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

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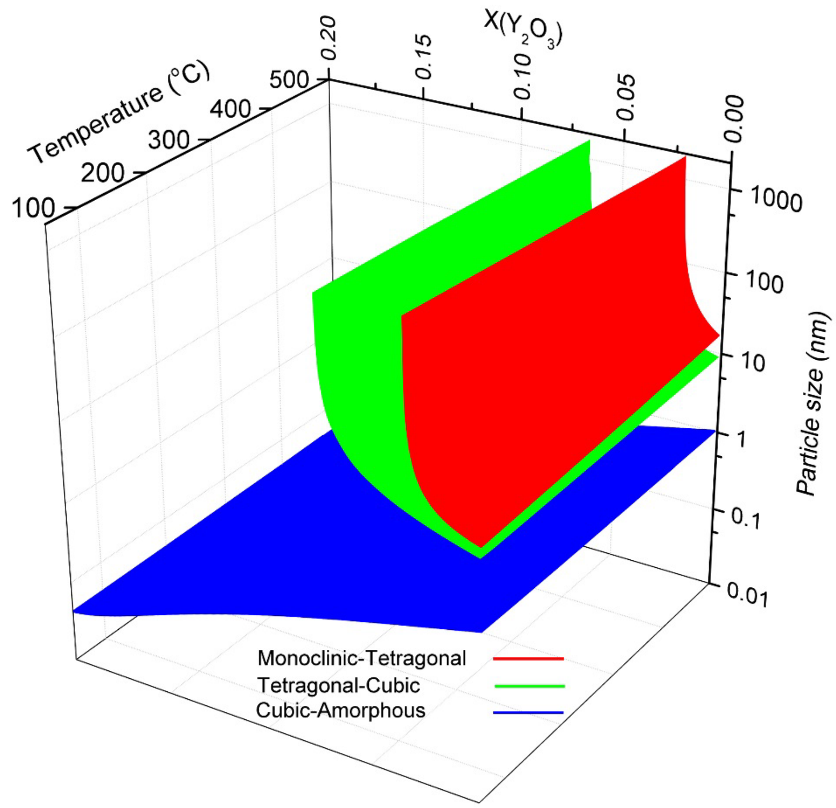
Self Introduction

- Ph.D. Penn State 2005
  - ICME approach to design new high creep resistance Mg alloys
- Saint Gobain HPM 2005-2013
  - Structural Ceramics: SiC, B_4C, Si_3N_4
  - 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



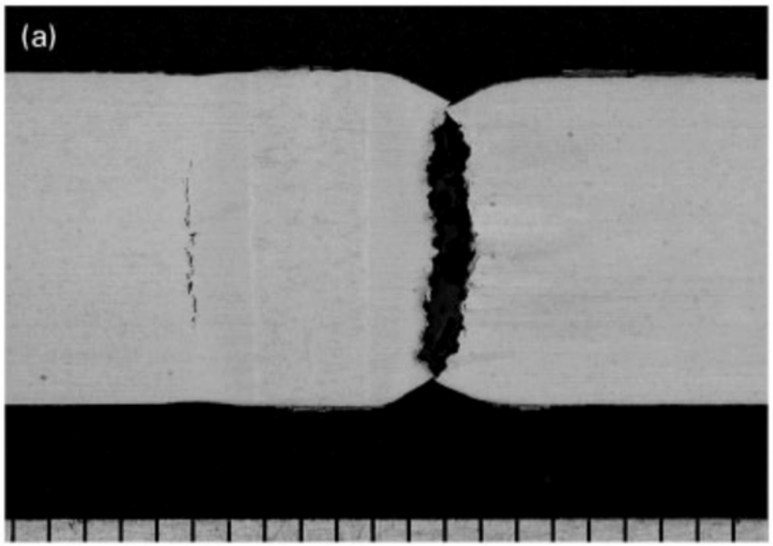
Outline

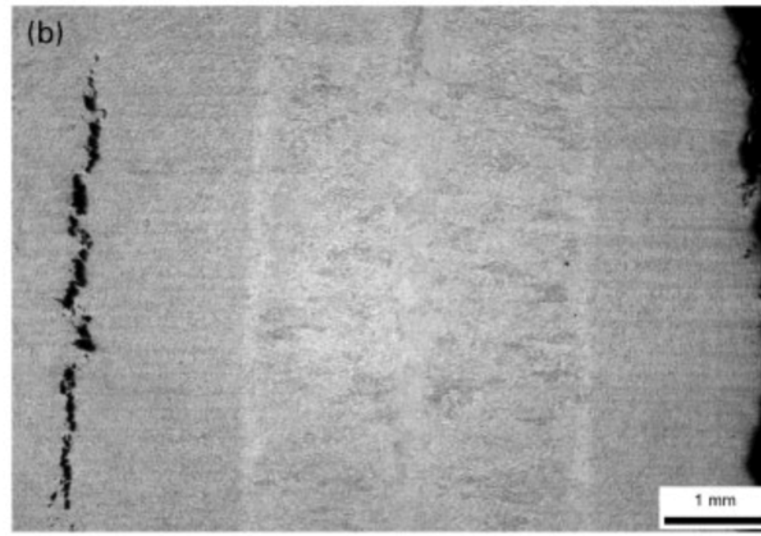
- Objective/Vision
- Background
- Team Description and Assignments
- Gantt Chart
- Milestones
- Previous Work (Creep Resistance of Mg alloys)

