Computational design and development of a new, lightweight cast alloy for advanced cylinder heads in high-efficiency, light-duty engines

FOA 648-3a

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General Motors
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Overview

Timeline
Start date – February 2013
End date – March 2017
Percent complete – 25%

Budget
• Total funding $5,145,073
  – DOE share $3,498,650
  – Contractor share $1,646,423
• Funding received in FY13
  – (02/13-09/13) $203,598
• Funding for FY14
  – (10/13-03/14) $247,462

Barriers and Targets
Changing ICE regimes
  – Material property improvements required to accommodate increases in:
    • Peak cylinder pressure
    • Exhaust Temperature and Combustion Dome Temperature

Partners
• QuesTek Innovations LLC
• Northwestern University
• American Foundry Society
• Dr. Fred Major
• Dr. Geoffrey Sigworth (2013)
• Camanoe Associates
• MIT
• Project lead General Motors
## Milestones 2013-2014

<table>
<thead>
<tr>
<th>Date</th>
<th>Description</th>
<th>Status</th>
</tr>
</thead>
<tbody>
<tr>
<td>03/27/2014</td>
<td>Task 2. Generate Alloy Concepts and Select Alloy Models</td>
<td>Complete</td>
</tr>
<tr>
<td></td>
<td>Milestone 1: Alloy Requirement Matrix Established</td>
<td></td>
</tr>
<tr>
<td>04/01/2014</td>
<td>Task 2. Milestone 3: Alloy Models Selected for Casting</td>
<td>Complete</td>
</tr>
<tr>
<td>04/30/2014</td>
<td>Task 3. Cast and Characterize Sub-scale Alloy Models</td>
<td>Complete</td>
</tr>
<tr>
<td></td>
<td>Milestone 4: Sub-scale Castings Completed</td>
<td></td>
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<tr>
<td>07/31/2014</td>
<td>Task 3. Milestone 5: Sub-scale Data Development Completed</td>
<td>On-track</td>
</tr>
<tr>
<td>11/26/2014</td>
<td>Go/No Go Decision: Do models and experiments agree? Can models be used to move forward to continue to develop alloy?</td>
<td></td>
</tr>
</tbody>
</table>
To meet energy efficiency targets, peak engine pressures and temperatures will greatly exceed current material properties and therefore needs to be improved.

### DOE FOA 648-3a Material Property Targets

<table>
<thead>
<tr>
<th>Property</th>
<th>Cast Aluminum Baseline</th>
<th>Cast Non-Ferrous Alloy Targets</th>
<th>Key Properties</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tensile Strength (Ksi)</td>
<td>33 KSI</td>
<td>40 KSI</td>
<td>Key</td>
</tr>
<tr>
<td>Yield Strength (Ksi)</td>
<td>24 KSI</td>
<td>30 KSI</td>
<td>Key</td>
</tr>
<tr>
<td>Elongation (%)</td>
<td>3.5 %</td>
<td>3.5 %</td>
<td>Key</td>
</tr>
<tr>
<td>Shear Strength</td>
<td>26 KSI</td>
<td>30 KSI</td>
<td>Key</td>
</tr>
<tr>
<td>Endurance Limit</td>
<td>8.5 KSI</td>
<td>11 KSI</td>
<td>Key</td>
</tr>
<tr>
<td>Fluidity (Die Filling Capacity/Spiral Test)</td>
<td>Excellent</td>
<td>Excellent</td>
<td>Key</td>
</tr>
<tr>
<td>Hot Tearing Resistance</td>
<td>Excellent</td>
<td>Excellent</td>
<td>Key</td>
</tr>
<tr>
<td>High Temperature Performance</td>
<td>@ 250C</td>
<td>@ 300 C</td>
<td></td>
</tr>
<tr>
<td>Tensile Strength (KSI) @ 250 C</td>
<td>7.5 KSI</td>
<td>9.5 KSI @ 300 C</td>
<td>Key</td>
</tr>
<tr>
<td>Yield Strength (KSI)</td>
<td>5 KSI @ 250 C</td>
<td>6.5 KSI @ 300 C</td>
<td>Key</td>
</tr>
<tr>
<td>Elongation in 2”</td>
<td>20% @ 250 C</td>
<td>&lt; 20% @ 300 C</td>
<td></td>
</tr>
</tbody>
</table>
Relevance – 2013 Objectives

Define and rank material properties necessary to meet project targets and optimal engine requirements

- Provide a framework for alloy development to meet objectives.

