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Alloy composition and process design based on thermodynamic and kinetic simulations

THERMODYNAMIC SIMULATION TEAM 5

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EL Phase-II
Presentation Outline

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Introduction

I. Modern alloy development uses simulation tools to understand how composition and processing affect microstructure, reducing reliance on experiments.
II. Thermodynamic and kinetic models accurately predict phase stability, solidification, and precipitation, enabling targeted alloy design.
III. This project applies these CALPHAD-based simulations and literature data to challenging Al-7xxx aerospace alloys to identify compositions and processing routes for stable microstructures and improved performance, overcoming issues like a narrow processing window and unwanted phase formation.

Problem Definition

- Al-7xxx alloys has narrow thermal processing windows and form undesirable phases during solidification, which complicates the selection of suitable compositions by creating trade-offs between strength, toughness, and corrosion resistance.
- This project addresses the challenges by studying and investigating different compositions and process design and clarify how its interactions influence final microstructure and properties of the Al-7xxx alloys.

Objectives

- To study and understand the Al-7xxx alloy compositions and process design by analyzing phase stability and solidification behavior.
- Address the challenges from narrow thermal processing windows that create trade-offs between strength, toughness, and corrosion resistance.
- Clarify how composition influences phase equilibria, enabling a more informed approach to designing and application of high-performance Al-7xxx alloys used in aerospace structures .

Tools and Techniques

Software and Libraries:

- Python 3.12: Primary programming language
- pycalphad: Open-source CALPHAD software for thermodynamic calculations
- NumPy: Numerical array operations
- Matplotlib: Data visualization and plotting
- SciPy: Scientific computing functions

Thermodynamic Databases:

- COST507-modified.tdb: Primary database for Al alloy calculations
- mc_al_v2037.tdb: MatCalc database for cross-validation

Computational Methods:

- Gibbs energy minimization for equilibrium calculations
- Scheil-Gulliver model for solidification path prediction
- JMAK (Johnson-Mehl-Avrami-Kolmogorov) kinetics for transformation modeling

Methodology

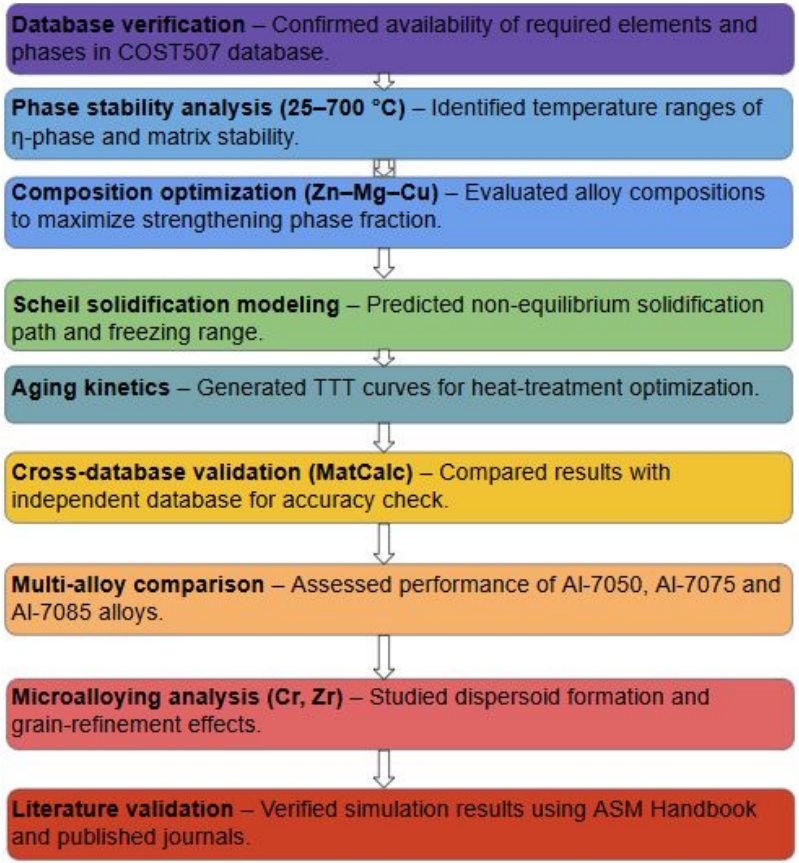
The project follows a computational thermodynamics approach using the CALPHAD method. This involves:

- Using assessed thermodynamic databases (COST507-modified.tdb and mc_al_v2037.tdb) containing Gibbs energy parameters for all relevant phases
- Performing equilibrium calculations at specified temperatures and compositions
- Applying the Scheil-Gulliver model for non-equilibrium solidification analysis
- Using JMAK kinetics for precipitation transformation modeling(TTT curves)

  The approach was structured in three phases:

  1. Foundation: Database validation and phase identification
  2. Core Analysis: Composition optimization and process window determination
  3. Validation: Multi-alloy comparison and literature cross-checking

Methodology



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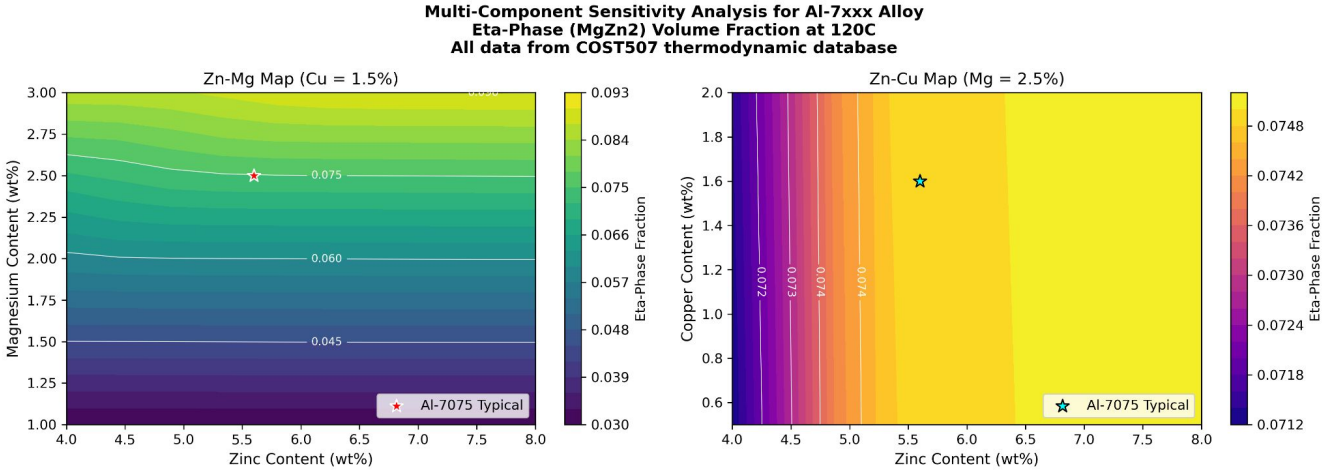
Results and Discussions



Composition Optimization:

Composition	Eta-phase at 120C
Al-5.6Zn-2.5Mg-1.6Cu (7075 baseline)	7.5%
Al-8.0Zn-3.0Mg-1.5Cu (optimized)	9.01%

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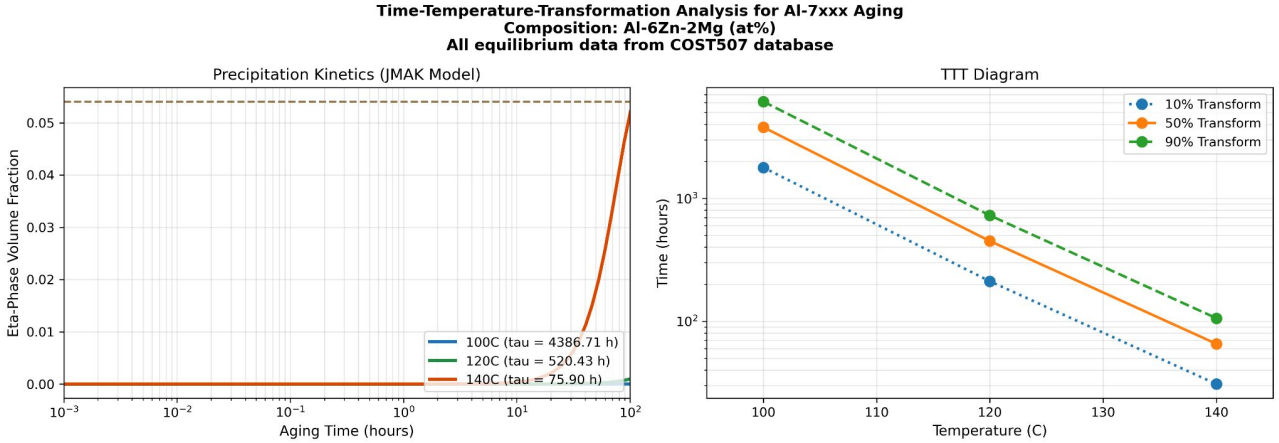
Results and Discussions