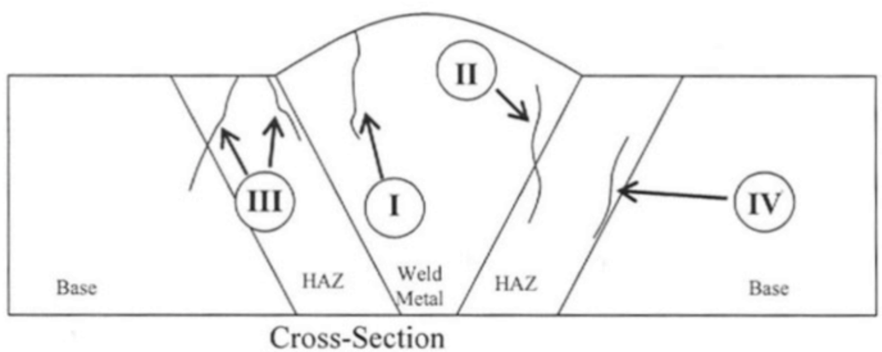
Objective/Vision

- 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

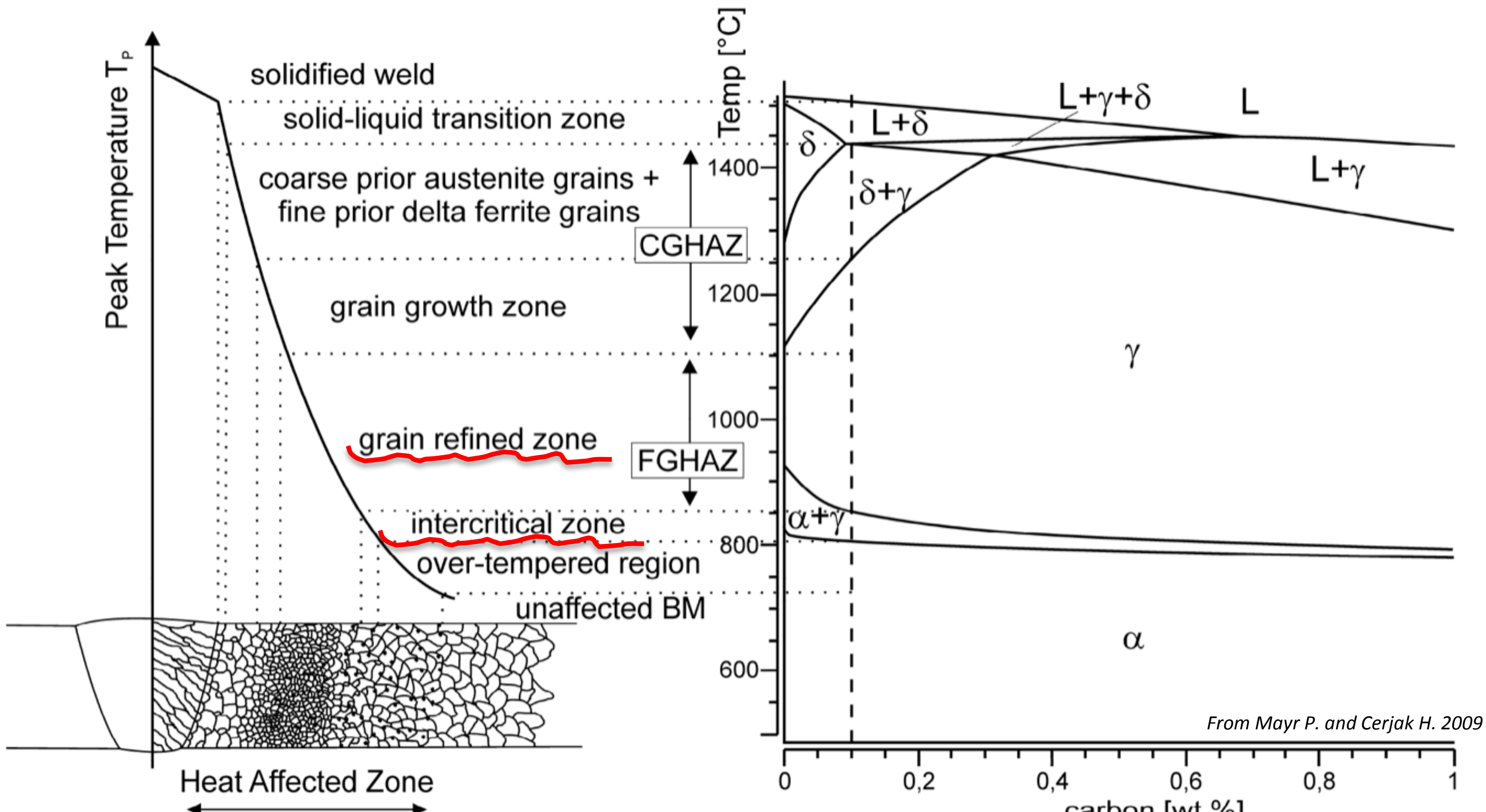






From D. J. Abson and J. S. Rothwell 2013

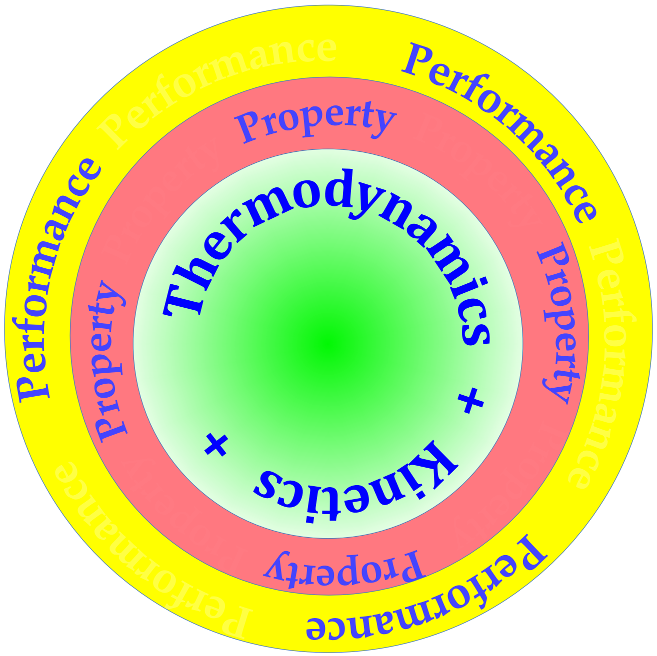
Microstructure of HAZ

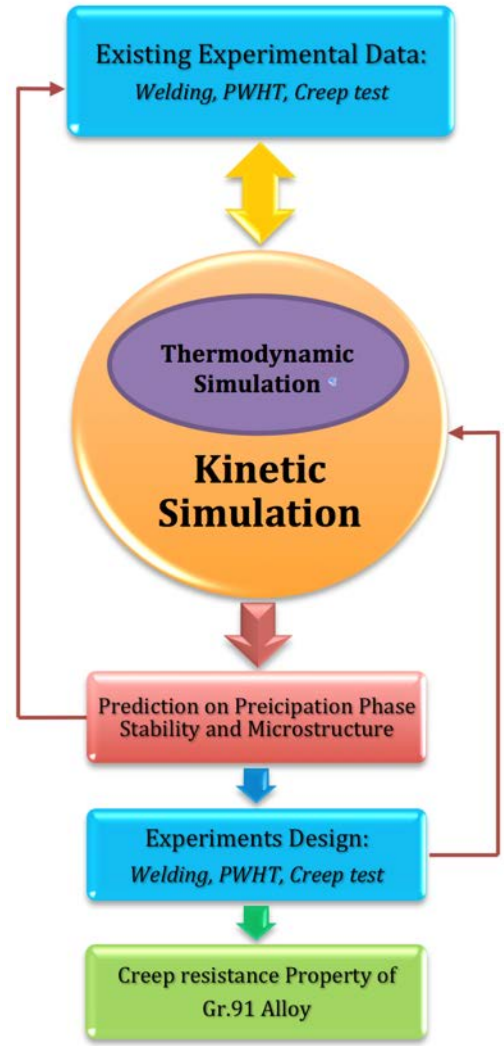


The fine $M_{23}C_6$ phase has the strengthen effect in the early life of the steels but it will coarsen quickly and therefore should not be treated as strengthen phase in the long-term operations

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





Team Description and Assignments

PI
Dr. Yu Zhong
FIU

Effective Communications

Subcontract
Prof. Wei Zhang
OSU

Graduate Student/Post-Doc

Graduate Student

Task 2. Literature Review

Task 3. Thermodynamic/Kinetic Simulations

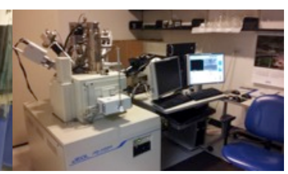