Research current alloys systems and develop concept models

Create castings to test stability of alloy concepts and validate model systems

Generate experimental data for input into concept models
Approach

Identify and rank most critical properties to meet high performance engine head requirements

- Milestone 1  Alloy Requirement Matrix

Use models and expert knowledge to identify and create alloy concepts that can contribute to the overall high temperature strength and fatigue requirements.

- Milestone 2, 3 Alloy Concept Generation and Selection

Produce castings for data generation, testing, and validation of models

- Milestone 4, 5 Subscale casting and data development

Validate alloy concepts by microstructural analysis, hardness testing and mechanical property testing

- Milestone 6 Subscale concept and model validation

Develop Parametric Designs of New Alloys
- Develop alloy combinations from alloy concepts, introduce elements for increased high temperature stability, ductility, fatigue strength and castability.
- Milestones 7-9 Parametric alloy generation, casting, testing and model validation.

Create Final Embodiment of New alloy
- Milestone 10-14 Computational design, lab scale castings and component casting trial, recyclability analysis, final alloy testing and model validation

Develop alloy and component production cost models
- Milestone 15 Final cost models.
Apply Design for Six Sigma (DFSS) methodology to establish the most critical material properties to meet engine requirements.

**Control Factors:**
- Coefficient Thermal Expansion
- Thermal Conductivity
- Young’s Modulus
- Specific Heat
- Density

**Noise Factors:**
- Coolant Temperature
- Peak Cylinder Pressure
- Combustion Temperature
- Architecture

**Output:**
- Flatness
- Mean Stress
- Alternating Stress
- Temperature Distribution (from GED)

**Symptoms:**
- Temperature increase in aluminum

**Phase I Physical Properties**

Min.: 287.2 deg C
Max.: 297.2 deg C

**Front**
Approach: Material Requirement Matrix (Milestone 1)

Phase II Mechanical Properties and Thermal Conductivity

Control Factors:
- Ultimate Tensile Strength
- Cyclic Strength Coefficient
- Cyclic Strain Hardening Exponent
- Low Cycle Fatigue Strength
- High Cycle Fatigue Strength
- Thermal Conductivity

System
- Cylinder Head
- FEA, GED and GETC

Output
- Temperature Distribution
- Mean Stress
- Alternating Stress
- Safety Factor

Noise Factors:
- Coolant Temperature
- Peak Cylinder Pressure
- Combustion Temperature

Symptoms:
- Temperature increase in aluminum
Approach: Alloy Concepts
Milestones 2-6

- Identify Alloy structures by Density Functional Theory
- Scheil simulation of concept alloy solidification
- Calculate diffusivity of Elements
## Technical Accomplishments

### Material Requirement Matrix

<table>
<thead>
<tr>
<th>Property</th>
<th>Temperature</th>
<th>DOE Cast Lightweight Alloy</th>
<th>High Temp Alloy Requirements</th>
<th>Rank</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tensile Strength (MPa)</td>
<td>25 C</td>
<td>275.8</td>
<td>300</td>
<td>19</td>
</tr>
<tr>
<td></td>
<td>150 C</td>
<td>N/A</td>
<td>280</td>
<td>15</td>
</tr>
<tr>
<td></td>
<td>250 C</td>
<td>N/A</td>
<td>100</td>
<td>17</td>
</tr>
<tr>
<td></td>
<td>300 C</td>
<td>65.5</td>
<td>65.5</td>
<td>21</td>
</tr>
<tr>
<td>Yield Strength (MPa)</td>
<td>25 C</td>
<td>206.8</td>
<td>210</td>
<td>13</td>
</tr>
<tr>
<td></td>
<td>150 C</td>
<td>N/A</td>
<td>200</td>
<td>14</td>
</tr>
<tr>
<td></td>
<td>250 C</td>
<td>N/A</td>
<td>75</td>
<td>12</td>
</tr>
<tr>
<td></td>
<td>300 C</td>
<td>44.8</td>
<td>45</td>
<td>20</td>
</tr>
<tr>
<td>Plastic Elongation (%)</td>
<td>25 C</td>
<td>3.5</td>
<td>≥ 3.5</td>
<td>11</td>
</tr>
<tr>
<td></td>
<td>300 C</td>
<td>&lt; 20</td>
<td>N/A</td>
<td>22</td>
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<tr>
<td>Fatigue Strength at 10^7 cycles (MPa)</td>
<td>25 C</td>
<td>75.8</td>
<td>N/A</td>
<td>23</td>
</tr>
<tr>
<td></td>
<td>150 C</td>
<td>N/A</td>
<td>70</td>
<td>7</td>
</tr>
<tr>
<td></td>
<td>250 C</td>
<td>N/A</td>
<td>50</td>
<td>9</td>
</tr>
<tr>
<td>Fatigue Strength at 10^8 cycles (MPa)</td>
<td>150 C</td>
<td>N/A</td>
<td>140</td>
<td>8</td>
</tr>
<tr>
<td></td>
<td>250 C</td>
<td>N/A</td>
<td>60</td>
<td>10</td>
</tr>
<tr>
<td>Density (g/cm³)</td>
<td>25 C</td>
<td>&lt; 6.4</td>
<td>&lt; 3.0</td>
<td>5</td>
</tr>
<tr>
<td>Shear Strength</td>
<td>25 C</td>
<td>206.8</td>
<td>206.8</td>
<td>24</td>
</tr>
<tr>
<td>Thermal Conductivity (mw / mm-C)</td>
<td>150 C</td>
<td>N/A</td>
<td>202</td>
<td>6</td>
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<tr>
<td>Coefficient of Thermal Expansion (mm / mm-C)</td>
<td>150 C</td>
<td>N/A</td>
<td>2.20E-05</td>
<td>16</td>
</tr>
<tr>
<td>Fluidity (Die Filling Capacity / Spiral Test)</td>
<td>150 C</td>
<td>N/A</td>
<td>Excellent</td>
<td>3</td>
</tr>
<tr>
<td>Hot Tearing Resistance</td>
<td>Excellent</td>
<td>≥ 319</td>
<td>4</td>
<td></td>
</tr>
<tr>
<td>Manufacturing cost including alloy and processing</td>
<td>&lt; 110% Baseline</td>
<td>&lt; 110% Baseline</td>
<td>2</td>
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<tr>
<td>Corrosion resistance</td>
<td>GMW15272 for Underhood Vehicle Requirements</td>
<td>18</td>
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<tr>
<td>Recyclability</td>
<td>Must comply with GMW3059 GMW3116 Recyclability / Recoverability</td>
<td>1</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Technical Accomplishments
Alloy Concepts

