ADBA Computer Science
Cutting-Edge Scientific Solutions

e-ISSN: 3023-8544
RESEARCH ARTICLE
Vol.2 / No.2 / 2025 / pp.36-42
https://doi.org/10.69882/adba.cs.2025072

Computational Study of the Effect of Aluminum Content on the Thermodynamic Properties and Phase Stability of Mg-Al-Zn Alloys

Yusuf Uzunoğlu *,[1]
*Mechanical and Metal Technologies, OSB Vocational School, Bitlis Eren University, Bitlis, Türkiye.

ABSTRACT This study investigates the effect of varying aluminum (Al) content on the thermodynamic properties and phase stability of Mg-Al-Zn alloys using Computational Materials Science techniques. Three Mg-Al-Zn alloys were modeled with 3 wt%, 6 wt%, and 9 wt% Al, while the zinc (Zn) content was fixed at 1 wt% and magnesium (Mg) made up the remaining balance. Phase fraction diagrams were generated using the JMatPro software to analyze the phase transformations and their evolution with temperature. Additionally, the phase compositions and thermodynamic behavior of the alloys at a fixed temperature of 300 ℃ were examined. The chemical potential ($M\mu$) of each element was calculated to assess the energy state and stability of Mg, Al, and Zn in the alloys. Furthermore, the activity values of the elements were determined to evaluate their deviations from ideal behavior and effective thermodynamic concentrations within the alloys. The results reveal that increasing Al content significantly influences the phase stability and transformation behavior of the Mg-Al-Zn system. Higher Al concentrations led to a greater proportion of the intermetallic phase ($Mg_{17}Al_{12}$) at 300 ℃, which in turn affected the chemical potential and activity of the constituent elements. This computational investigation provides insights into the role of Al in tailoring the thermodynamic properties and phase constitution of Mg-Al-Zn alloys, offering valuable guidance for alloy design and optimization in lightweight structural applications.

KEYWORDS
Computational materials science
Magnesium alloys
Thermodynamic properties

INTRODUCTION

Magnesium alloys, particularly Mg-Al-Zn systems, have garnered significant attention in recent years due to their exceptional properties such as lightweight, high specific strength, and excellent corrosion resistance, making them ideal candidates for structural applications in automotive, aerospace, and electronic industries (Huang *et al.* 2023; Luo *et al.* 2012). The precise control of alloy composition, particularly the content of aluminum and zinc, plays a pivotal role in optimizing the thermodynamic and mechanical properties of these alloys. This study investigates the influence of varying aluminum concentrations (3 wt.%, 6 wt.%, and 9 wt.%) on the phase transformation behavior and thermodynamic stability of Mg-Al-Zn alloys, with zinc content fixed at 1 wt.%, through computational modeling using the JMatPro software. Previous studies have highlighted the critical role of aluminum in enhancing strength and reducing density, yet the detailed phase stability mechanisms remain underexplored (Kaya 2020; David *et al.* 2016).

The utilization of computational thermodynamics, particularly Computational Materials Science (CMS)-based software like JMatPro, has revolutionized the design and analysis of alloy systems. It provides valuable insights into phase diagrams, phase fractions, and thermodynamic properties under varying conditions (Avedesian and Baker 1999). Prior investigations have shown the effectiveness of such simulations in predicting phase equilibrium in Mg-Al-Zn alloys; however, the combined effects of aluminum variation on specific phase fractions and thermodynamic activities at intermediate temperatures, such as 300°C, remain inadequately studied (Brubaker and Liu 2004). This study aims to bridge this knowledge gap by analyzing the phase transformation diagrams, thermodynamic properties, and chemical potential of alloy components at 300°C.

In this research, the Mg-Al-Zn alloys with 3 wt.%, 6 wt.%, and 9 wt.% aluminum were simulated, and the results were compared to provide a comprehensive understanding of aluminum's impact on the alloy's phase behavior and thermodynamic stability. Additionally, the activity and chemical potential values were computed to evaluate the deviation from ideal behavior, offering insights into the energetic and interaction dynamics of the constituent elements within the alloy matrix. Previous works have shown that increased aluminum content can enhance mechanical strength but also alter the thermodynamic equilibrium (Yuzbekova *et al.* 2019; Dai *et al.* 2013). Our findings align with this observation and further elucidate the quantitative effects on phase stability and phase fraction at elevated temperatures.