Subtask 4.2 Post-Weld Heat Treatment (PWHT)

Task 6. Characterization

Task 7. Model development and BEYOND

Subtask 4.1 Welding

Task 5. Creep Test



Subtask 7.1 Model Verification

Subtask 7.2 Prediction on the effect of Processing parameters

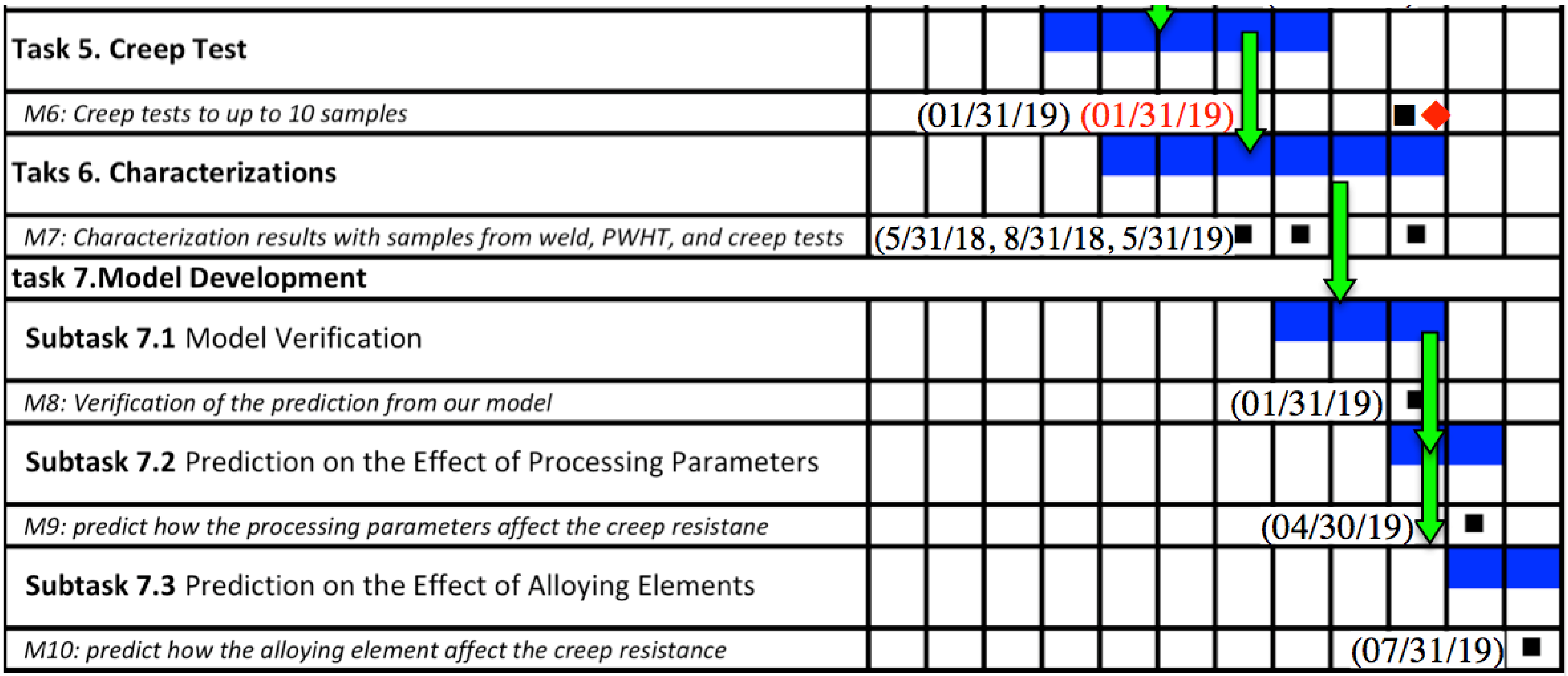
Subtask 7.3 Predictions on the effect of alloying elements

Mechanical and Materials Engineering
FLORIDA INTERNATIONAL UNIVERSITY

Gantt Chart

Task/Milestone	Project Timeline											
	Q1	Q2	Q3	Q4	Q5	Q6	Q7	Q8	Q9	Q10	Q11	Q12
Task 1. Project Management and Planning												
D1: Quarterly Reports	•	•	•	•	•	•	•	•	•	•	•	•
D2: Annual Progress Reports				•				•				
D3: Final Technical Report												•
Task 2. Literature Review												
M1: sceening all 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)					