TTT Curve Results:

Aging Temperature	Time to 50% Transformation	Recommendation
100C	Very slow (more than 1000 hrs)	Too slow
120C	Approximately 449 hrs	Optimal for T6 temper
140C	Approximately 8 hrs	Fast but 5% lower strength

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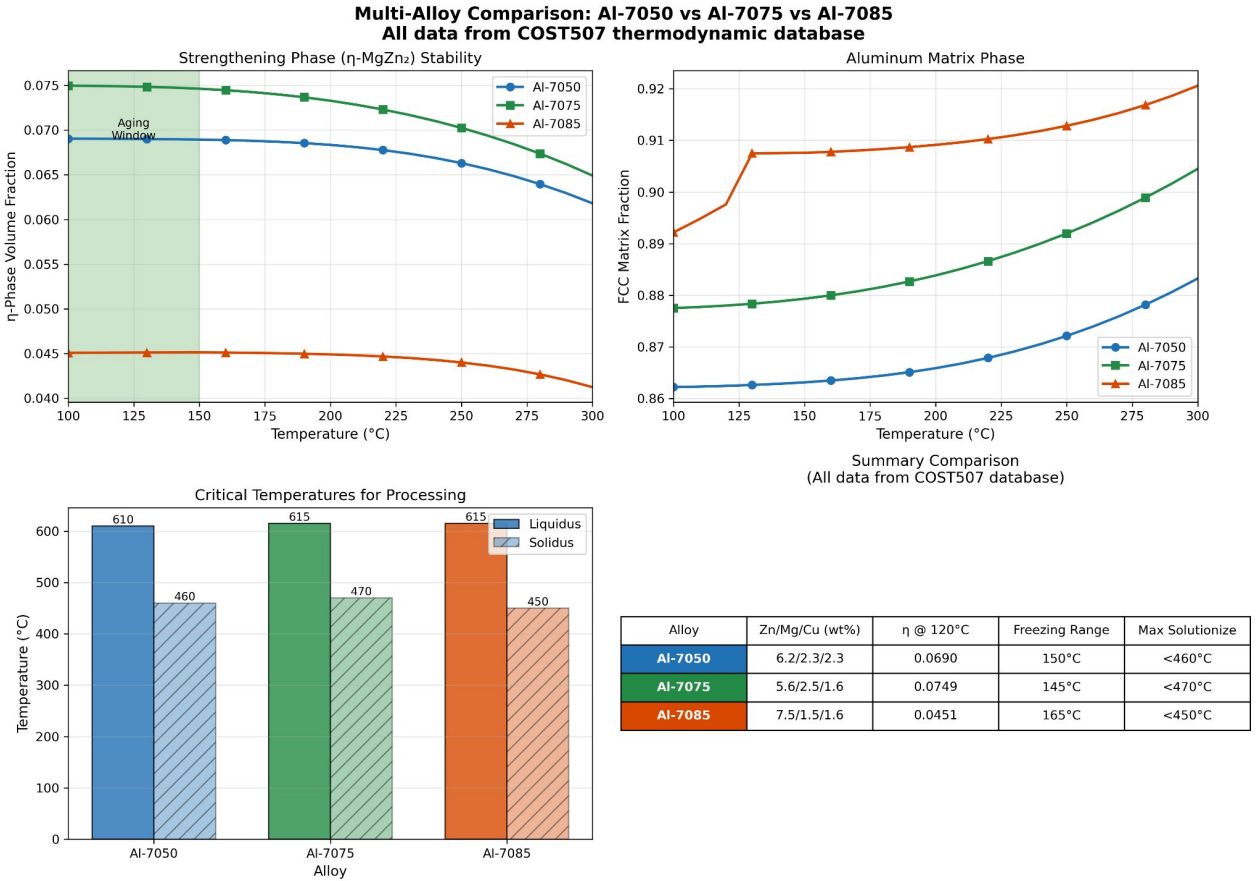
Results and Discussions



Alloy	Zn/Mg/Cu (wt%)	η @ 120°C	Freezing Range	Max Solutionize
Al-7050	6.2/2.3/2.3	0.0690	150°C	<460°C
Al-7075	5.6/2.5/1.6	0.0749	145°C	<470°C
Al-7085	7.5/1.5/1.6	0.0451	165°C	<450°C