Manuscript received: 28 March 2025,
Revised: 7 June 2025,
Accepted: 5 July 2025.

[1]yuzunoglu@beu.edu.tr (**Corresponding author**)

The results of this study contribute significantly to the understanding of thermodynamic behavior in Mg-Al-Zn alloys, enabling improved alloy design strategies for structural applications. By comparing the outcomes with existing literature, such as works on Mg-Zn-Al ternary phase diagrams and thermodynamic models (Hayashi *et al.* 2020; Li *et al.* 2010), this research underscores the importance of aluminum content in determining phase stability and highlights the utility of computational methods in alloy design (Uzunoğlu and Alaca 2025b; Emin *et al.* 2025). Computational methods provide significant efficiency and convenience in generating the datasets required for artificial intelligence applications in alloy design. In particular, the findings from our previous studies involving the integration of artificial intelligence with computational methods demonstrate the potential for further advancement of this approach and highlight the facilitative role of computational materials science techniques in AI-assisted alloy design (Uzunoğlu *et al.* 2025; Alaca *et al.* 2025; Uzunoğlu and Alaca 2025a).

MATERIALS AND METHODS

In this study, the thermodynamic behavior and phase stability of Mg-Al-Zn alloys were analyzed using computational materials science techniques. The JMatPro software was employed to model and simulate three different alloy systems with varying aluminum (Al) content of 3 wt%, 6 wt%, and 9 wt%, while zinc (Zn) content was held constant at 1 wt%, and the remaining balance was magnesium (Mg). The primary objective was to investigate the influence of increasing Al content on phase transformations, chemical potential, and activity of the constituent elements within the Mg-Al-Zn system.

The methodology involved three key steps, as illustrated in the Proposed Model (Figure1):

- Alloy Modeling: The alloys were constructed by systematically varying the Al content to 3 wt%, 6 wt%, and 9 wt%, while fixing Zn at 1 wt%.
- Simulation: Phase fraction diagrams were generated for each alloy composition using JMatPro to identify the phase evolution across a temperature range. This provided insight into phase transformations as a function of Al concentration.
- Thermodynamic Calculations at 300°C: To further analyze the thermodynamic properties at a single temperature, the weight fractions of the phases, chemical potential (Mμ), and activity values of Mg, Al, and Zn were calculated at 300°C.

The results were evaluated to determine how increasing Al content influenced the formation and stability of phases, specifically the $Mg_{17}Al_{12}$ intermetallic phase. Additionally, the chemical potential and activity values provided a quantitative measure of the energy state and the thermodynamic behavior of each element in the alloys. This integrated approach, as summarized in Figure 1, provides a systematic framework to evaluate the effect of Al content on the thermodynamic properties of Mg-Al-Zn alloys, offering critical insights for alloy design and optimization.

Alloy Modeling

The alloy compositions were designed by varying the aluminum content to 3 wt.%, 6 wt.%, and 9 wt.%, with the zinc content fixed at 1 wt.%, and the balance being magnesium. This compositional range was selected based on previous studies that have explored the effects of Al and Zn concentrations on the microstructure and properties of Mg-based alloys. For instance, Yu and Li investigated the precipitated phases in Al-Zn-Mg-Cu alloys, highlighting the significance of Al content in phase formation (Yu and Li 2011). Similarly, Liang et al. provided a thermodynamic description of the Al-Mg-Zn system, emphasizing the role of Al in phase stability (Liang *et al.* 1997).

Simulation

Phase fraction diagrams for each alloy composition were generated using JMatPro, a computational tool that has been extensively utilized for modeling phase transformations in multicomponent alloys (JMatPro Sense Software Accessed in 2024). The simulations were conducted over a temperature range of 200 ° C to 600 ° C to capture the evolution of various phases, including the intermetallic phase $Mg_{17}Al_{12}$, which is known to influence the mechanical properties of Mg-Al-Zn alloys (Alidoust *et al.* 2020). The accuracy of JMatPro in predicting phase equilibria has been validated in studies such as those by Yu and Li, who modeled precipitated phases in Al-Zn-Mg-Cu alloys (Yu and Li 2011).

