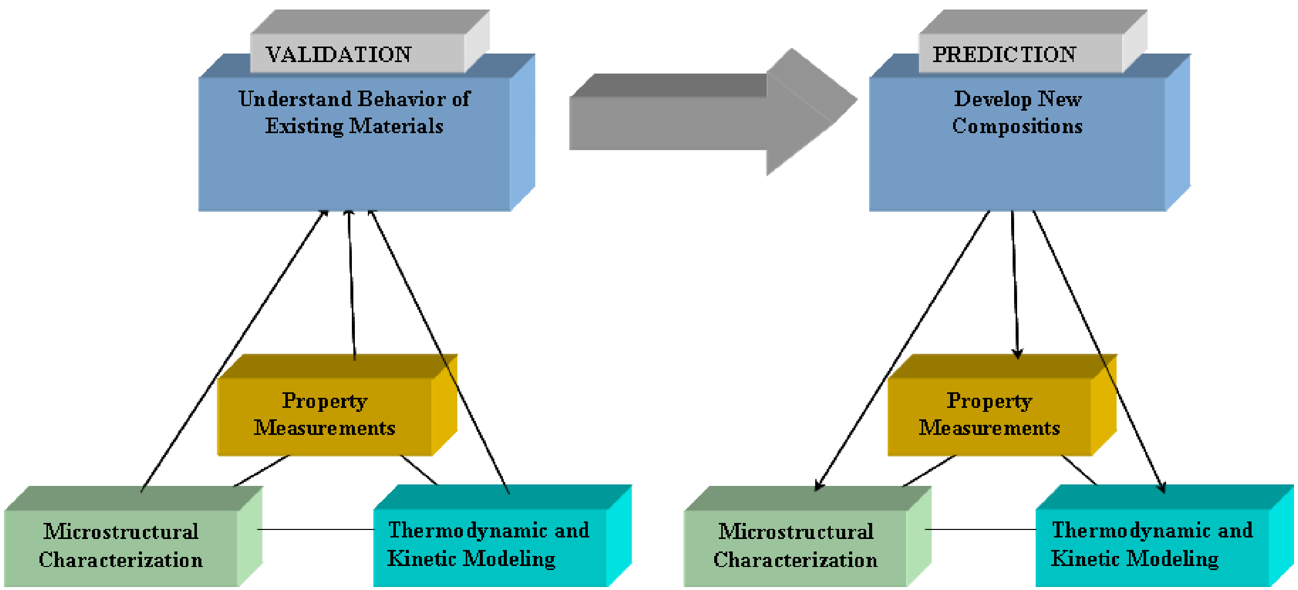
FY14-FY15 Milestones

Month/ Year	Milestone/ Go-No Go Decision	Description	Status
June 2014	Milestone	Evaluate the effect of increasing temperatures on strength of selected alloys up to 900ºC	Complete
Sept. 2014	Milestone	Identify initial target microstructural constituents (strengthening phases) for new Ni-based alloys up to 900ºC	Complete
Dec. 2014	Milestone	Evaluate oxidation resistance and high temperature strength properties of large scale heats fabricated by commercial manufacturer	Complete
March 2015	Milestone	Identify initial target composition range of new alloys for desired oxidation resistance	Complete
June 2015	Milestone	Complete oxidation testing and tensile testing of alloys prepared in laboratory scale at temperatures up to 950ºC	On Track
Sept. 2015	Milestone	Down-select atleast two promising alloys for processing large scale heats with strength and oxidation resistance at 950ºC comparable to commercial alloy and lower cost	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 above **~850°C** due to 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 (Alloy 520) 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**

Typical Commercial Ni-Based Alloys and their Compositions

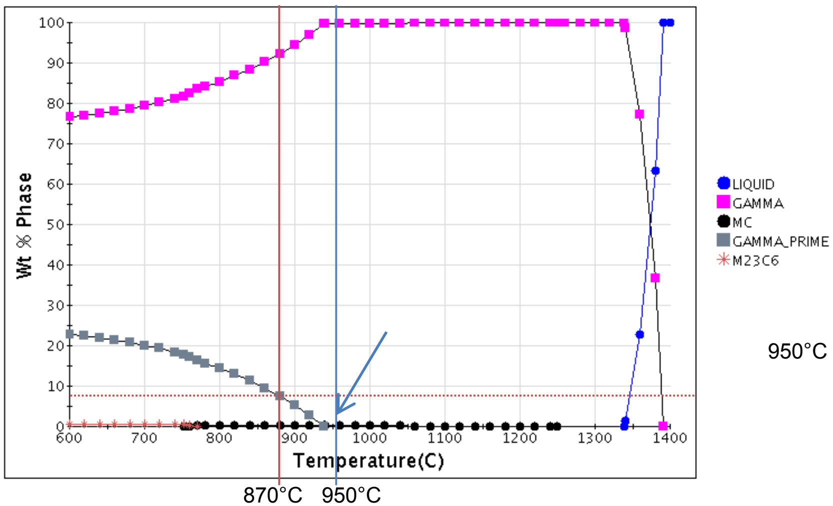
Alloy	C	Si	Mn	Al	Co	Cr	Cu	Fe	Mo	Nb	Ni	Ta	Ti	W	Zr
X750	0.03	0.09	0.08	0.68	0.04	15.7	0.08	8.03	-	0.86	71.84	0.01	2.56	-	-
Nimonic 80A	0.08	0.1	0.06	1.44	0.05	19.6	0.03	0.53	-	-	75.58	-	2.53	-	-
IN 751	0.03	0.09	0.08	1.2	0.04	15.7	0.08	8.03	-	0.86	71.32	0.01	2.56	-	-
Nimonic 90	0.07	0.18	0.07	1.4	16.1	19.4	0.04	0.51	0.09	0.02	59.65	-	2.4	-	0.07
Waspaloy	0.03	0.03	0.03	1.28	12.5	19.3	0.02	1.56	4.2	-	58.03	-	2.97	-	0.05
Rene 41	0.06	0.01	0.01	1.6	10.6	18.4	0.01	0.2	9.9	-	56.01	-	3.2	-	-
Udimet 520	***0.04***	***0.05***	***0.01***	***2.0***	***11.7***	***18.6***	***0.01***	***0.59***	***6.35***	***-***	***57.65***	***-***	***3.0***		
Udimet 720	0.01	0.01	0.01	2.5	14.8	15.9	0.01	0.12	3.0	0.01	57.25	-	5.14	1.23	0.03

