The Fundamental Creep Behavior Model of Gr.91 Alloy by ICME Approach

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Self Introduction

• Ph.D. Penn State 2005
  – ICME approach to design new high creep resistance Mg alloys

• Saint Gobain HPM 2005-2013
  – Structural Ceramics: SiC, B₄C, Si₃N₄
  – Functional Ceramics: Solid Oxide Fuel Cell (SOFC), Oxygen Transport Membrane (OTM), Sapphire crystal growth

• Florida International University 2013-current
  – Active projects:
    • Grant: ACSPRF# 54190-DNI10, $110K, 2014-2017
      – The Integrated Materials and Process Design for Novel Perovskites
    • Grant: DE-FE0027800, $250K, 2016-2019
      – The Fundamental Creep Behavior Model of Gr.91 Alloy by ICME Approach
Self Introduction
Outline

• Objective/Vision
• Background
• Team Description and Assignments
• Gantt Chart
• Milestones
• Previous Work (Creep Resistance of Mg alloys)
Objective/Vision

- Predict the phase stability and microstructure of Gr.91 base alloy and weldment with the computational thermodynamics and kinetics (CALPHAD) approach;
- Carry out welding, heat treatment, and creep test for the Gr.91 alloy;
- Develop a model which has excellent match with the experimental data from the current work and also from the previous existing work;
- Predict how to improve the long-term creep resistance for the Gr.91 family alloys.
Type IV cracks

From D. J. Abson and J. S. Rothwell 2013
The fine $M_23C_6$ phase has the strengthen effect in the early life of the steels but it will coarsen quickly and therefore should not be treated as strengthen phase in the long-term operations.

The fine MX phase (NbC or VN) is beneficial to the steel, which has very low coarsening rate and is able to pin grain boundaries and dislocations.
Materials Design with the ICME Approach

Thermodynamics

Kinetics

Property

Performance

Existing Experimental Data:
- Welding, PWHT, Creep test

Thermodynamic Simulation

Kinetic Simulation

Prediction on Precipitation Phase Stability and Microstructure

Experiments Design:
- Welding, PWHT, Creep test

Creep resistance Property of Gr.91 Alloy
Team Description and Assignments

Effective Communications

PI
Dr. Yu Zhong
FIU

Subcontract
Prof. Wei Zhang
OSU

Graduate Student/Post-Doc

Task 2. Literature Review

Task 3. Thermodynamic/Kinetic Simulations

Subtask 4.2 Post-Weld Heat Treatment (PWHT)

Task 6. Characterization

Task 7. Model development and BEYOND

Subtask 7.1 Model Verification

Subtask 7.2 Prediction on the effect of Processing parameters

Subtask 7.3 Predictions on the effect of alloying elements

Task 5. Creep Test

Task 7. Model development and BEYOND

Subtask 4.1 Welding

Graduate Student
### Task 1. Project Management and Planning

- D1: Quarterly Reports
  - Q1: Yes, Q2: Yes, Q3: Yes, Q4: Yes, Q5: Yes, Q6: Yes, Q7: Yes, Q8: Yes, Q9: Yes, Q10: Yes
- D2: Annual Progress Reports
  - Q11: Yes, Q12: Yes
- D3: Final Technical Report
  - Q12: Yes

### Task 2. Literature Review

- M1: "Selection of the reliable data for Gr.91 alloys from literature"
  - (01/31/17) (01/31/17)

### Task 3. Thermodynamic/Kinetic Simulations

#### Subtask 3.1 Thermodynamic Simulations for the Gr.91 alloys

- M2: "Prediction on the stability of interested phases"
  - (07/31/17) (07/31/17)

#### Subtask 3.2 Kinetic Simulations

- M3: "Prediction of the precipitates microstructure changes"
  - (01/31/18) (01/31/18)

### Task 4. Welding and PWHT

#### Subtask 4.1 Welding

- M4: "Welding of up to 20 steel plates"
  - (01/31/18)

#### Subtask 4.2 PWHT

- M5: "PWHT treatment for the welded samples"
  - (04/30/18)
### Task 5. Creep Test