Thermodynamic Calculations at 300℃

At a fixed temperature of 300 ° C, detailed thermodynamic calculations were performed to determine the weight fractions of the existing phases, as well as the chemical potential (μ) and activity values of Mg, Al, and Zn. These parameters are crucial for understanding the thermodynamic stability and the deviation from ideal behavior of each element within the alloy matrix. The selection of 300 ° C is pertinent, as it aligns with temperatures commonly encountered in the processing and application of Mg-Al-Zn alloys (Zhang *et al.* 2024). The methodologies employed for these calculations are consistent with those used in prior thermodynamic analyses of similar alloy systems (Silva *et al.* 2022).

The selection of 300 ° C as evaluation temperature is highly relevant for industrial applications, particularly in the automotive and aerospace sectors, where magnesium alloys are increasingly employed for structural components that demand both lightweight and high thermal stability. Components such as engine blocks, transmission cases, and aircraft interior structures are commonly exposed to service temperatures ranging between 200°C and 350°C. At this intermediate temperature regime, the stability of intermetallic phases, such as $Mg_{17}Al_{12}$, and the thermodynamic behavior of alloying elements become critical for maintaining mechanical performance and dimensional stability. Therefore, understanding the phase constitution and chemical potential characteristics of Mg-Al-Zn alloys at 300 ° C provides practical insight into their suitability for high-temperature service conditions and helps in the development of alloys with optimized phase stability and mechanical reliability under operational stresses.

The chemical potential (Mμ) quantifies an element's propensity to integrate into or separate from an alloy, influenced by factors such as concentration, temperature, and pressure within the alloy matrix. A more negative chemical potential signifies a lower free energy state, indicating greater stability of the element within the alloy (Matsushita and Mukai 2018).

Activity (α) measures the deviation of an element's behavior from ideality in an alloy. In an ideal solution, an element's activity equals its mole fraction; however, real alloys often exhibit deviations due to interactions among constituent elements (Chen 2019). Activity reflects the effective concentration of an element, contingent upon the alloy's composition, temperature, and the presence of other elements. An activity value close to 1 signifies