- **Target for development is a low-cost Alloy 520 equivalent (strength and oxidation resistance)**

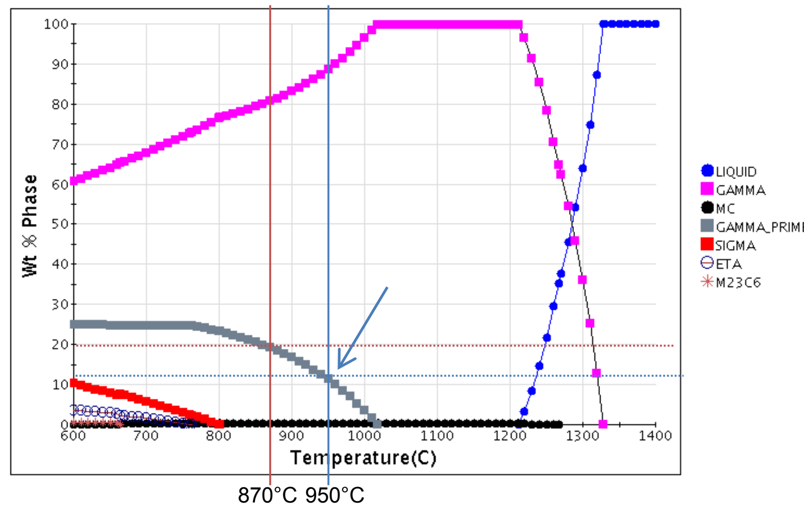
Computational Thermodynamics Predictions are Used to Guide Alloy Development

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

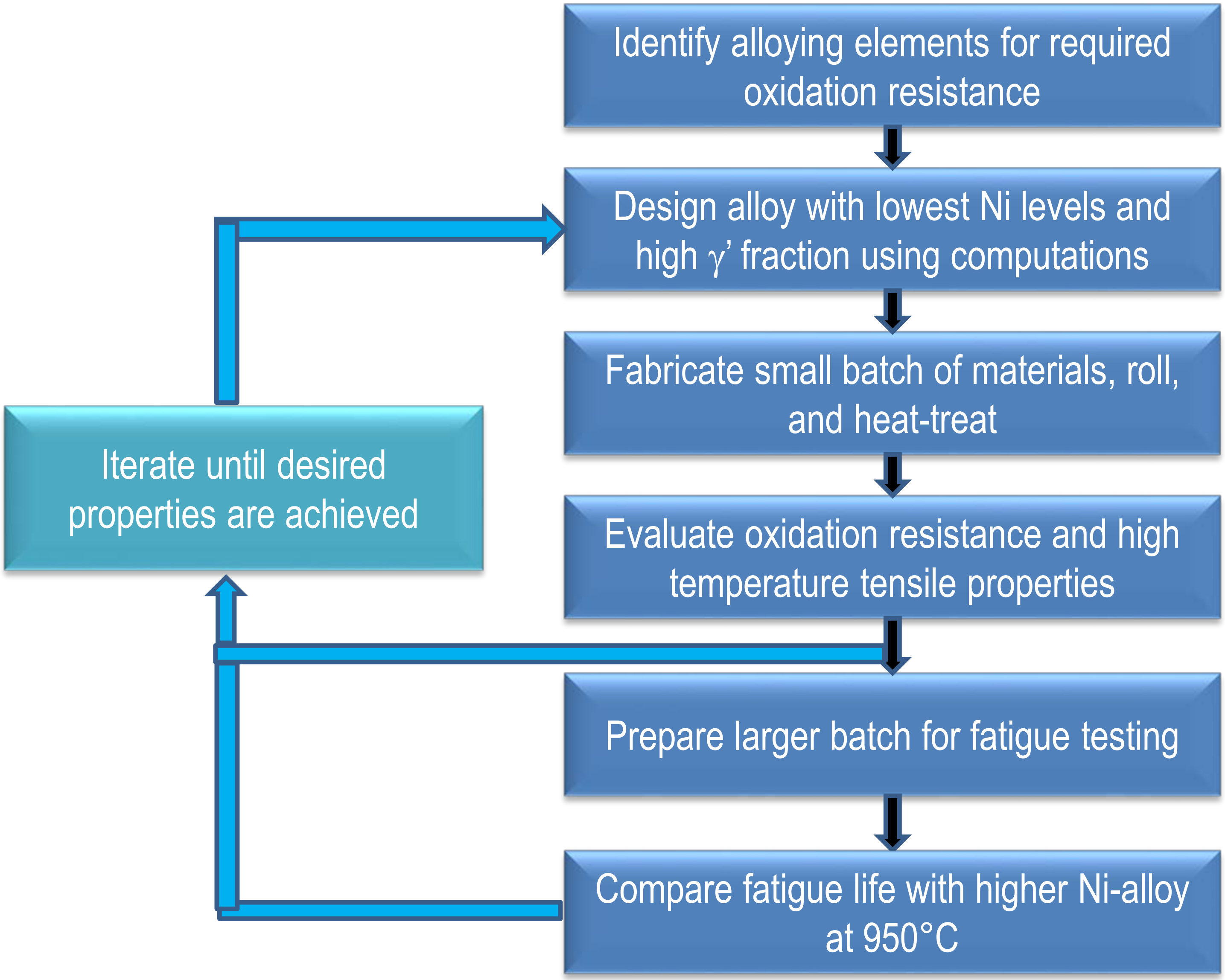


Phase Equilibria Predicted in Existing Commercial Alloy 751 Shows Dissolution of Strengthening Phase at 950°C