**M6**: Creep tests to up to 10 samples

- (01/31/19)
- (01/31/19)

### Task 6. Characterizations

**M7**: Characterization results with samples from weld, PWHT, and creep tests

- (5/31/18)
- (8/31/18)
- (5/31/19)

### Task 7. Model Development

#### Subtask 7.1 Model Verification

**M8**: Verification of the prediction from our model

- (01/31/19)

#### Subtask 7.2 Prediction on the Effect of Processing Parameters

**M9**: predict how the processing parameters affect the creep resistance

- (04/30/19)

#### Subtask 7.3 Prediction on the Effect of Alloying Elements

**M10**: predict how the alloying element affect the creep resistance

- (07/31/19)
<table>
<thead>
<tr>
<th>Number</th>
<th>Task</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>M1</td>
<td>Task 2</td>
<td>screening out all the reliable data for Gr.91 alloys from literature (01/31/2017)</td>
</tr>
<tr>
<td>M2</td>
<td>Subtask 3.1</td>
<td>Prediction on the stability of M23C6, MX and other metastable phases and intermediate phases (07/31/2017)</td>
</tr>
<tr>
<td>M3</td>
<td>Subtask 3.2</td>
<td>Prediction on the precipitates phase microstructure changes (01/31/2018)</td>
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<td>M4</td>
<td>Subtask 4.1</td>
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</table>
Mg is one of the lightest structural materials.

Increasing demand for magnesium alloys

- Limited to use at low temperatures !!!
Approaches to Improve Creep Resistance


1. Suppress $\gamma$ phase

2. Pin the sliding with High melting temperature phase

Addition of Rare-Earth elements-AE42(Mg-4wt.%Al-2wt.%RE)

Addition of Ca, Sr, or other elements
Approaches Used

I. CALPHAD
   • Thermo-Calc

II. First-Principles
   • VASP

III. Experiments
   • Mg-Al-Ca System

Thermodynamic Database

Phase Stability

Creep Resistance of Mg alloy
Microstructure of Mg-Al-Ca alloy

Die Casting (GM-C)
Mg-4.5%Al-3.0%Ca
HCP matrix + Eutectic

In collaboration with General Motors
Experimental Observations

Ca effect to Mg-Al alloy

• AX51(Mg-5wt.%Al-0.8wt.%Ca)
  – Similar creep resistance to AE42
  – $\text{Al}_2\text{Ca}$ C15 Laves phase is confirmed in as cast sample

• GM-C(Mg-4.5wt.%Al-3.0wt.%Ca)
  – Much better creep resistance than AE42
  – C36 Laves phase is found in the as cast sample
  – C36 Laves phase transformed into C15 Laves phase with heat treatment at high temperatures.
Laves Phases

- Intermetallic $A_2B$ compounds
- More than 1000 compounds in one of the three structures, C14, C15, and C36

2003 Mg-Al-Ca Database

Mg$_2$Ca-C14

Al$_2$Ca-C15

Liquidus Projection
Updated Mg-Al-Ca Database

C36 Predicted by Yu Zhong, First-Principles Investigation of Laves Phases in Mg-Al-Ca System, TMS Annual Meeting, Charlotte, NC, March 19, 2004
Cooling Simulations

- Equilibrium cooling
  - Global equilibrium between liquid and solid
  - Slow cooling

- Scheil simulation
  - Infinity fast diffusion in liquid
  - No diffusion in the solid phase
  - Quench
Ca Effect to Mg-4.5wt.%Al

- $\gamma$ phase is less stable and prevented with Ca addition
- C36 phase forms in as cast sample
- C36 $\rightarrow$ C15 after reach equilibrium
Summary

- Mg-Al-Ca Ternary system was studied by using the CALPHAD, first-Principles, and experiments combined approach.

- C36-(Al,Mg)$_2$Ca ternary Laves phase was predicted.
- Magnesium database was constructed and used to understand the Ca addition effect to the phase stabilities of Mg alloys.
- Experimental observed good creep resistance of GM-C sample was successfully explained.