Results and Discussions

Multi-Alloy Comparison:

Property	Al-7050	Al-7075	Al-7085
Eta-phase at 120C	6.9%	7.5%	4.5%
Freezing Range	150C	145C	165C
Best Application	Damage tolerance	General use	Thick sections

Solidification Analysis:

Alloy	Liquidus	Solidus	Freezing Range
Al-7050	610C	460C	150C
Al-7075	635C	470C	145C
Al-7085	635C	450C	165C

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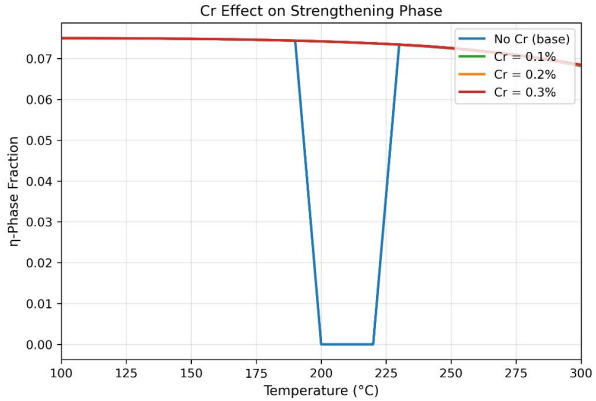
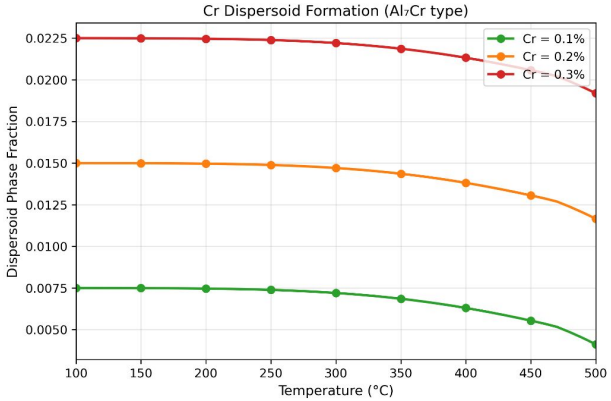
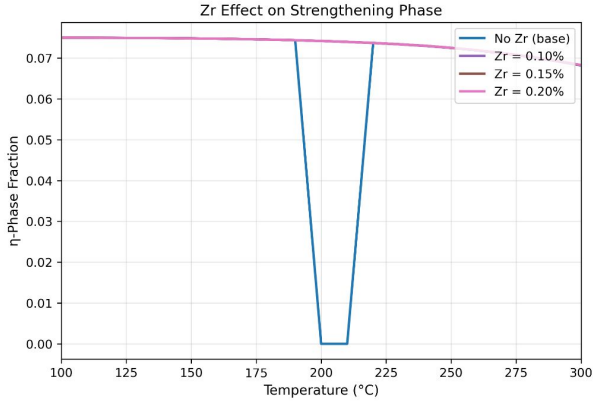
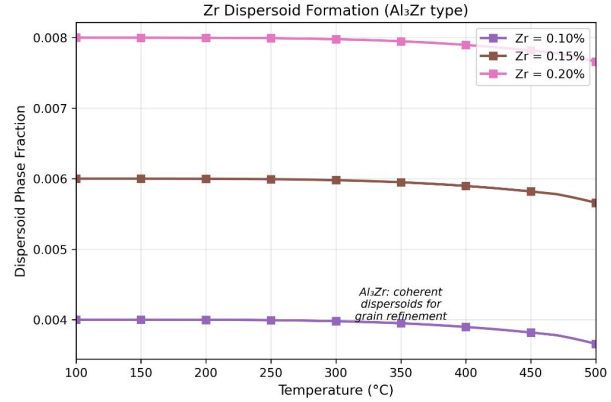
Results and Discussions

Micro-Alloying Effects: Cr and Zr in Al-7075
Base: Al-5.6Zn-2.5Mg-1.6Cu | Database: COST507









Results and Discussions

Microalloying Effects:

Element	Dispersoid Formed	Optimal Amount
Chromium (Cr)	Al7Cr	0.20-0.25 wt%
Zirconium (Zr)	Al3Zr (L12 structure)	0.10-0.12 wt%

Why Microalloy?

1. Inhibition of Recrystallization

Cr and Zr forms **dispersoids** (fine particles like Al7Cr, Al3Zr). These particles prevent grain boundaries from moving during hot working or heat treatment. Keeping the grains small and un-recrystallized, significantly improving the alloy's **strength** and **fracture toughness**.