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

Example ICME-Based Methodology For New Alloy Development



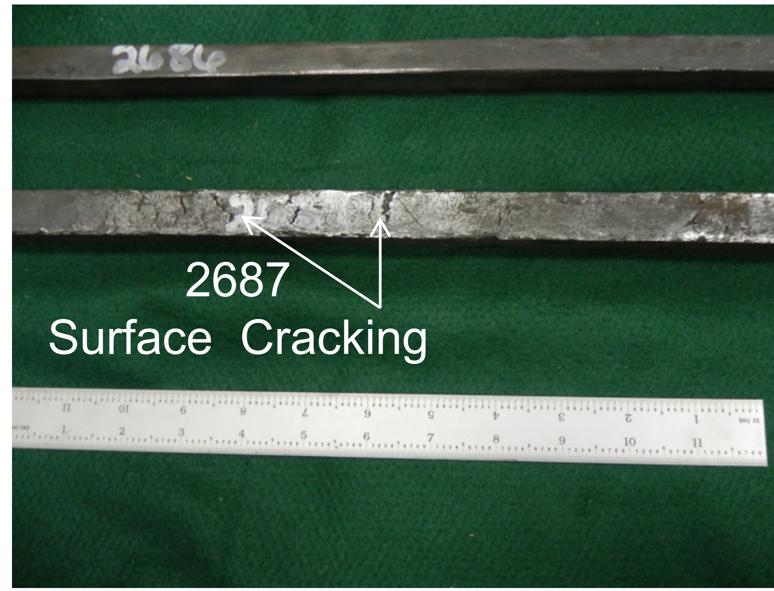
Previous Accomplishments and Progress: Initial Effect of Composition Was Evaluated and New Alloys Were Identified In FY 14

- Commercial valve alloy 751 shows better oxidation resistance at 900°C in air + 10% water vapor BUT has **inadequate strength** at 900°C compared to lower Ni-alloys developed at ORNL
- Two potential causes were initially identified for poorer oxidation performance of ORNL alloys at longer times
  - Excessive impurity levels in starting material
  - Low Cr/(Fe+Ni) ratio
- Three parallel paths were evaluated to improve oxidation resistance
  - Two alloy compositions were processed by Carpenter Technologies, adopting processing techniques designed for manufacture of higher purity Ni-based superalloys (vacuum processed)
  - Seven new alloys with higher Cr levels were identified, cast and processed at ORNL (**all similar lower Ni-levels**) (Gen 4 Alloys)
  - Improved purity feedstock was procured for future heats

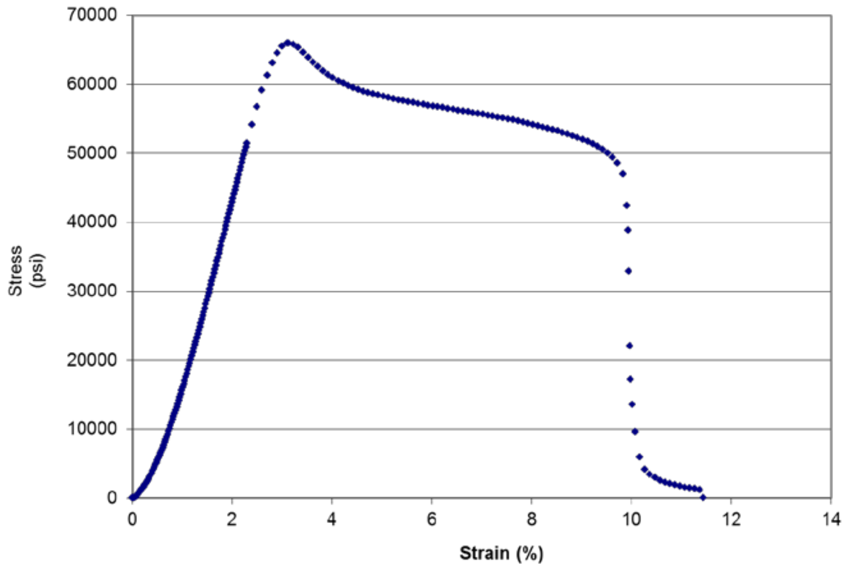
Two ORNL Alloys Were Prepared by Carpenter Technologies

- Key elements in Carpenter Heat #2686 (40Ni-19Cr-Al-Ti) and Heat # 2687 (47Ni-18Cr-higher Al-Ti)
- Initial ingot size: 4” square, Final size: 0.625”
- In initial trials Heat # 2687 was harder to forge resulting in surface cracking
  - Process modifications are required as is often the case with similar alloys

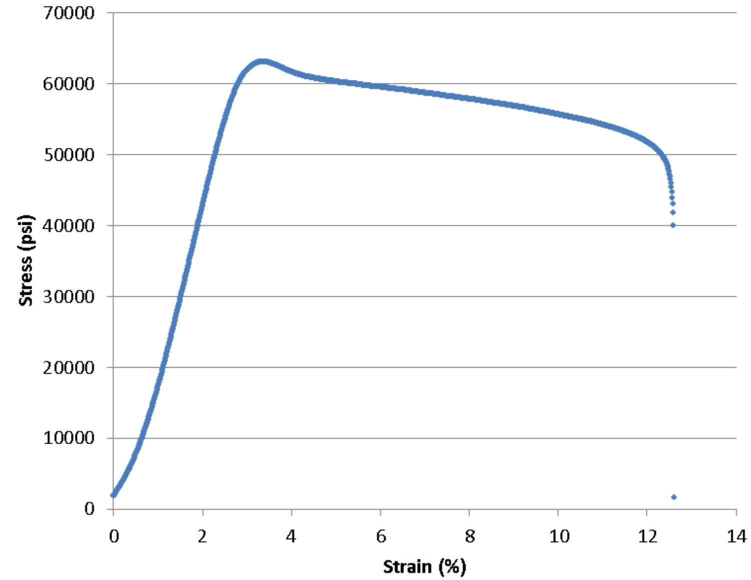
2686
No cracking



Good Agreement Has Been Obtained with Tensile Data From Laboratory Heat at 870°C(C2686)