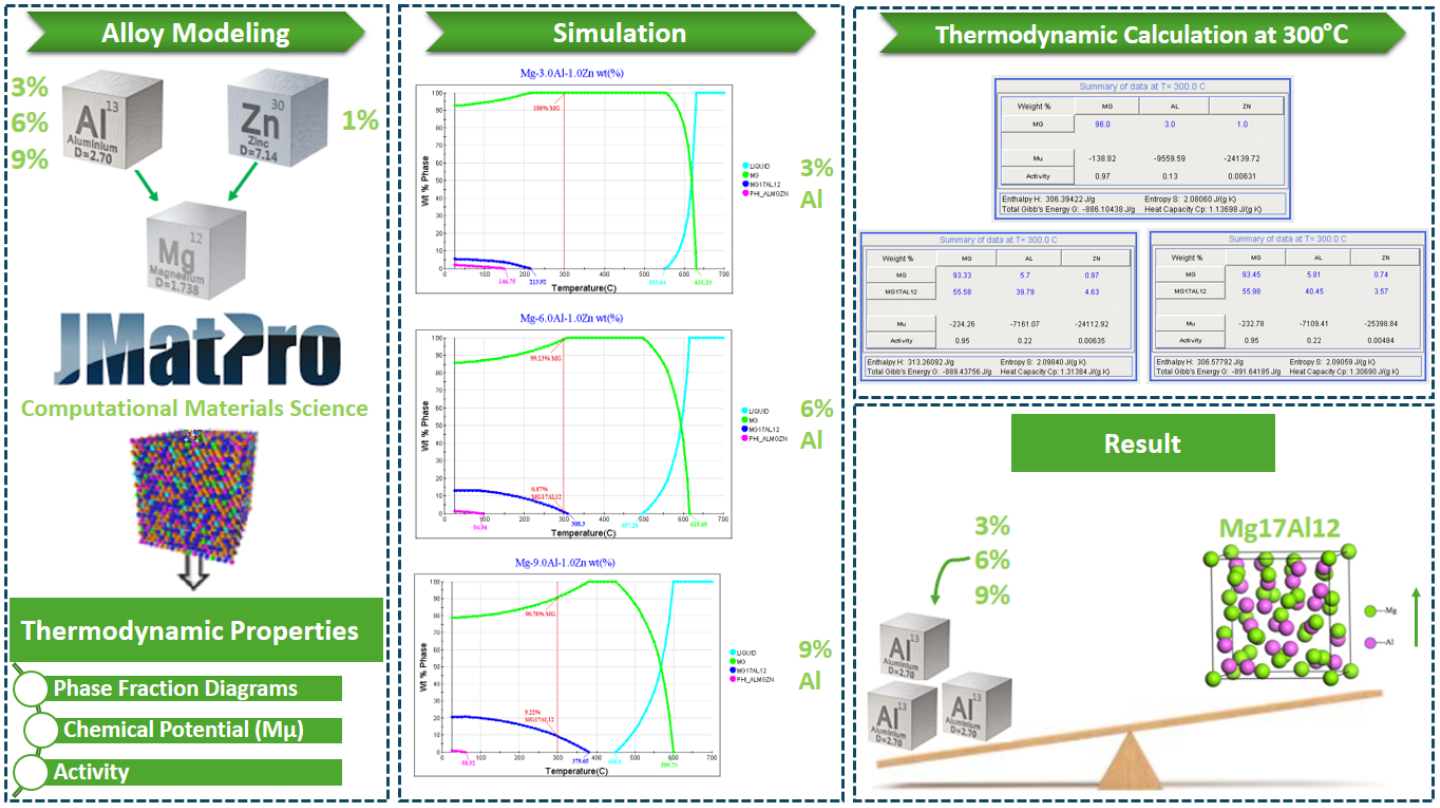

Figure 1 Proposed Model for Investigating the Thermodynamic Properties and Phase Stability of Mg-Al-Zn Alloys

ideal behavior, while values much lower than 1 indicate a significantly reduced effective concentration, meaning the element is only weakly dissolved in the alloy.

The relationship between chemical potential and activity is expressed by the equation:

$$\mu = \mu^{\circ} + RT \ln \alpha \tag{1}$$

where:

- μ: Chemical potential
- μ°: Standard chemical potential of the pure element
- R: Universal gas constant
- T: Absolute temperature (Kelvin)
- α: Activity

This equation illustrates that an increase in activity corresponds to a less negative chemical potential, signifying a higher energy state and reduced stability within the alloy (Sahoo *et al.* 2024). By integrating alloy modeling, phase diagram simulation, and thermodynamic calculations, this study provides a comprehensive understanding of how varying aluminum content affects the phase stability and thermodynamic properties of Mg-Al-Zn alloys. The findings contribute to the optimization of alloy compositions for enhanced performance in practical applications.

RESULTS AND DISCUSSION

In this section, the results of the computational simulations and thermodynamic analyses performed on the Mg-Al-Zn alloys are presented and discussed in detail. The primary focus is on understanding the influence of increasing aluminum (Al) content (3 wt%, 6 wt%, and 9 wt%) on phase stability, chemical potential (Mμ), and activity of the constituent elements.

First, the phase evolution behavior of the alloys was examined through phase fraction diagrams generated using JMatPro. These diagrams illustrate the formation and stability of phases such as the primary magnesium (Mg) matrix, the intermetallic $Mg_{17}Al_{12}$ phase, and the liquid phase over a temperature range. The results highlight the relationship between Al concentration and the increasing presence of the $Mg_{17}Al_{12}$ phase, which plays a critical role in the mechanical and thermal properties of the alloys. Second, thermodynamic calculations at a fixed temperature of 300 °C provide detailed insights into the chemical potential and activity values of Mg, Al, and Zn. These parameters offer a quantitative evaluation of the energy state, stability, and effective thermodynamic concentration of each element in the alloys. Comparisons between the three alloy compositions reveal significant trends, such as the decrease in Mg chemical potential and the increase in Al contribution to phase stability with rising Al content.

The findings are analyzed in light of previous studies on Mg-Al-Zn alloys to validate the results and highlight their implications for alloy design. Trends observed in phase stability and thermodynamic behavior are discussed, with emphasis on their impact on the structural integrity and application potential of the alloys. This section provides a comprehensive evaluation of the results, correlating phase transformations with thermodynamic properties to explain the role of Al in modifying the behavior of Mg-Al-Zn systems.

