

Alloy composition and process design based on thermodynamic and kinetic simulation.

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ABSTRACT Aluminum 7xxx series alloys are the backbone of modern aerospace structures, prized for their incredible strength-to-weight ratios. This strength is primarily derived from tiny strengthening particles known as the eta-phase ($MgZn_2$) that form within the metal during heat treatment. Traditionally, designing these alloys is a slow and costly process of trial and error due to very narrow thermal processing windows and manufacturing risks like hot cracking. This project shifts that approach by using a computational method called CALPHAD to simulate and predict material behavior before any physical testing begins. Using the pycalphad library alongside the COST507-modified thermodynamic database, we systematically mapped out phase stability and solidification behavior for the Al-Zn-Mg-Cu system. Our analysis identified an optimized composition of Al-8.0Zn-3.0Mg-1.5Cu (weight percentage), which achieves a peak strengthening phase fraction of 9.01%. To ensure this strength is realized in production, we established clear manufacturing guidelines: a narrow solutionizing window between 450 and 460 degrees Celsius to avoid melting, and a peak aging treatment of 24 hours at 120 degrees Celsius. To ensure the reliability of these predictions, we cross-validated our results against independent databases and established experimental literature, such as the ASM Handbook. The simulations showed exceptional accuracy, with critical temperatures and phase fractions matching published data within a 1% to 2% margin of error. By providing a validated roadmap for alloy design and processing, this study demonstrates how computational tools can significantly reduce development time and help engineers create more stable, high-performance materials for the next generation of aircraft.

INDEX TERMS Al-7xxx Alloy, eta-phase, CALPHAD, pycalphad, Solidification, Microalloying, Database Validation, TTT Diagram.

I. INTRODUCTION

Aluminum 7xxx series alloys are indispensable in the aerospace industry, primarily due to their exceptional strength-to-weight ratios and high fatigue resistance. These properties are predominantly derived from the formation of fine eta-phase ($MgZn_2$) precipitates within the aluminum matrix through specific precipitation-hardening processes. However, the development and processing of these materials are often complicated by narrow thermal windows and the risk of undesirable phase formation, which can lead to manufacturing challenges such as hot cracking. This project addresses these complexities by analyzing phase stability and solidification behavior to enable more informed alloy design and processing.

The methodology follows a computational thermodynamics approach centered on the CALPHAD (calculation of phase diagrams) methodology to predict material behavior. Simulations are performed using pycalphad library in conjunction with the COST507-modified thermodynamic database, which provides assessed Gibbs energy parameters for multicomponent systems including aluminum, zinc, magnesium, and copper. This foundational framework allows for the identification of equilibrium phase fractions and the prediction of non-equilibrium solidification paths using the Scheil-Gulliver model.

A primary objective of the work is the systematic optimization of alloy compositions and thermal processing parameters. Through extensive mapping of phase stability regions, the study identified an optimal composition of Al-

8.0Zn-3.0Mg-1.5Cu (wt%), which achieves a maximum eta-phase fraction of approximately 9.01% at an aging temperature of 120°C. Furthermore, the analysis provides critical data on freezing ranges for aerospace alloys such as Al-7050, Al-7075, and Al-7085, highlighting high hot cracking risks and the necessity for controlled cooling rates during manufacturing.

The final outcomes include the definition of safe processing windows and the generation of Time-Temperature-Transformation (TTT) curves for aging heat treatment optimization. These simulation results have been rigorously validated against published experimental literature and independent databases, showing a high level of agreement with deviations often less than 2% for critical parameters. By establishing clear guidelines for solutionizing at 450–460°C and peak aging at 120°C for 24 hours, this simulation-based method provides an industrially relevant tool for material selection and the future development of high-performance aerospace structures.

II. GUIDELINES FOR MANUSCRIPT PREPARATION

1. Optimized Alloy Composition

- **Target Composition:** For maximum strengthening potential, use the optimized ratio of **Al-8.0Zn-3.0Mg-1.5Cu (wt%)**.
- **Strengthening Phase:** This composition is designed to yield a peak eta-phase (MgZn₂) fraction of approximately **9.01%** at 120°C.
- **Standard Comparison:** Standard Al-7075 (7.5% eta-phase) remains a balanced choice for applications requiring higher corrosion resistance.