Gantt Chart

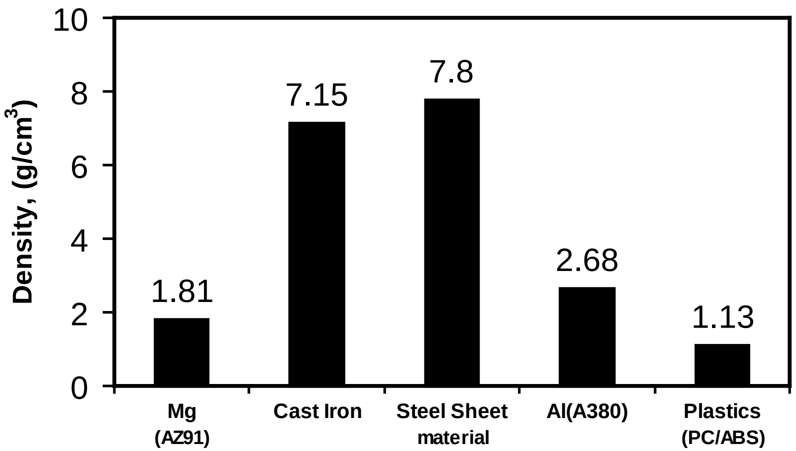

Task 5. Creep Test
M6: Creep tests to up to 10 samples
(01/31/19) (01/31/19)
Taks 6. Characterizations
M7: Characterization results with samples from weld, PWHT, and creep tests
(5/31/18, 8/31/18, 5/31/19)
task 7.Model Development
Subtask 7.1 Model Verification
M8: Verification of the prediction from our model
(01/31/19)
Subtask 7.2 Prediction on the Effect of Processing Parameters
M9: predict how the processing parameters affect the creep resistane
(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)

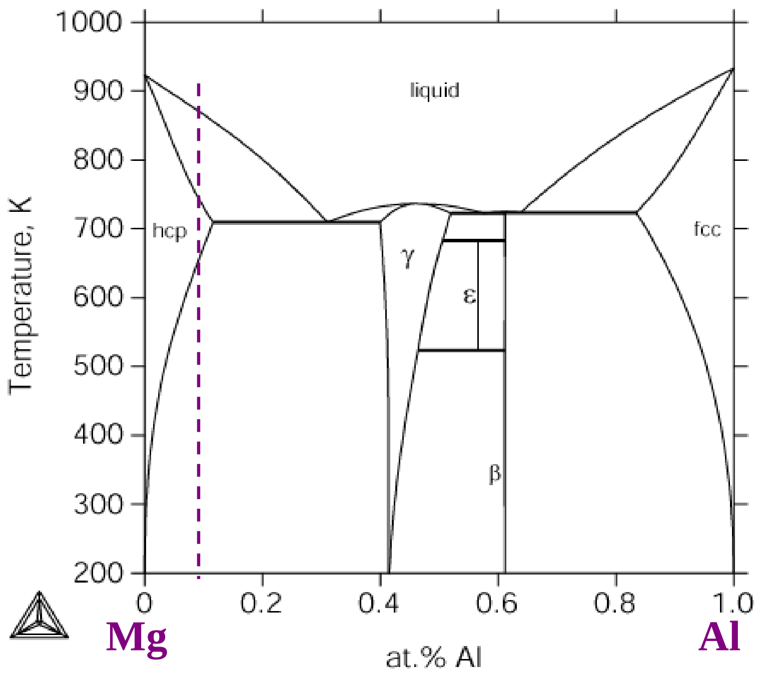
Milestones

Number	Task	Description
M1	Task 2	screening out all the reliable data for Gr.91 alloys from literature (01/31/2017)
M2	Subtask 3.1	Prediction on the stability of M23C6, MX and other metastable phases and intermediate phases (07/31/2017)
M3	Subtask 3.2	Prediction on the precipitates phase microstructure changes (01/31/2018)
M4	Subtask4.1	Welding of up to 20 steel plates (01/31/2018)
M5	Subtask 4.2	PWHT treatment for the welded samples (04/30/2018)
M6	Task 5	Creep test for up to 10 samples (01/31/2019)
M7	Task 6	Characterization results with samples from weld (05/31/2018), PWHT (08/31/2018), and creep tests (05/31/2019)
M8	Subtask 7.1	Verification of the prediction from our model (01/31/2019)
M9	Subtask 7.2	Prediction on the effect of processing parameters (04/30/2019)
M10	Subtask 7.3	Prediction on the effect of alloying elements (07/31/2019)

Previous Success on Mg Alloy

- ✓ Mg is one of the lightest structural materials.
- ✓ Increasing demand for magnesium alloys





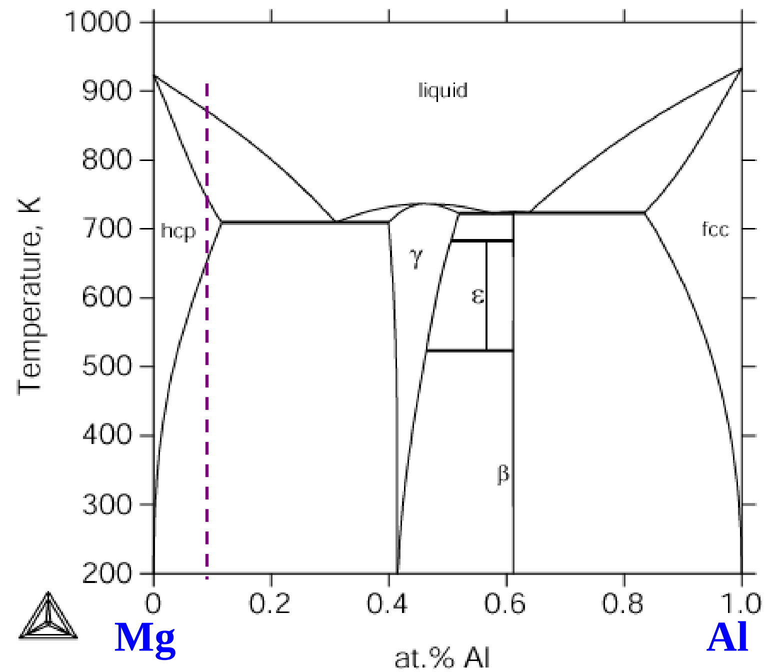
- Limited to use at low temperatures !!!