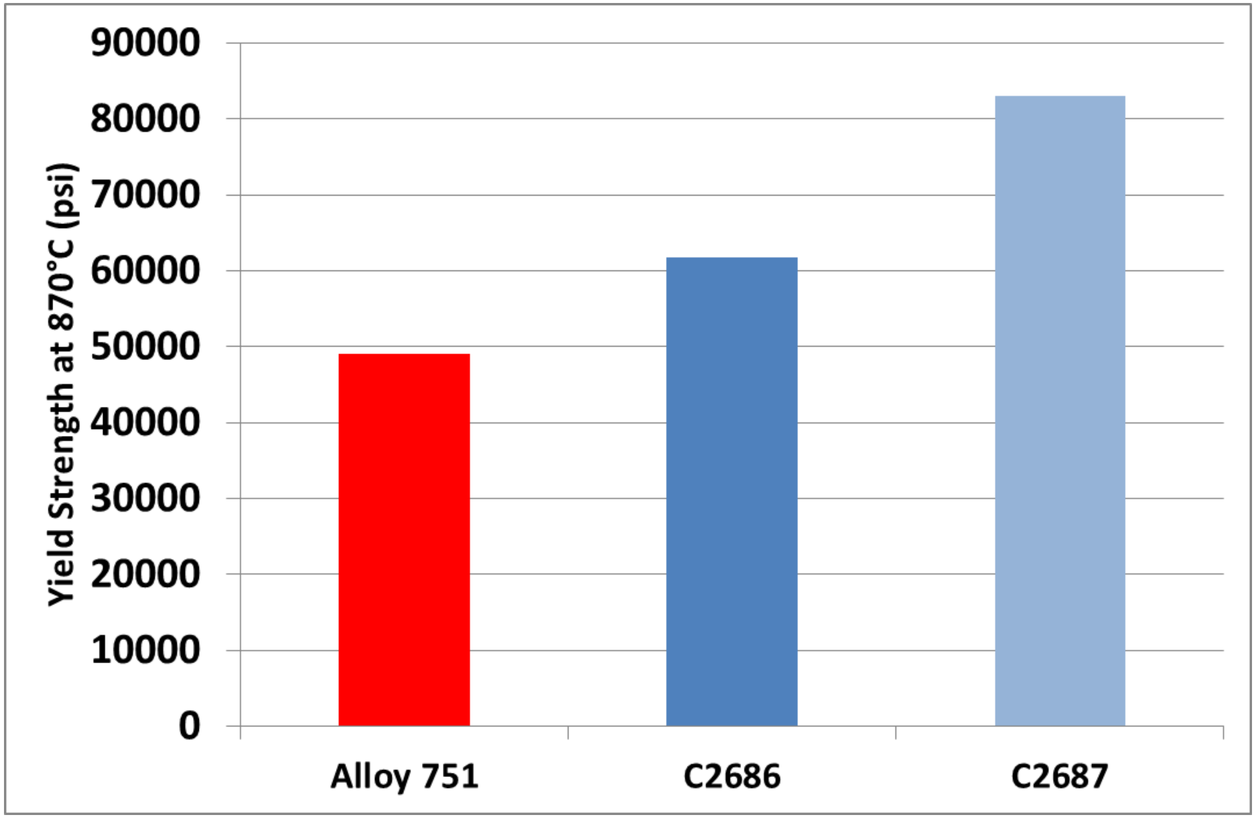
Laboratory Scale Heat



Industry Heat (C2686)

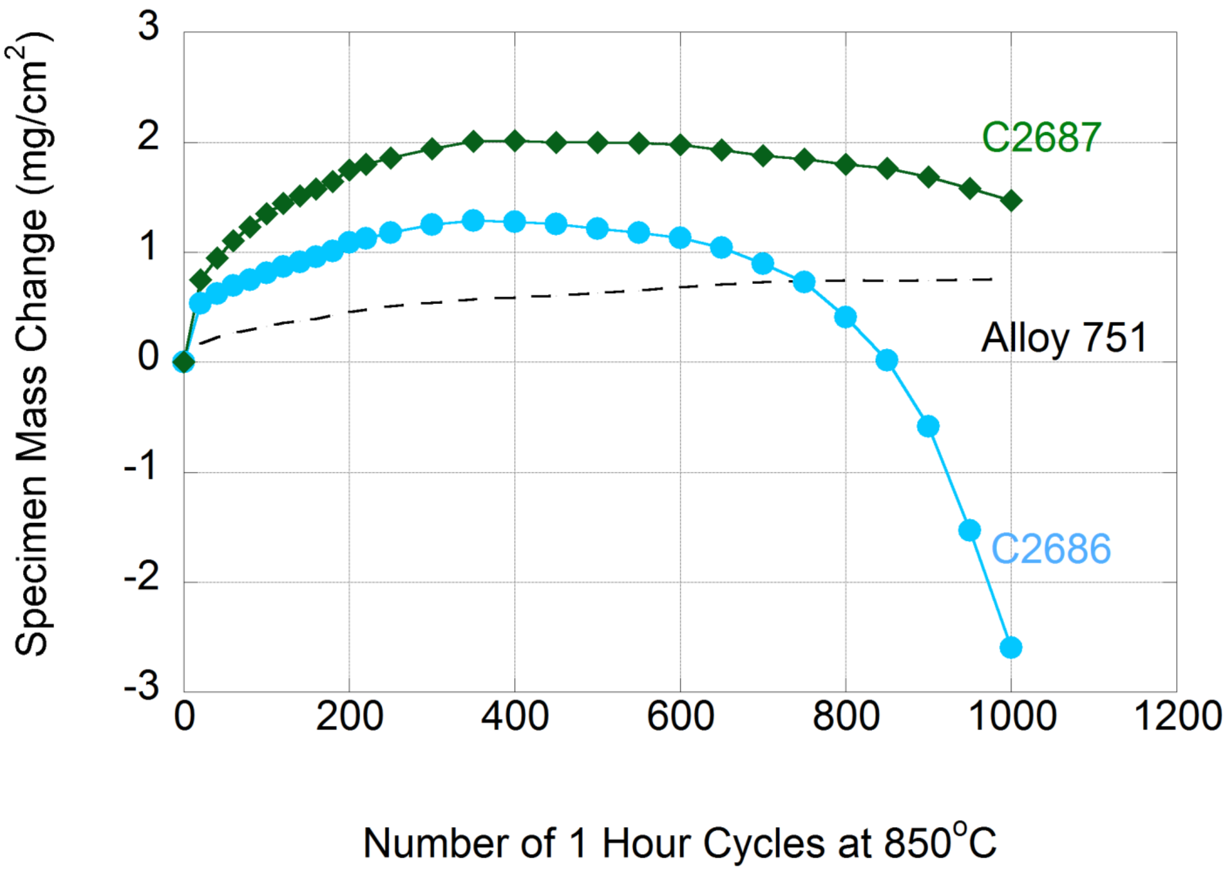
Translation of laboratory scale heats to industrial scale heats is proven to be feasible