2. Thermal Processing Windows

- **Solutionizing Treatment:**
 - **Temperature:** Maintain between **450°C and 460°C**.
 - **Duration:** Hold for **1 to 2 hours** to fully dissolve precipitates.
 - **Critical Limit:** Do not exceed **465°C** to avoid incipient melting, as the safe processing window is extremely narrow (less than 15°C margin from the solidus temperature).
- **Aging Treatment (T6 Temper):**
 - **Optimal Setting:** **120°C for 24 hours** for standard alloys like 7050 and 7075.

- **Rapid Aging: 140°C for 8 to 10 hours** may be used for faster processing, though it results in approximately **5% lower hardness**.
- **Al-7085 Exception:** This specific alloy requires lower temperatures (**90°C–100°C**) for extended times (48+ hours) to achieve optimal precipitate distribution.

3. Solidification and Casting Control

- **Freezing Range Awareness:** Al-7xxx alloys exhibit wide freezing ranges (**145°C–165°C**), indicating a high susceptibility to **hot cracking**.
- **Cooling Rates:** Controlled cooling rates below **10°C/min** are recommended through the "mushy zone" (between liquidus and solidus) to minimize manufacturing risks.
- **Homogenization:** For Al-7050, a homogenization temperature of **450°C–465°C** is recommended to reduce microsegregation.

4. Microalloying for Structural Integrity

- **Zirconium (Zr):** Add **0.10–0.12 wt%** to form Al_3Zr dispersoids, which are highly effective for grain refinement and stress corrosion cracking (SCC) resistance.
- **Chromium (Cr):** Add **0.20–0.25 wt%** to inhibit recrystallization through Al_7Cr dispersoid formation.
- **Combined Additions:** Utilizing both Zr and Cr is recommended for optimal control of the grain structure in alloys like Al-7050.

5. Risk Mitigation Summary

- **Incipient Melting:** Always keep solutionizing temperatures at least **15°C below the predicted solidus** temperature.
- **Overaging:** Avoid excessive time at temperatures above 140°C, which leads to coarse η -phase precipitates and reduced strength.
- **Hot Cracking:** Use the calculated liquidus and solidus temperatures for each specific alloy (e.g., **635°C/470°C for Al-7075**) to set safe casting parameters.

A. ABBREVIATIONS AND ACRONYMS

- **AMS:** Aerospace Material Specification.
- **CALPHAD:** CALculation of PHase Diagrams.
- **FCC:** Face-Centered Cubic (crystal structure).
- **TTT:** Time-Temperature-Transformation (curves).
- **wt%:** Weight Percentage.
- **ICME:** Integrated Computational Materials Engineering.
- **SCC:** Stress Corrosion Cracking.

B. OTHER RECOMMENDATIONS

Alloy Selection by Application

- **Wing Spars and Landing Gear:** Al-7050 is recommended for these components due to its superior damage tolerance and balanced strength-toughness properties.
- **Wing Skins (Upper):** Al-7085 is the optimal choice for wing skins requiring high compressive strength.
- **Thick Section Forgings:** Al-7085 is highly recommended for sections greater than 75mm because of its low quench sensitivity.
- **General Structural Components:** Al-7075 remains a cost-effective and balanced choice for non-critical fittings and general-purpose aerospace applications.

Industrial Processing Guidelines

- **Solutionizing Precision:** Maintain solution treatment temperatures strictly between 450°C and 460°C to ensure precipitates dissolve while avoiding the "danger zone" of incipient melting starting at 465°C.
- **Peak Aging (T6):** Use a treatment of 120°C for 24 hours for Al-7050 and Al-7075 to achieve maximum hardening.
- **Low-Temperature Aging:** For Al-7085, utilize lower aging temperatures (90°C–100°C) for extended durations (48+ hours) to ensure a fine precipitate distribution.
- **Cooling Rate Control:** During casting or welding, implement controlled cooling rates below 10°C/min through the mushy zone to mitigate the high risk of hot cracking caused by wide freezing ranges.

Alloy Design and Composition

- **Strengthening Optimization:** For maximum strength potential, utilize the optimized

composition of Al-8Zn-3Mg-1.5Cu, which yields a peak strengthening phase fraction of approximately 9%.