Phase Fraction Diagrams

The phase fraction diagrams for the three Mg-Al-Zn alloys, corresponding to 3 wt% Al (Figure 2), 6 wt% Al (Figure 3), and 9 wt% Al (Figure 4), were generated using JMatPro to investigate the effect of increasing Al content on the phase stability and evolution across a

temperature range. These diagrams provide detailed insights into the phase transformations, including the stability of the primary magnesium (Mg) phase, the $Mg_{17}Al_{12}$ intermetallic phase, and the liquid phase.

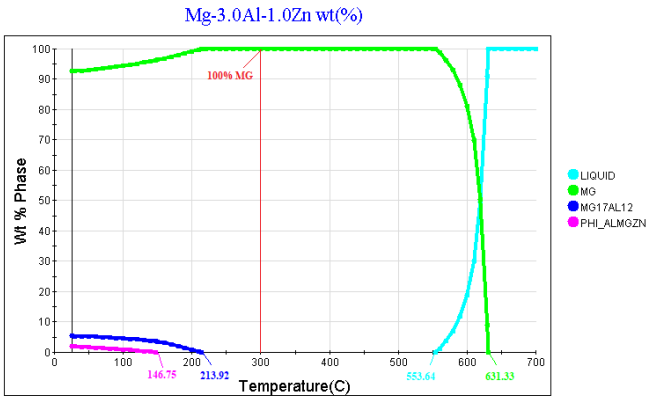

Figure 2 Phase Fraction Diagram of Mg-3.0Al-1.0Zn Alloy. LIQUID: Represents the molten phase where the alloy constituents exist in a fully liquid state above the solidus temperature. MG: Denotes the primary magnesium-rich solid solution phase that forms the matrix of the alloy. $Mg_{17}Al_{12}$: A hard and brittle intermetallic phase known to enhance high-temperature strength but reduce ductility in magnesium alloys. PHI_AlMgZn: A ternary intermetallic phase that forms at low temperatures in the Al-Mg-Zn system, with limited thermodynamic stability and relatively low prevalence.

The phase fraction diagram for the Mg-3.0Al-1.0Zn alloy shows that the primary Mg phase (green line) dominates at low and intermediate temperatures up to approximately 553.64 °C. At this temperature, the liquid phase (cyan line) begins to form, reaching full transformation at approximately 631.33 °C. The $Mg_{17}Al_{12}$ phase (blue line) appears at lower temperatures and remains relatively low, accounting for only a small fraction (less than 5%) below 213.92 °C. This indicates that at 3 wt% Al, the alloy remains primarily composed of the Mg matrix phase, with minimal formation of the intermetallic $Mg_{17}Al_{12}$. The PHI_AlMgZn phase (magenta line) is observed only at very low temperatures (146.75 °C) and remains negligible.

The results suggest that at 3 wt% Al, the alloy exhibits high phase stability dominated by the primary Mg phase, with limited precipitation of the $Mg_{17}Al_{12}$ intermetallic. This behavior aligns with findings reported in similar Mg-Al-Zn systems, where lower Al contents result in negligible formation of secondary phases (Yu and Li 2011; Liang *et al.* 1997).

For the Mg-6.0Al-1.0Zn alloy, a notable increase in the $Mg_{17}Al_{12}$ phase fraction is observed. The primary Mg phase (green line) still dominates the microstructure but begins to decline slightly as the temperature decreases below approximately 308.3 °C. At 300 °C, the Mg phase accounts for 99.13%, with the $Mg_{17}Al_{12}$ phase (blue line) contributing 0.87%. The liquid phase (cyan line) begins to form at around 497.28 °C and becomes fully dominant by approximately 615.69 °C. The PHI_AlMgZn phase (magenta line) remains insignificant, forming only at temperatures below 100 °C and at a negligible fraction. Compared to the 3 wt% Al alloy, the increase in Al content to 6 wt% promotes the formation of the $Mg_{17}Al_{12}$ phase, albeit still at a relatively low fraction. This trend agrees with the literature, where Al is identified as a key element in the formation of intermetallic phases, which can enhance mechanical strength at