Industry-Processed Alloys Have Higher Strength Compared to Alloy 751



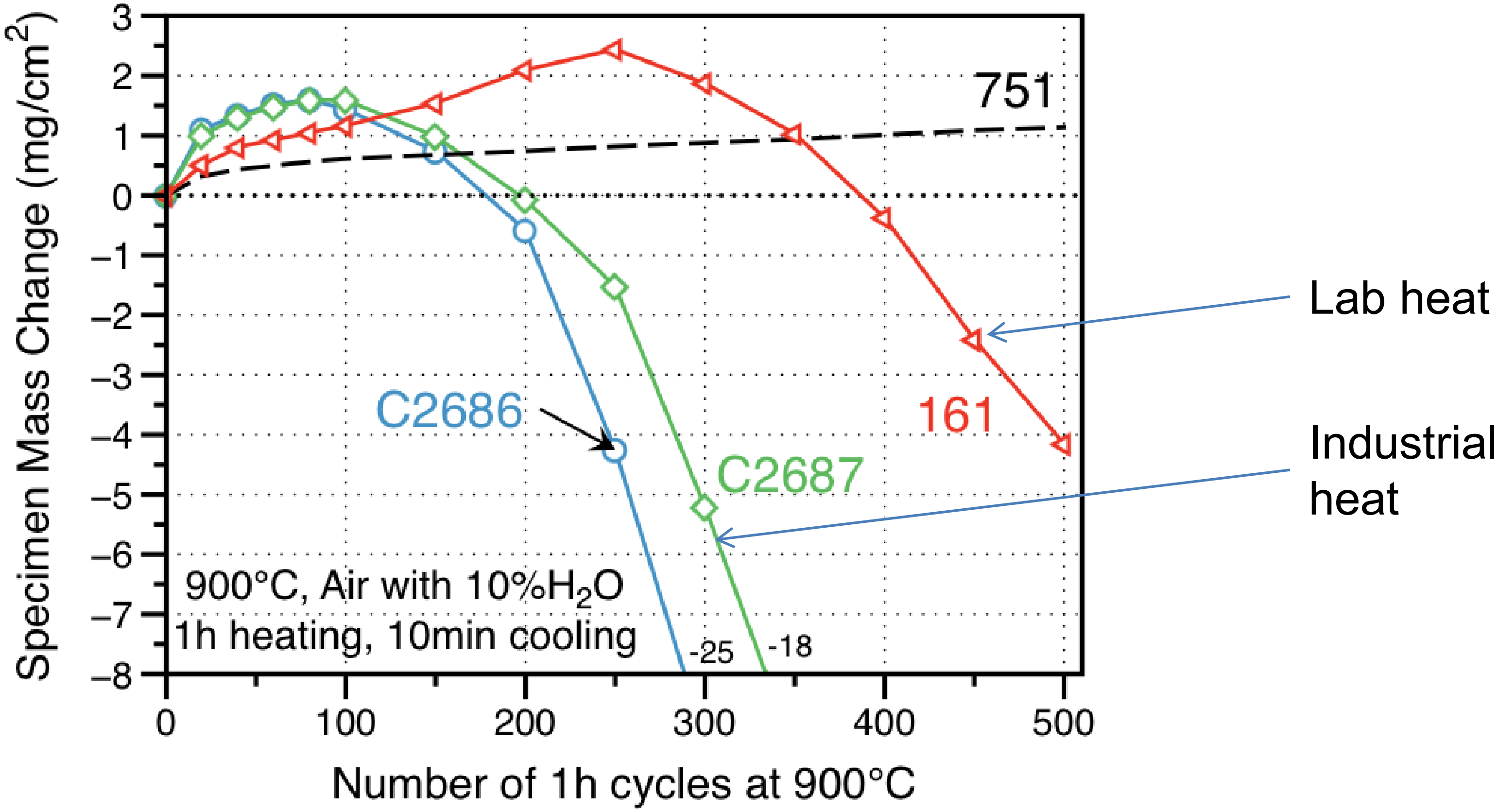
Alloy 751 has ~25%-70% lower strength than ORNL alloys at 870°C and is not an option for exhaust valve applications at the higher temperatures

Oxidation Resistance of Industry-Processed Alloys at 850°C in Air + 10% Water Vapor Environment Varied With Ni and Al Contents