Approaches to Improve Creep Resistance

A. A. Luo, M. P. Balogh and B. R. Powell, *Metall. Mater. Trans. A*, 33, (2002) 567-574.

1. Suppress γ phase

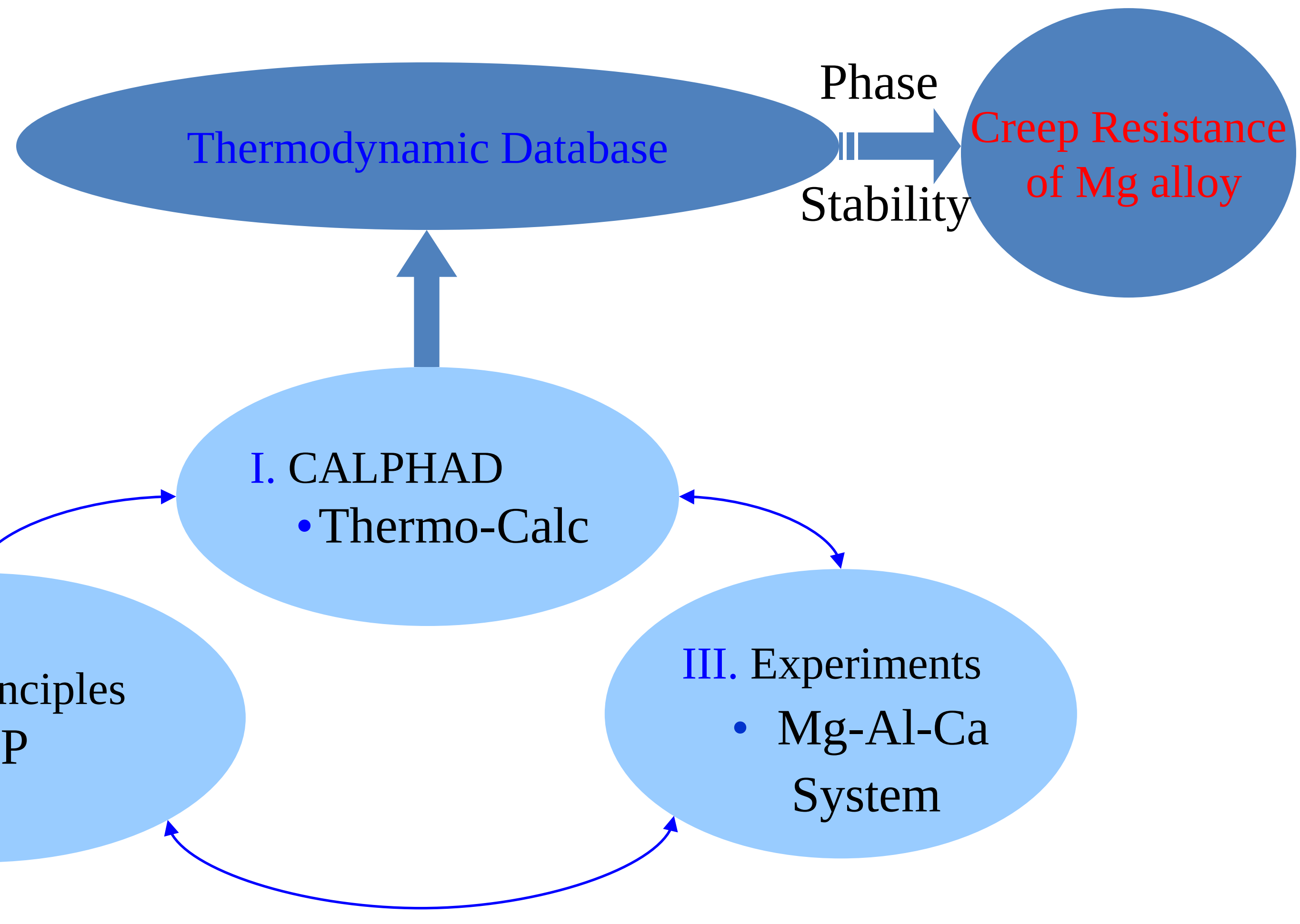
2. pin the sliding with High melting temperature phase



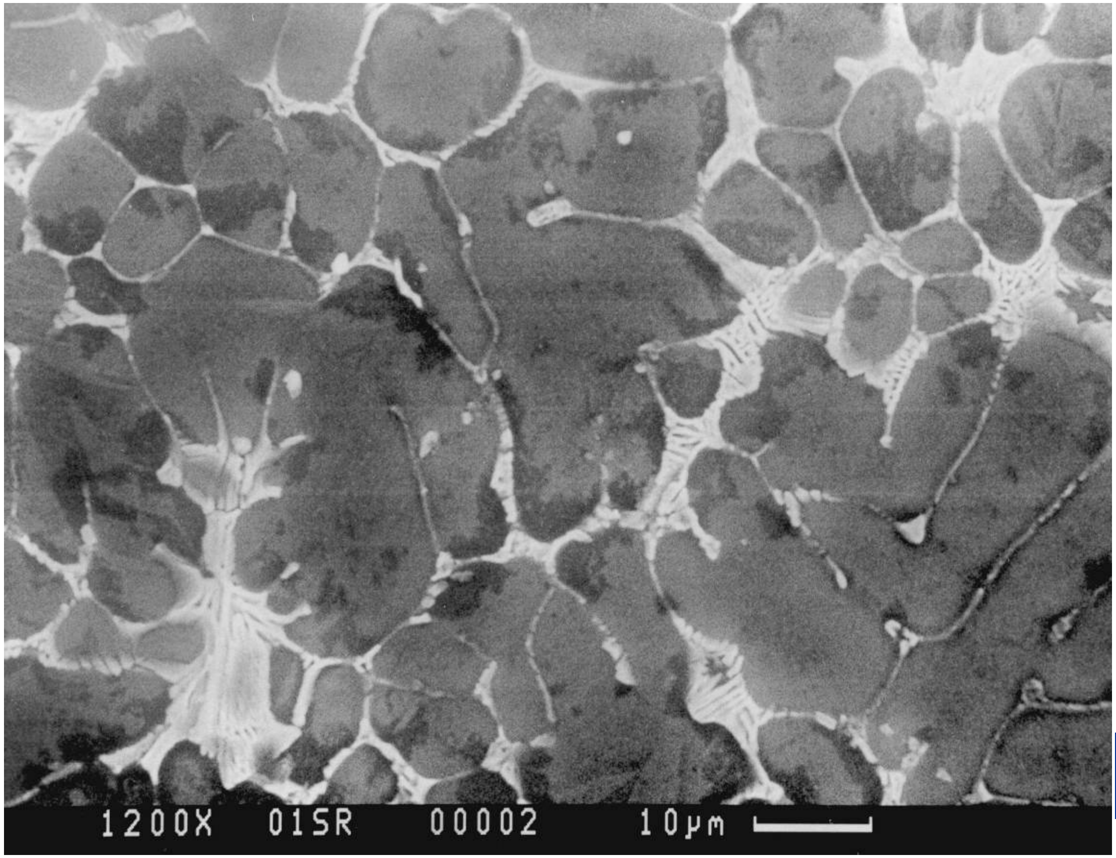
Addition of Rare-Earth elements-AE42(Mg-4wt.%Al-2wt.%RE)