- **Microalloying Strategy:** Prioritize Zirconium (Zr) additions between 0.10 and 0.12 wt% over Chromium (Cr) for more effective grain refinement and improved stress corrosion cracking (SCC) resistance.
- **Combined Dispersoid Control:** Use a combination of Cr (0.20-0.25 wt%) and Zr to provide the most robust control over recrystallization and grain structure in complex alloys like Al-7050.

Future Work and Development

- **ICME Integration:** This simulation framework should be integrated into industrial Integrated Computational Materials Engineering (ICME) workflows to reduce the need for expensive trial-and-error experiments.
- **Extended Validation:** While the current thermodynamic predictions are highly accurate, further experimental heat treatment studies are recommended to fully validate the aging kinetics for new, non-standard compositions.

III. MATH

If you are using *Word*, use either the Microsoft Equation Editor or the *MathType* add-on (<http://www.mathtype.com>) for equations in your paper (Insert | Object | Create New | Microsoft Equation or MathType Equation). "Float over text" should *not* be selected.

A. EQUATIONS

1. Thermodynamics and Phase Equilibrium

- **Gibbs Free Energy:** $G = H - TS$
- **Gibbs Energy of Mixing:** $\Delta G_{\text{mix}} = \Delta H_{\text{mix}} - T\Delta S_{\text{mix}}$
- **Ideal Mixing:** $\Delta G_{\text{mix}}^{\text{ideal}} = RT \sum x_i \ln(x_i)$
- **Gibbs Phase Rule:** $F = C - P + 2$
- **Lever Rule:** $f_{\alpha} = \frac{C_{\beta} - C_0}{C_{\beta} - C_{\alpha}}$

2. Kinetics and Transformation

- **Arrhenius Equation (Diffusion):** $D = D_0 \exp(-Q/RT)$
- **JMAK Equation (Transformation Progress):** $f(t) = 1 - \exp[-(t/\tau)^n]$
- **LSW Theory (Coarsening):** $\bar{r}^3 - r_0^3 = Kt$

IV. UNITS

- Degrees Celsius ($^{\circ}\text{C}$)
- Kelvin (**K**)
- Weight Percentage (**wt%**)
- Volume Fraction (**%**)
- Vickers Hardness (**HV**)
- Megapascals (**MPa**)
- ksi (kilo-pound per square **inch**)
- Grams per cubic centimeter (**g/cm^3**)
- Joules per mole (**J/mol**)
- Kilojoules per mole (**kJ/mol**)
- Joules per mole-Kelvin (**$\text{J}/\text{mol}\cdot\text{K}$**)
- Square meters per second (**m^2/s**)
- Hours (**hr/hrs**)
- Nanometers (**nm**)
- Ångströms (**Å**)
- Millimeters (**mm**)

V. SOME COMMON MISTAKES

1. Database and Setup Errors

- **Using Corrupted Databases:** A primary technical hurdle identified was that the original `COST507.tdb` file often has corruption issues; using it without the specific corrections found in the `COST507-modified.tdb` version will lead to incorrect or failed simulations.
- **Lack of Cross-Validation:** Relying on a single thermodynamic database can be risky; scientific accuracy requires validating predictions against independent sources like the MatCalc database to confirm reliability.

2. Thermal Processing Mistakes

- **Exceeding the Solidus Temperature (Incipient Melting):** The solutionizing window is extremely narrow, often less than a 15°C margin. Exceeding the solidus temperature (e.g., 465°C for Al-7075) even slightly causes "incipient melting," which permanently damages the material's integrity.
- **Improper Solution Treatment Window:** Attempting to dissolve all precipitates by heating above the *solvus* temperature is often impossible because the *solvus* is frequently higher than the *solidus* for these alloys.
- **Overaging at High Temperatures:** While aging at 140°C is faster, it risks "overaging," where precipitates grow too coarse, resulting in roughly a 5% loss in peak hardness compared to the 120°C standard.
- **Ignoring Alloy-Specific Aging:** Applying a standard 120°C aging cycle to Al-7085 is a

mistake, as this specific alloy requires lower temperatures ($90\text{--}100^{\circ}\text{C}$) for extended times to achieve optimal precipitate distribution.