C2687 (higher Ni, higher Al alloy) has better oxidation resistance than C2686

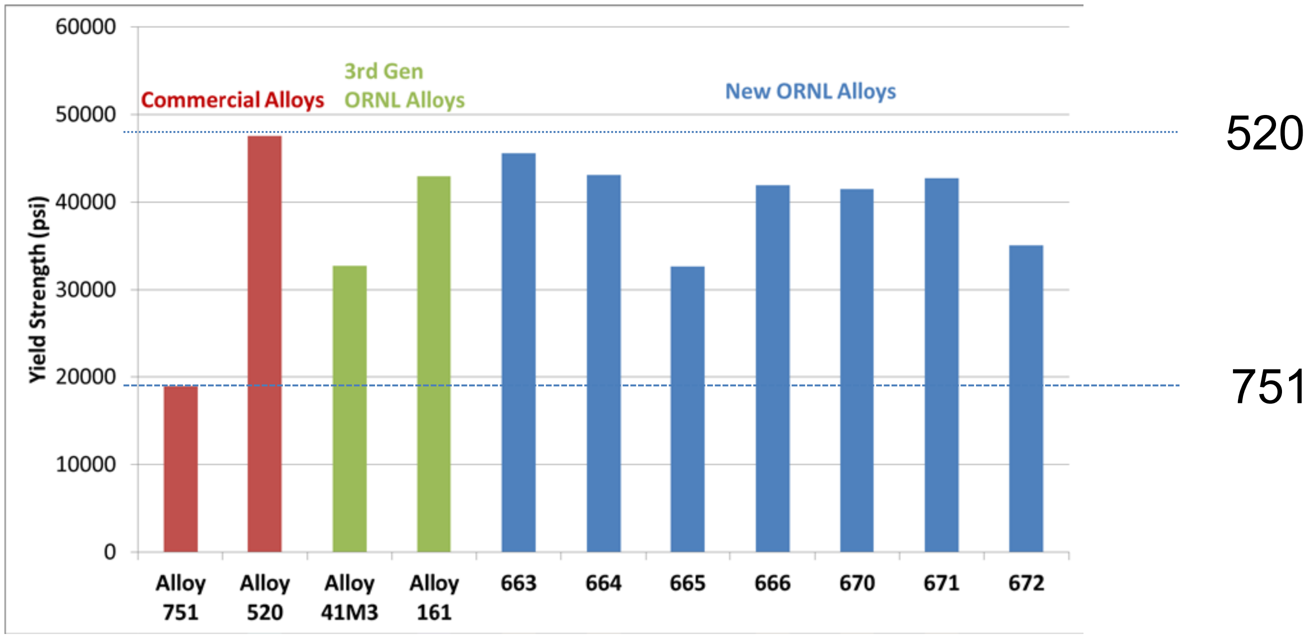
Oxidation Behavior Of Higher Purity Industry-Processed Alloys and Lab Alloys are Similar at 900°C in Air + 10% Water Vapor Environment



Oxidation resistance of industry processed alloy was not improved over lab heat

- **Impurities were not the limiting factor in alloy oxidation behavior**

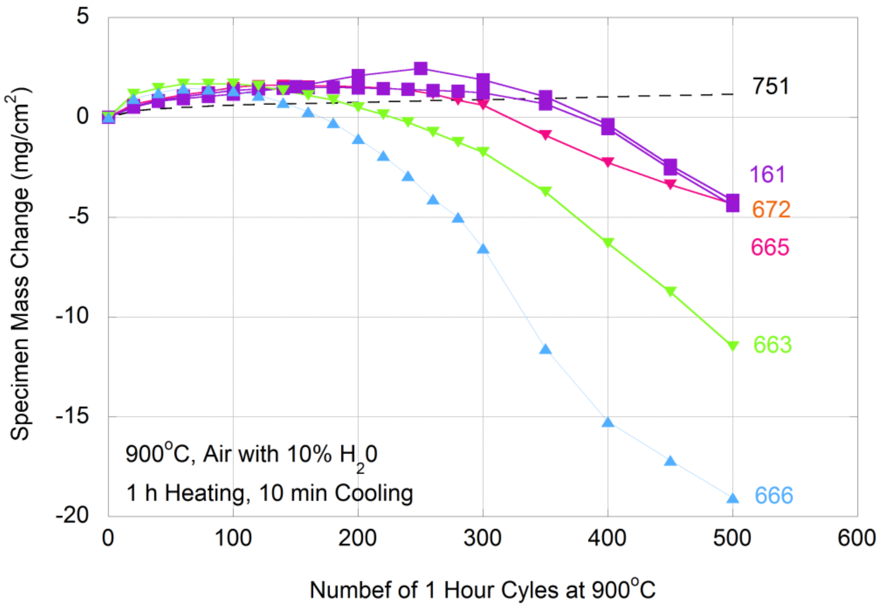
Accomplishments and Progress: New Lab-Scale Alloys Have High Strengths at 950°C



Alloy 751: 71 wt. %(Ni +Co), Alloy 520 : 69.3 wt. % (Ni+ Co), New ORNL alloys: < ~50 wt.% Ni+Co

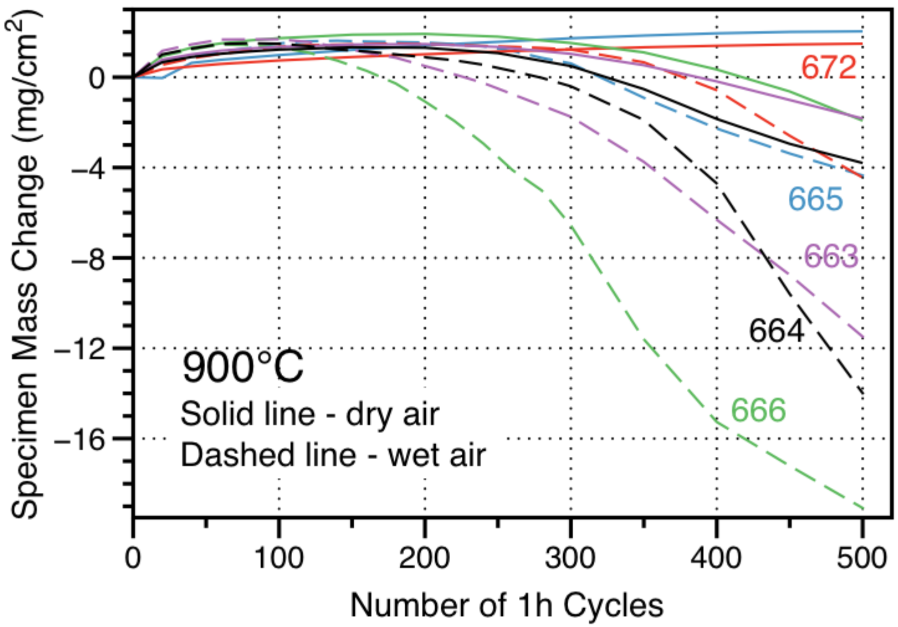
- **Strength levels of best alloy (663) within 5% of Alloy 520 (target) and 140% better than that of 751**