Addition of Ca, Sr, or other elements

Approaches Used



Microstructure of Mg-Al-Ca alloy



Die Casting (GM-C)

Mg-4.5%Al-3.0%Ca

HCP matrix + Eutectic

In collaboration with

GM General Motors

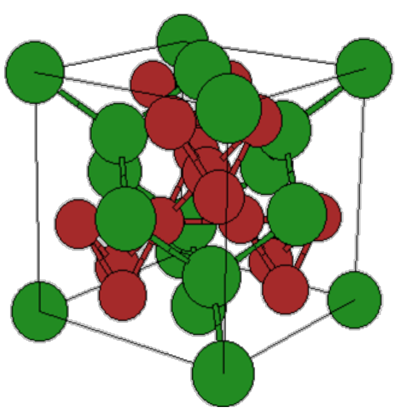
Experimental Observations

Ca effect to Mg-Al alloy

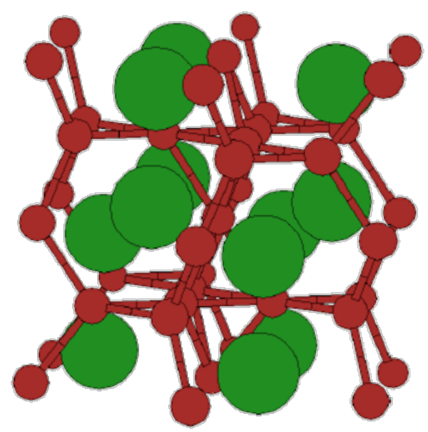
- AX51(Mg-5wt.%Al-0.8wt.%Ca)
  - Similar creep resistance to AE42
  - Al_2Ca C15 Laves phase is confirmed in as cast sample
- GM-C(Mg-4.5wt.%Al-3.0wt.%Ca)
  - Much better creep resistance than AE42
  - C36 Laves phase is found in the as cast sample
  - C36 Laves phase transformed into C15 Laves phase with heat treatment at high temperatures.

Laves Phases

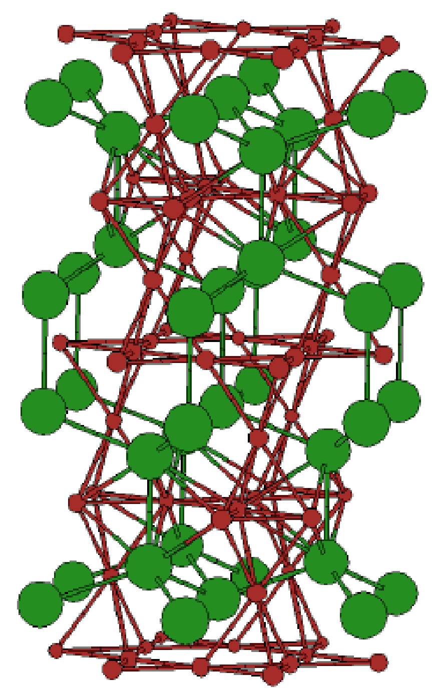
- Intermetallic A_2B compounds
- More than 1000 compounds in one of the three structures, C14, C15, and C36