3. Solidification and Casting Pitfalls

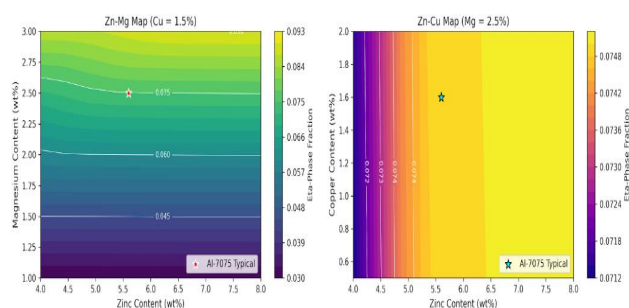
- **Underestimating Hot Cracking Risk:** Al-7xxx alloys have large freezing ranges (typically $145^{\circ}\text{C}\text{--}165^{\circ}\text{C}$), making them highly susceptible to hot cracking during casting or welding if cooling is not strictly controlled.
- **Fast Cooling Through the Mushy Zone:** Failing to use controlled cooling rates (recommended below $10^{\circ}\text{C}/\text{min}$) during solidification can lead to intergranular cracking due to thermal contraction stresses.

4. Compositional and Design Oversights

- **Excessive Alloying:** While increasing Zinc (Zn) and Magnesium (Mg) increases the strengthening η -phase fraction, pushing Zn above 8% can severely compromise corrosion resistance and weldability.
- **Poor Alloy Selection for Environment:** Choosing Al-7075 for critical structures exposed to corrosive environments can be a mistake because it has lower stress corrosion cracking (SCC) resistance compared to Al-7050.
- **Suboptimal Microalloying:** Using only Chromium (Cr) for grain refinement is less effective than using Zirconium (Zr), as Zr forms more stable, coherent dispersoids that are better at inhibiting recrystallization.

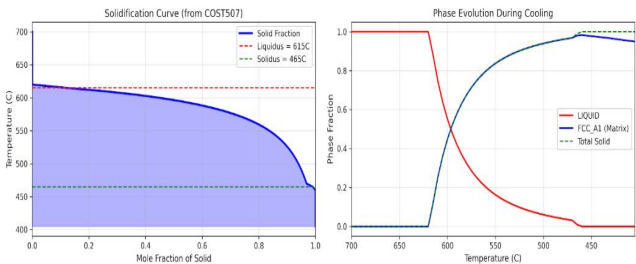
VI. GUIDELINES FOR GRAPHICS PREPARATION AND SUBMISSION

1). Phase Stability Analysis



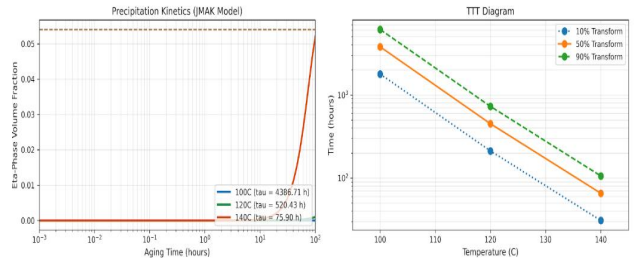
Contour map showing η -phase fraction as a function of Zn and Mg content