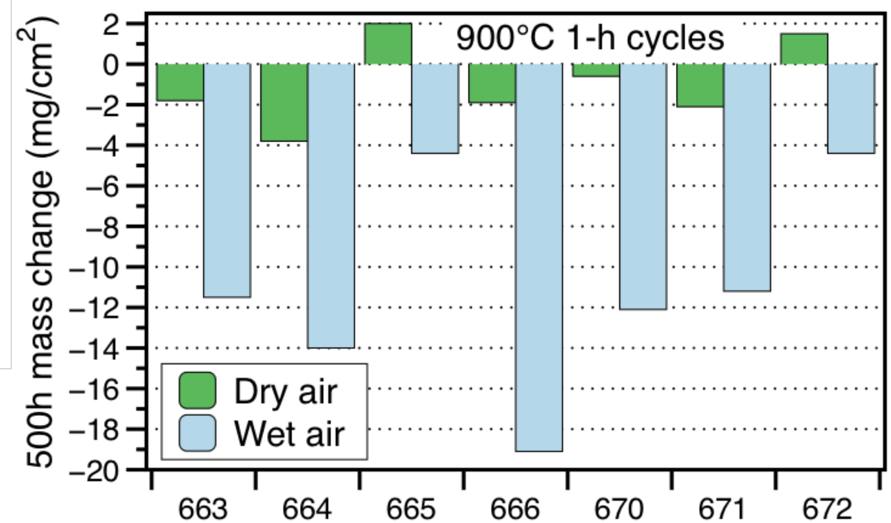
Accomplishments and Progress: New ORNL Alloys Show Effect of Composition Oxidation Resistance in Air + 10% water vapor environment at 900°C



- **Strong composition-dependence but no significant improvement in oxidation behavior**
  - **Oxidation behavior does not correlate with Cr levels only**
  - **Alloys with higher Al (665, 672) perform the best in this group but no improvement over 161**
  - **Spallation is observed in all alloys**

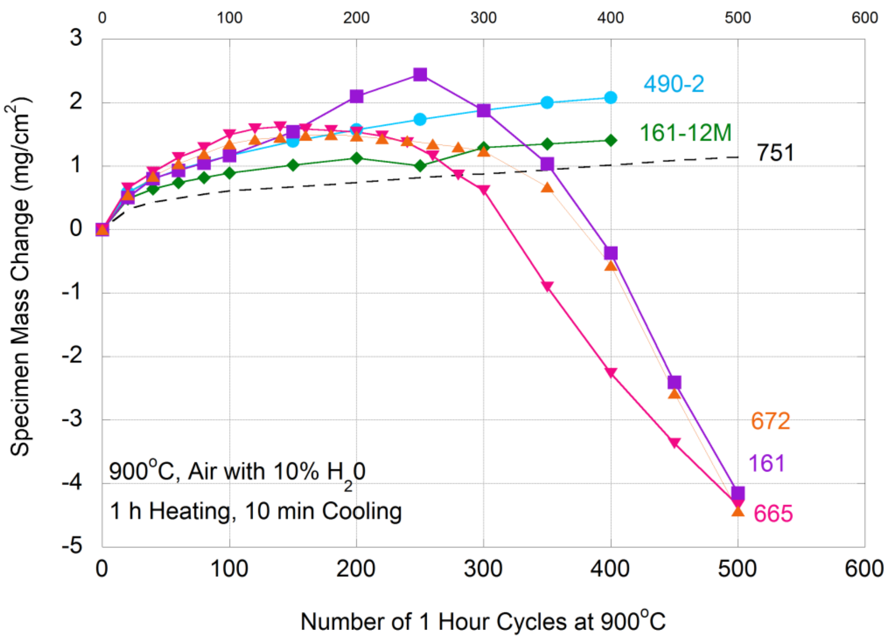
Accomplishments and Progress: Water Vapor Content Has Significant Effect on Oxidation Resistance at 900°C

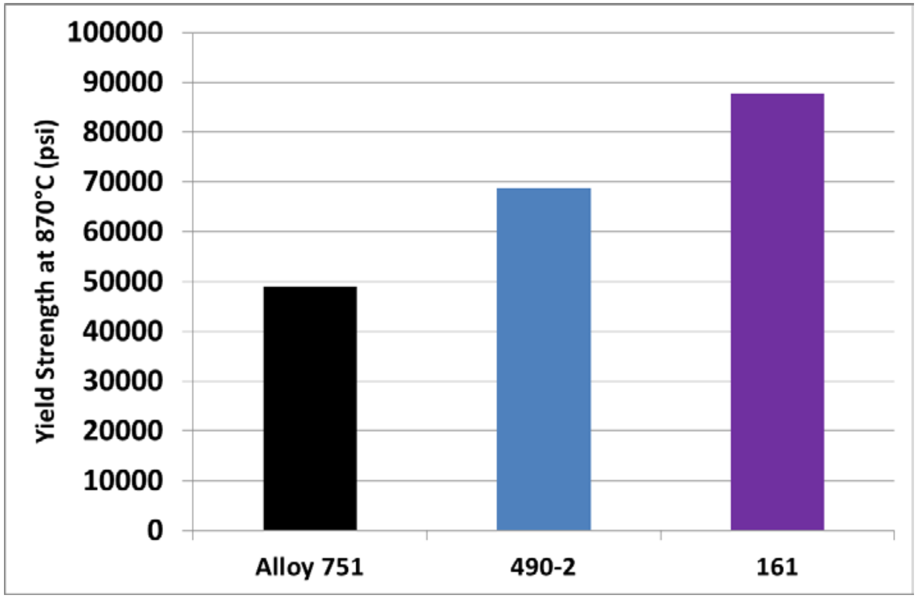




- All alloys show much lower specific mass change in dry air
- **Alloys 672 and 665 show acceptable behavior in dry air**
  - Moisture content in exhaust gas can significantly affect valve oxidation

Accomplishments and Progress: Other Alloys Show Improved Oxidation Behavior in On-going Tests





Spallation is not observed even after 400 cycles in Alloy 490-2 and 161-12M

Alloy 490-2 is 40% stronger than 751 at 870°C but with much lower Ni-levels

Strategy used in design of 490-2 and 161-12M will now be adopted for improving oxidation resistance in future alloys

Response to Reviewer's Comments

Comments were generally positive regarding objectives, approach, and progress in the early portion of the project

Comment: "The reviewer noted concerns over how results were measured and compared to previous research and what would be considered correct by the industry. For example, if possible, the weight gain of oxygen or the weight loss by flaking could both be resolved by the weight of oxide and the removal of the oxide after each cycle.