Seven alloy concepts have been created.

Four alloy concepts have been modelled in a thermodynamic framework, and heat treatment processing conditions identified.

Three alloy concepts have been identified by Density Functional Theory.

Metallurgical buttons have been cast for each of the alloy concepts.

Hardness studies at 200 C and 250 C give indications of the high temperature stability of the concepts.

Microstructural analysis including local electron atom probe (LEAP) identify structures and can measure the coarsening kinetics of phases.
Technical Accomplishments

Hardness measurements on chemical buttons test temperature stability of four alloy concept models.

Local electron atom probe (LEAP) analysis of phase precipitation.
Collaboration and Coordination

General Motors – Principle Investigator
– Project administration, casting simulation, casting experiments, mechanical properties, microstructural evaluation

QuesTek Innovations LLC – Industrial sub-partner
– Industrial Sub-partner
– ICME calculations – thermodynamics, kinetics, DFT alloy generation, alloy concept generation, parametric and final alloy designs, heat treatment process recommendations

Northwestern University – University sub-partner
– DFT alloy generation, Phase Field modelling of microstructure, experimental validation - Optical, SEM, TEM, LEAP

Fred Major, Tom Prucha (AFS), Geoffrey Sigworth (2013 only) – Industrial sub-partners
– Technical advisors

Camanoe Associates – Industrial sub-partner
– Process Based Cost Modelling

MIT – University sub-partner
– Recyclability Analysis
Remaining Challenges and Barriers

Find chemical combinations that are able to hold properties up to 300 C.

Maintain castability requirements such as resistance to hot tearing, fluidity, and good shrinkage characteristics.

Develop complete alloy systems that are capable of meeting project targets for high temperature cylinder applications with excellent castability and low cost.
Future work in 2014

Validate alloy concept models through microstructural analysis and mechanical tests

Develop parametric alloy systems from the validated alloy concepts.

Introduce alternate chemical species to further improve high temperature stability, ductility, fatigue properties and castability.

Begin casting and test parametric alloys.
Summary

Objective: Develop a non ferrous alloy capable of withstanding the temperature and pressures associated with advanced combustion engines

Approach: (1) Determine key material properties required for engine designs. (2) Identify alloy sub-structures potentially capable of meeting requirements - through computational simulation, experimental analysis, and mechanical testing; and (3) validate and utilize ICME models to rapidly design and optimize alloy(s) to meet all requirements.

Accomplishments: Material Design Matrix and 7 alloy concepts have been created, modeled, cast, and are being tested.

Collaborations: GM, QuesTek Innovations, Northwestern University, Fred Major, AFS, MIT, and Camanoe Associates

Future Work: Model validation, parametric alloy design development, casting, microstructural analysis and thermo-mechanical testing.