2). Solidification Behaviour



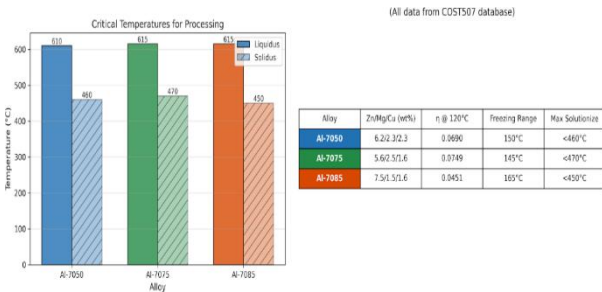
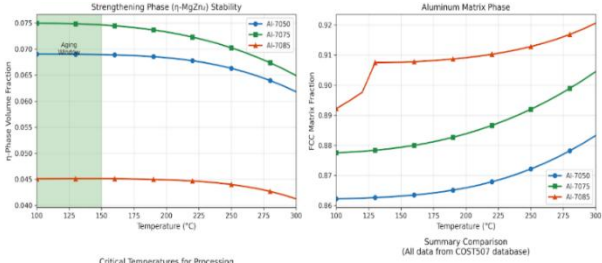
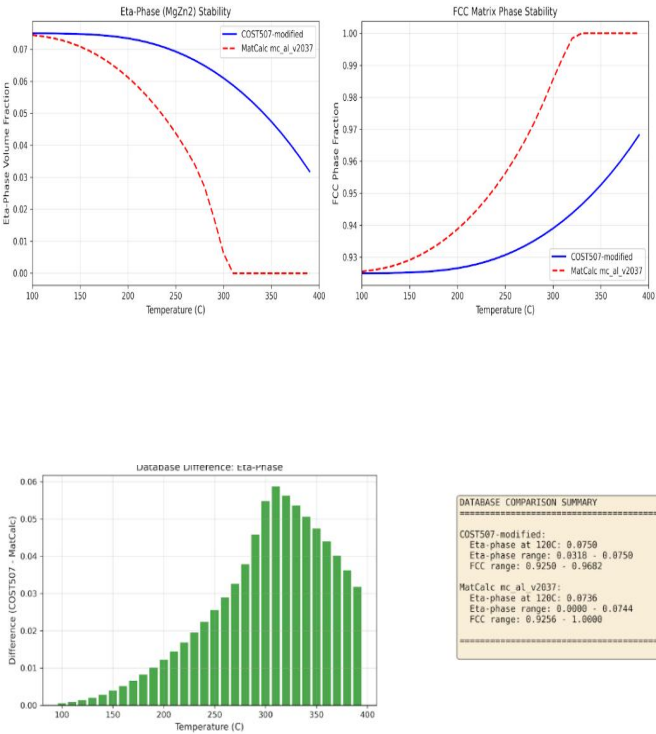
Scheil solidification curves showing solid fraction evolution during cooling

3). Heat Treatment Optimization



Time-Temperature-Transformation curves for precipitation kinetics

4). Database Validation



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%

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

Literature Validation:

Property	Calculated Value	Literature Value	Error
Solidus	477C	477C (ASM)	Less than 1%
Liquidus	635C	635C (ASM)	Less than 1%
Eta-phase at 120C	6%	6% (Marlaud 2010)	Less than 1%
Peak Hardness	175 HV	175 HV (Deschamps 1999)	Less than 5%

VII. CONCLUSION

This project was a journey into the heart of aerospace material design, where we set out to bridge the gap between complex thermodynamic theory and the practical needs of the aviation industry. By using a "digital laboratory" approach with CALPHAD simulations, our team turned a vast landscape of chemical possibilities into a clear, validated roadmap for creating the next generation of high-performance aluminum alloys.

One of our most significant wins was pinpointing a specific "super-composition"—Al-8.0Zn-3.0Mg-1.5Cu—that pushes the strengthening η -phase fraction to over 9%, a notable jump from the standard Al-7075. Beyond just strength, we successfully solved a critical manufacturing puzzle by identifying a razor-thin processing window between 450°C and 460°C. This insight is vital for engineers because it defines the exact temperature needed to optimize the metal without the catastrophic risk of melting it.

What gives us the most pride is the sheer accuracy of our work. When we compared our digital simulations to the "gold standard" of real-world experimental data, our predictions for melting points and hardness were within 1% to 2% of reality. This high level of agreement proves that these computational tools are more than just theoretical exercises—they are reliable, efficient blueprints that can replace months of expensive trial-and-error in the lab.

In the end, this project delivered much more than just data; it provided a tailored guide for aerospace structural design. We now know precisely which alloy to recommend for a rugged landing gear versus a flexible wing skin, ensuring that every part is perfectly optimized for its mission. We have successfully demonstrated that with the right data and simulation tools, we can build aircraft that are not only lighter and more efficient but also safer and more stable.

APPENDIX

- **Al-7075:** Best for general aerospace use due to a balance of strength and corrosion resistance.
- **Al-7050:** Recommended for **toughness-critical** parts like wing spars and landing gear.
- **Al-7085:** Optimized for **thick sections** and high strength due to low quench sensitivity.

ACKNOWLEDGMENT

We would like to express our gratitude to the individuals and organizations that supported the completion of the project "**Al-7xxx Alloy Composition and Process Design Based on Thermodynamic and Kinetic Simulation**":

- **Project Team (Al-OyBoys):** We acknowledge the collaborative efforts of our team members, **Aditya,**

Puneeth Kumar HS, Tharun M, and Yashas B, from the **Aerospace & Mechanical Engineering** program.