Response: In this study, importance is given to exposing the specimens to flowing air with water vapor by hanging the specimens. This does not allow measurement of weight of flaked oxide but allows rapid heating and cooling of the specimen which may simulate the transient exposure of the valve material better.

Comment: "The reviewer questioned how the ICME had sped the decision of new alloys."

Response: It is explained in this talk that ICME allowed rapid identification of alloy compositions that would have a certain desired amount of the strengthening phase.

Comment: "The chosen materials did not seem to be an improvement on the base alloy choice"

Response: The chosen materials are significantly stronger than the baseline alloy at temperatures of 870°C as shown in last year's and this year's presentation

Comment: "Reviewer questioned if there was room in the system to allow for higher rate of oxidation"

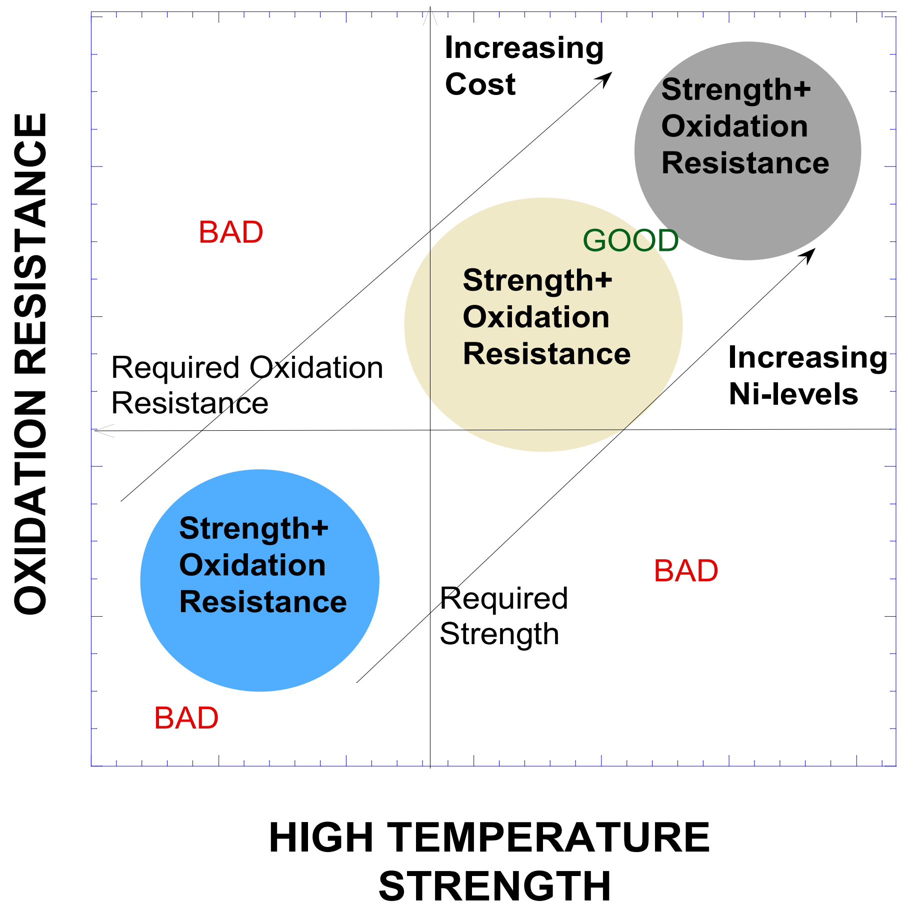
Response: One of the primary objectives of this work is to design alloys that have both the strength and oxidation resistance at the higher temperatures. Only alloys with rates of oxidation comparable to or better than base alloy but with much higher strength and lower cost will be down-selected

Collaborations and Coordination with Other Institutions

- Collaborations are on-going with Carpenter Technologies
  - Contributed two VIM heats of ORNL alloys
- Conversations have been held with Caterpillar about needs and potential future collaborations for valve manufacture and testing
- Discussions have been initiated with Eaton on potential path forward

Remaining Challenges and Barriers

- Strength levels at temperatures up to 950°C have to be maintained while also achieving adequate oxidation resistance
- Oxidation resistance at temperatures up to 950°C has to be evaluated and improved
  - *Increase aluminum contents*
  - *Increase nickel contents*
  - *Trace additions of rare earths (Y, Hf, La)*
- Microstructural stability must be evaluated and optimized to achieve desired fatigue life at temperatures up to 950°C



Need to find alloys desired combination of properties at the least required Ni-levels

Proposed Future Work

FY15

- Complete evaluation of oxidation resistance of new alloys at 950°C up to 500 hours
- Design and fabricate new alloys that balance oxidation resistance with strength at 950°C
- Complete tests on additional alloys to validate oxidation resistance and strength at 950°C
  - Down-select promising alloys for fabrication of larger heats to evaluate 950°C performance

FY16

- Fabricate, and test oxidation resistance and high temperature strength of larger batch of down-selected alloys that have the potential to meet oxidation resistance targets at temperatures up to 950°C
- Complete fatigue testing of most promising candidate at 950°C

Summary

- **Relevance:**
  - Temperatures are expected to increase from 870^{o}C to 950^{o}C in 2025 and to 1000^{o}C by 2050* in light-duty vehicles and from 700^{o}C to 900^{o}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^{o}C. Similar approach has been used previously to develop new cost-effective alloys for use at temperatures up to 870^{o}C.
- **Accomplishments:**
  - Based upon results on oxidation resistance of existing ORNL alloys, new alloys with minor variations Cr/Ni contents were designed, fabricated, and oxidation tests were completed at temperatures up to 900^{o}C and tensile tests were completed at temperatures up to 950^{o}C. It was observed that alloying element additions must carefully balance oxidation resistance with high temperature strength. Paths towards improved oxidation resistance were identified and will be used to design new alloys.
- **Collaborations:**
  - Collaborations are on-going with Carpenter Technologies
- **Proposed Future Work:**
  - New alloys capable of achieving desired oxidation resistance and mechanical properties at temperatures up to 950^{o}C will be designed.