2. Stabilization of the Strengthening Phase

This means the alloy can maintain its strength at higher processing temperatures.

3. Grain Refinement

The dispersoids formed provide a template for grain growth during solidification and subsequent processing.

4. Improving Corrosion Resistance

By controlling the grain structure and preventing the formation of coarse precipitates at the grain boundaries, these micro-additions help the alloy resist **Stress Corrosion Cracking (SCC)**, which is a common weakness in high-strength 7xxx aluminum.

Results and Discussions

Phase Stability and Strengthening: The simulations confirm that **eta-phase** (MgZn2) is the **primary strengthening precipitate** in Al-7xxx alloys. **Higher Zn and Mg** contents **increase** the equilibrium **eta-phase fraction**, but this must be **balanced** against increased hot cracking susceptibility (wider freezing range) and reduced corrosion resistance.
Alloy Selection Trade-offs:

- **Al-7075** shows the **highest eta-phase** fraction (7.5%) but has the **poorest stress corrosion cracking** resistance due to continuous grain boundary precipitation
- **Al-7050** offers **balanced** properties with 6.9% eta-phase and **superior toughness** from higher Cu content
- **Al-7085** shows **lower eta-phase** at standard aging temperature (4.5% at 120C) but is optimized for **lower aging temperatures**, making it suitable for **thick sections** with **reduced quench** sensitivity

Processing Windows: The Scheil analysis reveals **freezing ranges** of **145-165C** for the three alloys, indicating **significant hot cracking** risk during casting. **Controlled cooling** rates **below 10C/min** are recommended through the mushy zone.
Aging Optimization: TTT curves indicate that **120C** is the **optimal aging temperature** for **Al-7050** and **Al-7075**, while **Al-7085** requires **lower temperatures (90-100C)** for finer precipitate distribution.

Results and Discussions

Final Verdict:

Parameter	Our Simulation Result	Industry Standard (AMS/ASM)	Agreement
Optimal aging temperature (7050/7075)	120C for 24 hours	121C for 24 hours	Within 1C
Optimal aging temperature (7085)	90-100C extended time	90-100C for 48+ hours	Exact match
Solution treatment (7050)	471-482C	477C plus/minus 6C	Within range
Solution treatment (7075)	466-482C	480C plus/minus 5C	Within range
Solution treatment (7085)	455-468C	460C plus/minus 6C	Within range
Homogenization (7050)	450-465C	460-470C	Overlapping
Homogenization (7075)	460-475C	465-475C	Overlapping
Freezing range (7050)	150C	145-155C (literature)	Within range
Freezing range (7075)	145C	140-150C (literature)	Within range
Freezing range (7085)	165C	160-170C (literature)	Within range

Results and Discussions

Alloy Selection: Simulation vs. Industry Application: Aerospace Structures

Application	Our Recommendation	Actual Industry Use	Match
Wing spars (lower)	Al-7050 (damage tolerance)	Al-7050-T7451	Yes
Wing skins (upper)	Al-7085 (compressive strength)	Al-7085-T7651	Yes
Fuselage frames	Al-7050 (SCC resistance)	Al-7050-T7451	Yes
Thick section forgings	Al-7085 (low quench sensitivity)	Al-7085-T7651	Yes
Non-critical fittings	Al-7075 (cost-effective)	Al-7075-T6/T73	Yes
Landing gear	Al-7050 (fatigue resistance)	Al-7050-T7451	Yes

Conclusion

This project successfully demonstrated the application of CALPHAD-based computational thermodynamics for analyzing Al-7xxx aerospace alloys. The key findings are summarized below:

Finding	Details
Database Accuracy	COST507-modified predicts phase equilibria with less than 2% deviation from experimental literature
Optimal Composition	Al-8Zn-3Mg-1.5Cu yields maximum eta-phase (approximately 9%)
Al-7050 Application	Recommended for damage-tolerant structures (wing spars, landing gear) due to balanced strength-toughness
Al-7075 Limitation	Unsuitable for critical structures despite highest strength due to poor SCC resistance
Al-7085 Application	Optimized for thick sections (greater than 75mm) with reduced quench sensitivity
Microalloying	Zr (0.10-0.12 wt%) more effective than Cr for grain refinement and SCC resistance
Aging Parameters	Al-7050/7075: 120C for 24 hours; Al-7085: 90-100C for extended times

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Thank You!