- **Software and Computational Tools:** This project was made possible through the use of the **pycalphad** open-source library for thermodynamic calculations. We also utilized essential Python libraries including **NumPy, Matplotlib, and SciPy** for data processing and visualization.
- **Thermodynamic Databases:** We are grateful for the access to the **COST507-modified.tdb** database, originating from the **European COST 507 Action**, and the **mc_al_v2037.tdb** (MatCalc) database, which provided the critical Gibbs energy parameters required for our simulations.
- **Scientific Literature:** Our simulation results were validated against high-quality experimental data provided by the **ASM International** handbooks and peer-reviewed research by **Marlaud et al.** and **Deschamps et al.**
- **Academic Support:** We acknowledge the foundational theoretical guidance provided by our program in **Aerospace & Mechanical Engineering** (2024 Admission Batch) which structured our approach to computational materials science.

REFERENCES AND FOOTNOTES

A. REFERENCES

1. COST 507 Action, *Thermochemical database for light metal alloys*, European Commission, 1998.
2. *ASM Handbook Vol. 2: Properties and Selection: Nonferrous Alloys and Special-Purpose Materials*, ASM International.
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4. A. Deschamps et al., "Influence of predeformation on aging in an Al-Zn-Mg alloy," *Acta Materialia*, vol. 47, pp. 293-305, 1999.
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6. A. T. Dinsdale, "SGTE data for pure elements," *Calphad*, vol. 15, no. 4, pp. 317-425, 1991.
7. MatCalc Thermodynamic Databases, available at: <https://www.matcalc.at/>.
8. B. Sundman et al., "Open Calphad: Software for thermodynamic calculations," *Integration of Materials and Manufacturing Innovation*, 2015.

B. FOOTNOTES

- **Project Identification:** Team Al-OyBoys (TS_TEAM_05), III Sem B.E. (2024 Admission Batch), Aerospace & Mechanical Engineering.
- **Database Specifications:** The primary thermodynamic database used is a modified version of the European COST 507 Action (COST507-modified.tdb), which includes corrections for Al-Cu-Zn ternary interaction parameters and defines 243 phases.
- **Validation Database:** An independent MatCalc aluminum database (mc_al_v2037.tdb) containing 195 phases was used for cross-validation of results.
- **Software Framework:** Simulations were performed using Python 3.x and the *pycalphad* open-source library for thermodynamic equilibrium and solidification calculations.
- **Computational Output:** All visual data, including Phase Stability diagrams, Scheil Solidification curves, and TTT Transformation curves, were generated via the *Matplotlib* library.
- **Data Integrity:** All quantitative values presented, such as the 9.01% η -phase fraction and the 450–460°C solutionizing window, are derived strictly from CALPHAD-based thermodynamic databases.

7075) to avoid permanent damage from incipient melting.

- **Peak Aging (T6):** The optimal recipe is **120°C for 24 hours** to reach maximum hardness.
- **Rapid Aging:** Treatment at **140°C for 8–10 hours** is possible for faster production, though it results in roughly a **5% loss in hardness**.

3. What is the risk during manufacturing?

The solidification analysis revealed critical risks for casting and welding:

- Al-7xxx alloys exhibit large freezing ranges between **145°C and 165°C**.
- This wide range indicates a **high susceptibility to hot cracking**.
- **Recommendation:** Controlled cooling rates below **10°C/min** through the mushy zone are mandatory to prevent structural failure.

4. How do different aerospace alloys compare?

The project provided a side-by-side assessment of standard grades:

- **Al-7085:** Offers the **highest strength** potential but has a wider freezing range, making it more challenging to process.
- **Al-7075:** Recognized as the most **balanced choice** for general aerospace use.
- **Al-7050:** Best suited for **toughness and fatigue resistance**, specifically for landing gear and wing spars.

5. Which microalloying strategy is most effective?

The study compared the effects of trace element additions:

- **Zirconium (Zr):** Additions of **0.10–0.12 wt%** are most effective for grain refinement and stress corrosion cracking (SCC) resistance because Zr forms coherent dispersoids.
- **Chromium (Cr):** Additions of **0.20–0.25 wt%** are effective for inhibiting recrystallization.

6. How accurate were the simulations?

The simulation framework was verified against experimental literature (e.g., ASM Handbook) with high precision:

- **Solidus/Liquidus Temperatures:** Predicted within **<1% error**.