C15



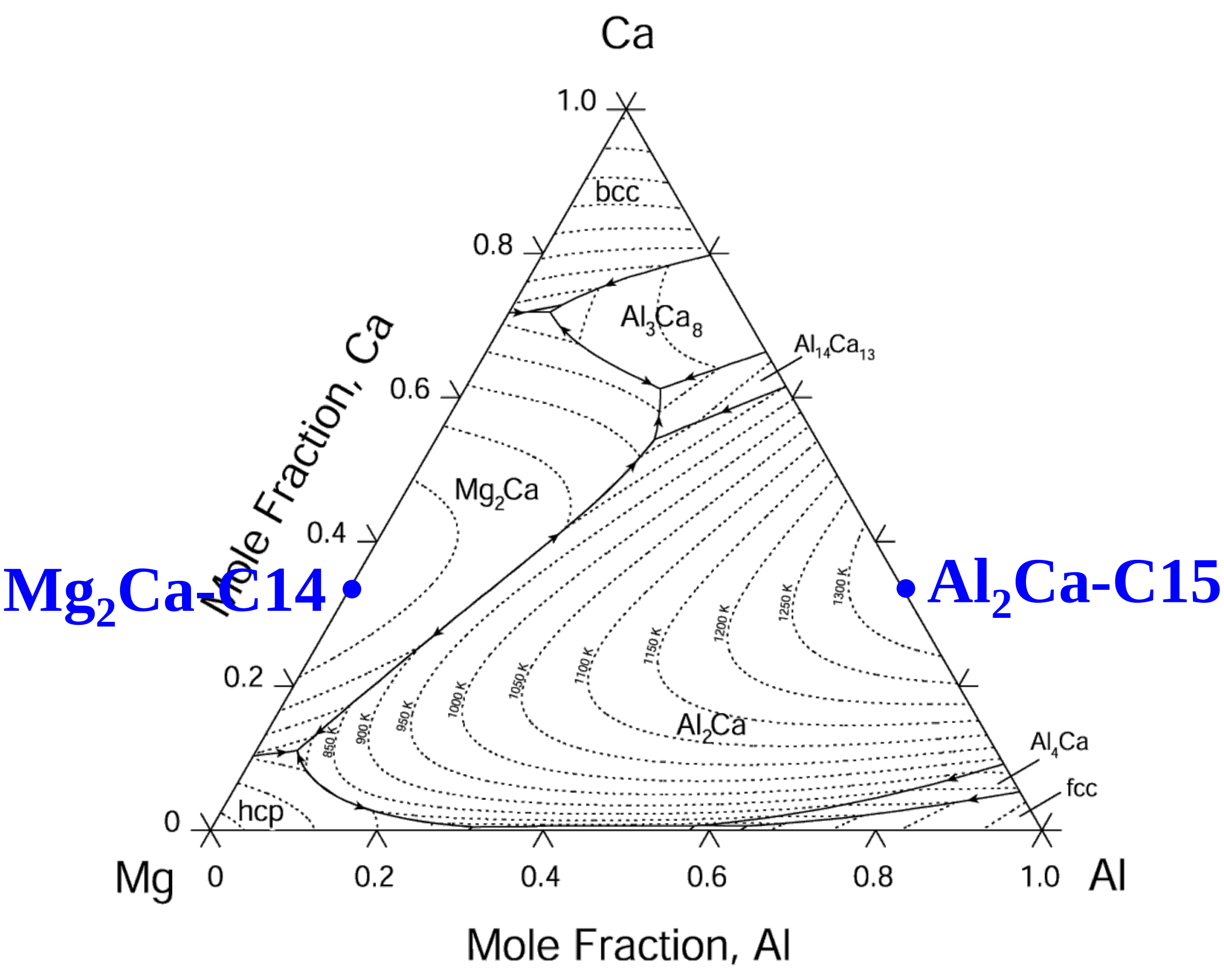
C14



C36

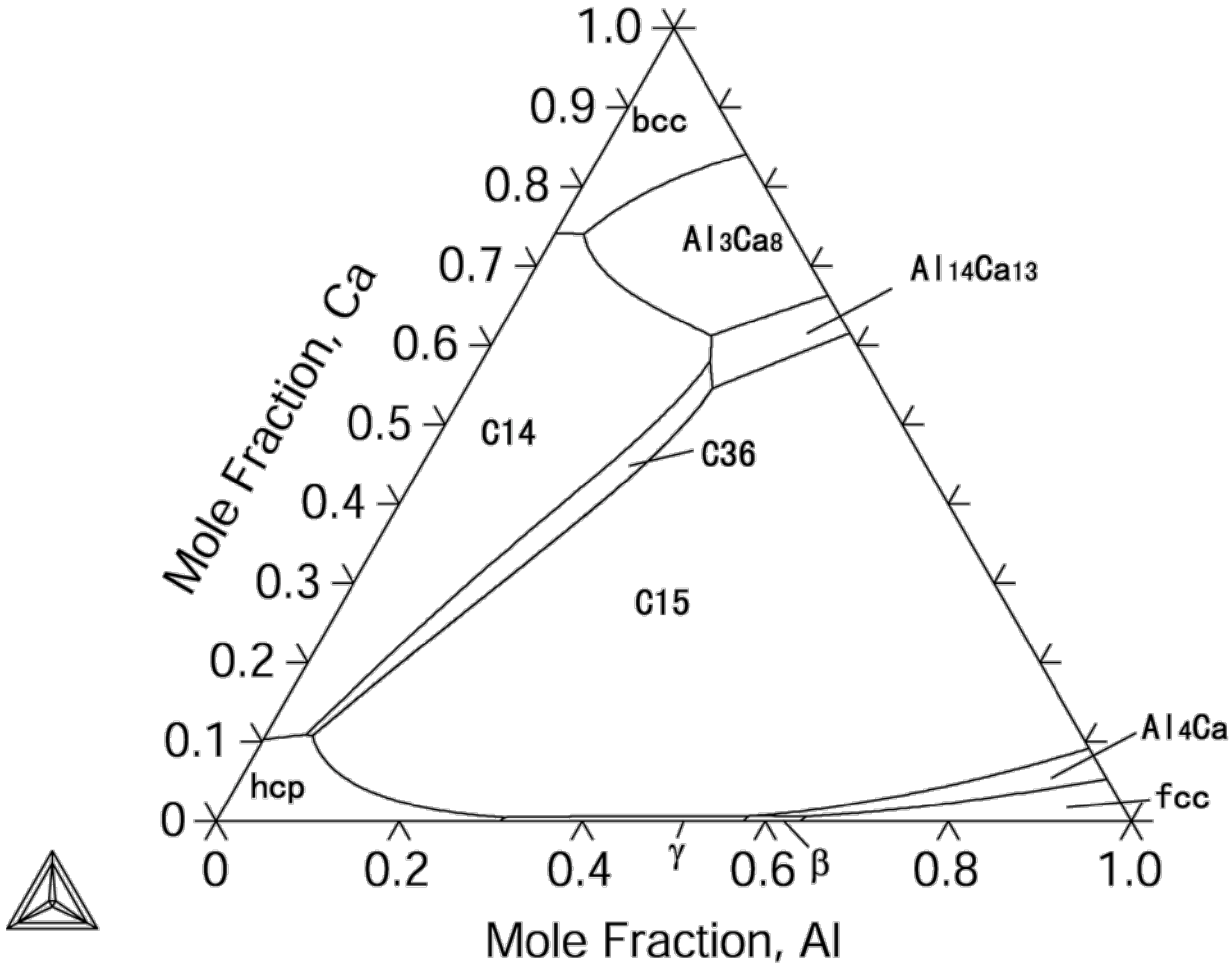
http://cst-www.nrl.navy.mil/lattice

2003 Mg-Al-Ca Database



Liquidus Projection

Updated Mg-Al-Ca Database

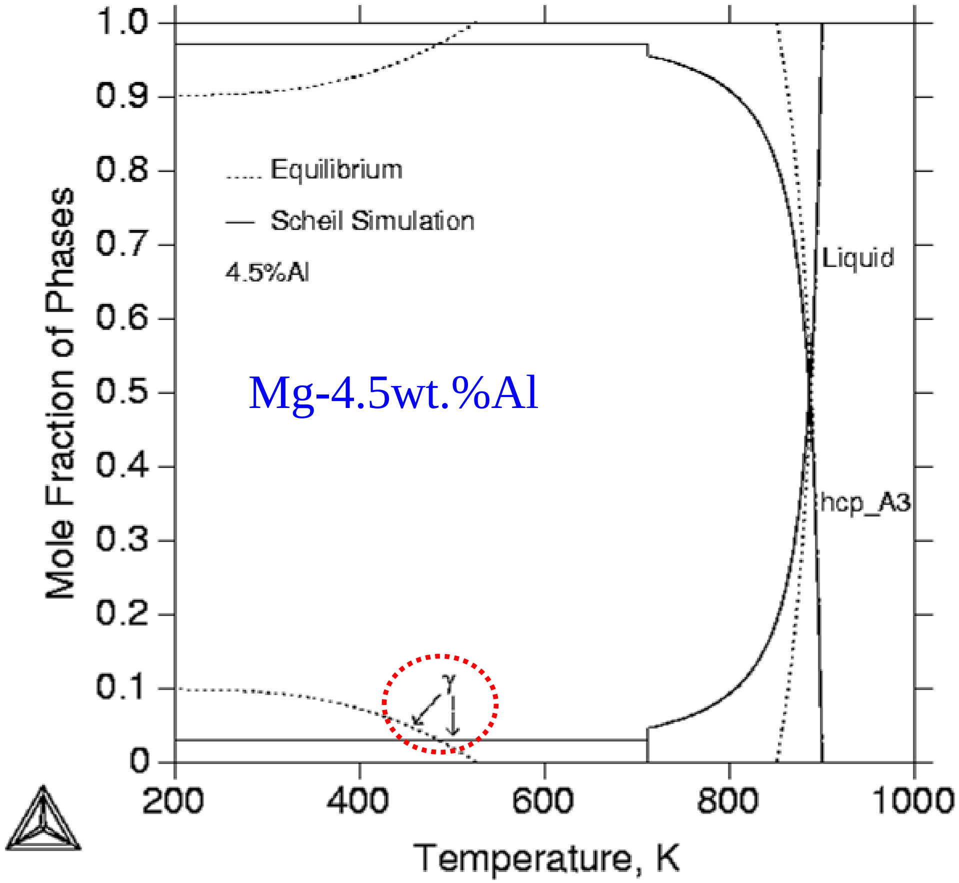


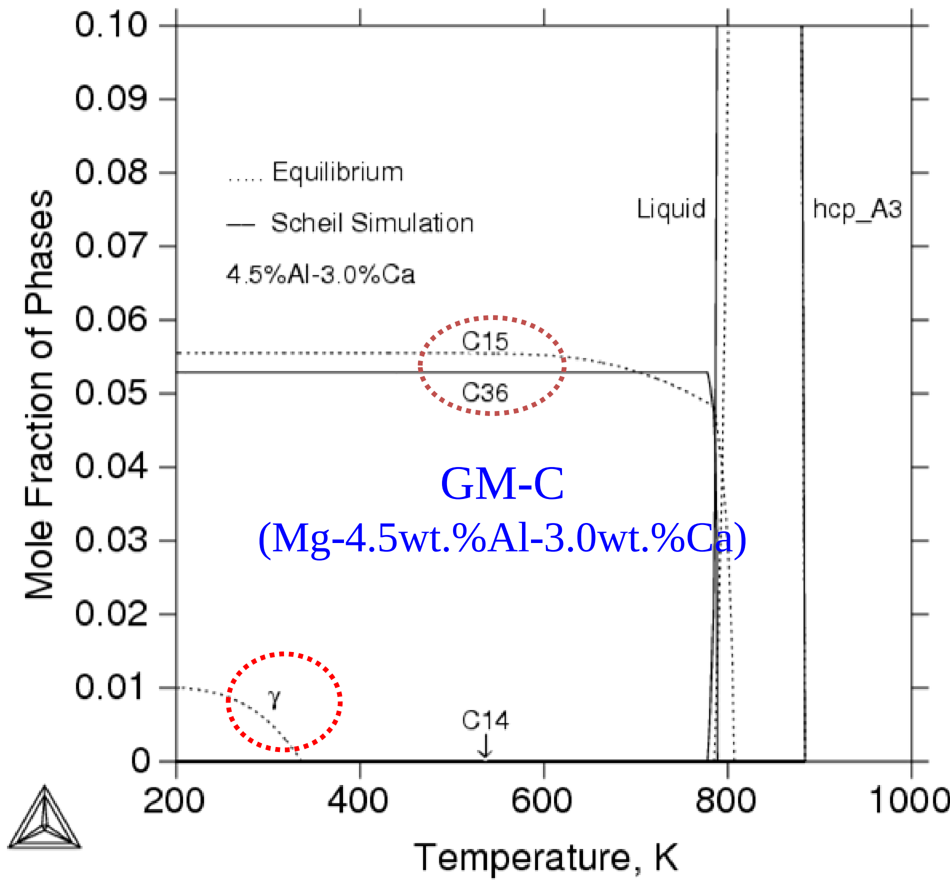
C36 Predicted by **Yu Zhong**, *First-Principles Investigation of Laves Phases in Mg-Al-Ca System*, TMS Annual Meeting, Charlotte, NC, March 19, 2004

Cooling Simulations

- Equilibrium cooling → Slow cooling
  - Global equilibrium between liquid and solid
- Scheil simulation → quench
  - Infinity fast diffusion in liquid
  - No diffusion in the solid phase

Ca Effect to Mg-4.5wt.%Al





- γ phase is less stable and prevented with Ca addition
- C36 phase forms in as cast sample
- C36 ➔ C15 after reach equilibrium

Summary

- Mg-Al-Ca Ternary system was studied by using the CALPHAD, first-Principles, and experiments combined approach.
    - C36-$(Al,Mg)_2Ca$ 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