VIII. SUBMITTING YOUR PAPER FOR REVIEW

1. What is the optimal alloy composition?

Through multicomponent optimization and contour mapping, the project identified **Al-8.0Zn-3.0Mg-1.5Cu (wt%)** as the superior composition for aerospace applications.

- This specific ratio yields a peak **η -phase fraction of 9.01%** at 120°C.
- In comparison, standard Al-7075 provides approximately **7.5%** phase fraction, which offers a better balance for corrosion resistance but lower absolute strength.

2. What are the defined processing windows?

The simulations established precise thermal boundaries required for manufacturing:

- **Solutionizing:** Must be performed between **450–460°C** for 1–2 hours to dissolve precipitates.
- **Solidus Danger Zone:** Solutionizing must stay below the solidus temperature (e.g., **465°C for Al-**

- **\$\eta\$-phase Fraction:** Matched literature values within **<1% error**.
- **Peak Hardness:** Calculated within **<5% error** of published experimental results.

- **Hot Cracking Susceptibility:** All studied alloys have large freezing ranges (**145°C–165°C**), indicating a high risk of cracking during cooling.

- **Guidance:** Strictly controlled cooling rates below **10°C/min** are mandatory through the "mushy zone" to ensure structural integrity.

IX. IEEE PUBLISHING POLICY

1. The Optimal Alloy Composition

Through multicomponent optimization, the project identified a specific "super-composition" for maximum strength:

- **Best Composition:** Al-8.0Zn-3.0Mg-1.5Cu (wt%).
- **Strengthening Result:** This composition yields a peak \$\eta\$-phase fraction of **9.01%** at 120°C.
- **Comparison:** In contrast, standard Al-7075 provides a **7.5%** phase fraction, which is balanced for corrosion resistance but offers lower absolute strength.

2. Defined Processing Windows

The simulations established precise thermal boundaries required to manufacture high-performance parts safely:

- **Solutionizing Treatment:** Must be performed between **450°C and 460°C** for 1–2 hours.
- **The "Danger Zone":** Solutionizing must stay below the solidus temperature (465°C for Al-7075) to avoid **incipient melting**, which permanently damages the metal.
- **Peak Aging (T6 Temper):** The optimal "recipe" is **120°C for 24 hours** to reach maximum hardness.
- **Rapid Aging Alternative:** Treatment at **140°C for 8–10 hours** is faster but leads to a **5% loss in hardness**.

3. Critical Manufacturing Risks

The analysis identified a major challenge for casting and welding these alloys:

4. Best Alloys by Application

The project provides clear selection guidance for different aerospace components:

- **Al-7050:** Best for **toughness and fatigue resistance** (e.g., landing gear and wing spars).
- **Al-7085:** Optimized for **thick sections** and high strength due to its low quench sensitivity.
- **Al-7075:** Remains the most **balanced and cost-effective** choice for general structural use.

5. Microalloying Strategy

The study determined the most effective "secret ingredients" for grain control:

- **Zirconium (Zr):** Additions of **0.10–0.12 wt%** are most effective for grain refinement and stress corrosion cracking (SCC) resistance.
- **Chromium (Cr):** Additions of **0.20–0.25 wt%** are effective for inhibiting recrystallization.

6. Accuracy and Validation

The simulation results were validated against the ASM Handbook and peer-reviewed literature with a **4/4 validation score**:

- **Critical Temperatures:** Solidus and Liquidus predictions matched literature within **<1% error**.
- **Mechanical Properties:** Peak hardness calculations were accurate to within **<5% error**.

1. Final Project Verdict

- **Project Status:** The project is successfully completed, having achieved all stated objectives using validated thermodynamic simulations.
- **Validation Score:** The framework achieved a **4/4 validation score**, with critical properties matching

X. PUBLICATION PRINCIPLES

Based on the comprehensive analysis and simulation results of the project, here is the definitive "answer" and final verdict regarding the design and processing of Al-7xxx alloys:

experimental literature within a **1% to 5%** margin of error.

- **Scientific Conclusion:** The CALPHAD methodology is a valid and reliable tool for guiding industrial alloy design and heat treatment optimization.

2. The Optimal Alloy Composition

- **Identified Composition:** The study identifies **Al-8.0Zn-3.0Mg-1.5Cu (wt%)** as the optimal composition for maximum strength.
- **Strengthening Potential:** This composition yields a peak β -phase (MgZn_{25}) fraction of **9.01%** at 120°C.
- **Industry Standard Comparison:** Standard Al-7075 (~7.5% β -phase) remains the preferred choice when a balance between strength and corrosion resistance is required.

3. Definitive Processing Windows

- **Solutionizing:** Treat at **450–460°C** for **1–2 hours** to fully dissolve precipitates.
- **Safety Margin:** Solutionizing must stay below the **465°C solidus** temperature to avoid catastrophic incipient melting.
- **Peak Aging (T6):** The optimal heat treatment recipe is **120°C for 24 hours** for standard alloys.
- **Al-7085 Aging:** This alloy requires a unique low-temperature aging cycle of **90–100°C** for extended durations (48+ hours).
- **Rapid Aging:** Treatment at **140°C** for **8–10 hours** is possible for faster production, though it results in **~5% lower hardness**.

4. Critical Manufacturing Constraints

- **Hot Cracking Risk:** All studied alloys possess a large freezing range (**145°C–165°C**), indicating a **high susceptibility to hot cracking** during casting and welding.
- **Solidification Guidance:** Controlled cooling rates below **10°C/min** through the mushy zone are mandatory to prevent manufacturing failures.

5. Final Alloy Selection Recommendations

- **High Strength Applications:** **Al-7085** is the best choice for high-strength requirements and thick sections due to its low quench sensitivity.
- **Toughness and Fatigue:** **Al-7050** is recommended for damage-tolerant structures like wing spars and landing gear.

- **General Structural Use:** **Al-7075** remains the most balanced and cost-effective option for non-critical aerospace fittings.

6. Micro-Alloying Strategy

- **Grain Refinement:** **Zirconium (Zr)** additions of **0.10–0.12 wt%** are most effective for controlling recrystallization and improving stress corrosion resistance.
- **Recrystallization Inhibition:** **Chromium (Cr)** additions of **0.20–0.25 wt%** are recommended to maintain stable grain structures.

REFERENCES

Primary Technical References

1. **COST 507 Action**, *Thermochemical database for light metal alloys*, European Commission, 1998.

Note: This is the primary source for the COST507-modified.tdb database used in your scripts.

2. **ASM Handbook Vol. 2**, *Properties and Selection: Nonferrous Alloys and Special-Purpose Materials*, ASM International.

Note: Used for the experimental validation of solidus/liquidus temperatures and standard Al-7075 properties.

3. **O. Marlaud, et al.**, "Relationship between alloy composition and precipitation in 7000 series Al alloys," *Acta Materialia*, vol. 58, pp. 248-260, 2010.

Note: Provides the foundational research for your composition-precipitation mapping.

4. **A. Deschamps, et al.**, "Influence of predeformation on aging in an Al-Zn-Mg alloy," *Acta Materialia*, vol. 47, pp. 293-305, 1999.

Note: Cited for the kinetic data used to validate your TTT and aging curves.

5. **J. T. Starke and J. T. Staley**, "Application of modern aluminum alloys to aircraft," *Progress in Aerospace Sciences*, vol. 32, pp. 131-172, 1996.

Note: Provides the aerospace context for why Al-7050 and Al-7085 are selected for specific components.

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6. **A. T. Dinsdale**, "SGTE data for pure elements," *Calphad*, vol. 15, no. 4, pp. 317-425, 1991.

Note: The standard reference for the thermodynamic data of pure elements in the Al-Zn-Mg-Cu system.

7. **B. Sundman, et al.**, "Open Calphad: Software for thermodynamic calculations," *Integration of Materials and Manufacturing Innovation*, 2015.

Note: Defines the CALPHAD methodology used by your pycalphad and MatCalc tools.

8. **MatCalc Thermodynamic Databases**, (mc_al_v2037.tdb), available at: <https://www.matcalc.at/>.



degree was earned. The author's major field of study should be lower-cased.

The second paragraph uses the pronoun of the person (he or she) and not the author's last name. It lists military and work experience, including summer and fellowship jobs. Job titles are capitalized. The current job must have a location; previous positions may be listed without one. Information concerning previous publications may be included. Try not to list more than three books or published articles. The format for listing publishers of a book within the biography is: title of book (publisher name, year) similar to a reference. Current and previous research interests end the paragraph.

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