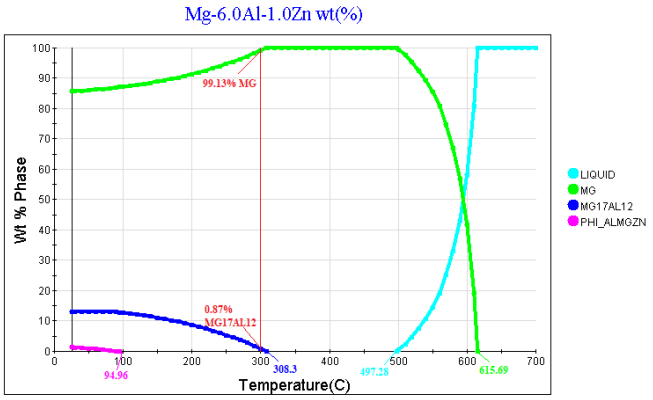

Figure 3 Phase Fraction Diagram of Mg-6.0Al-1.0Zn Alloy

elevated temperatures JMatPro Sense Software (Accessed in 2024), Alidoust *et al.* (2020). However, the dominance of the Mg phase indicates that the alloy remains largely single-phase at 300 °C.

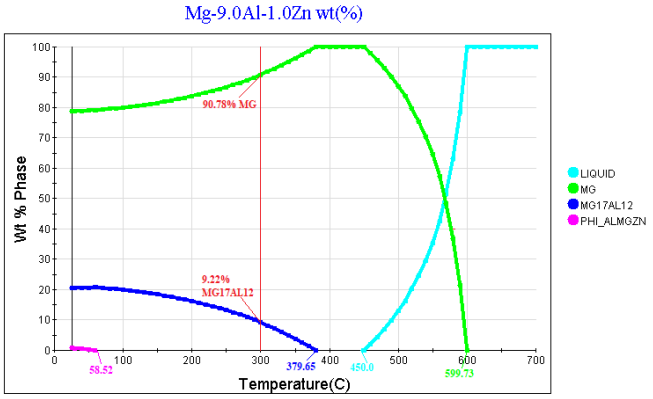

Figure 4 Phase Fraction Diagram of Mg-9.0Al-1.0Zn Alloy

The phase fraction diagram for the Mg-9.0Al-1.0Zn alloy reveals a significant increase in the $Mg_{17}Al_{12}$ phase compared to the previous two alloys. The primary Mg phase (green line) begins to decrease more noticeably below approximately 379.65 °C, contributing 90.78% at 300 °C. Simultaneously, the $Mg_{17}Al_{12}$ phase (blue line) grows to 9.22%, indicating a substantial increase in the intermetallic fraction as Al content rises. The liquid phase (cyan line) starts to form at approximately 450.00 °C and becomes fully dominant by 599.73 °C. Similar to the previous cases, the PHI_AlMgZn phase (magenta line) remains negligible, appearing only at very low temperatures (<60 °C).

The increased formation of $Mg_{17}Al_{12}$ at 9 wt% Al highlights the critical role of aluminum in promoting this intermetallic phase. This trend is consistent with prior studies, which have shown that higher Al concentrations in Mg-Al-Zn alloys significantly enhance the stability and volume fraction of the $Mg_{17}Al_{12}$ phase (Zhang *et al.* 2024; Silva *et al.* 2022). The presence of this intermetallic phase is known to influence the alloy's mechanical properties, such as hardness and creep resistance, which are desirable for structural applications (Liang *et al.* 1997).

The phase fraction diagrams demonstrate a clear correlation between increasing Al content and the formation of the $Mg_{17}Al_{12}$ phase. At 3 wt% Al, the Mg matrix remains dominant with min-

imal intermetallic formation. At 6 wt% Al, a slight increase in $Mg_{17}Al_{12}$ is observed, while at 9 wt% Al, the intermetallic phase grows substantially, accounting for approximately 9.22% of the microstructure at 300 °C. These results underscore the role of aluminum as a critical element in phase evolution within Mg-Al-Zn alloys, providing valuable insights into the alloy design process for enhanced mechanical and thermodynamic properties.

Single Calculations

To investigate the effect of aluminum (Al) content on the thermodynamic properties of Mg-Al-Zn alloys at a fixed temperature of 300 °C, single temperature calculations were performed. The weight percentages of Mg, Al, and Zn in each phase, as well as their chemical potential ($M\mu$) and activity values, were determined for the three alloy compositions: 3 wt%, 6 wt%, and 9 wt% Al. The results are presented in Figure 5, which combines the summary data for the three alloys.

a)

Mg-3%Al-1%Zn

Summary of data at T= 300.0 C

Weight %	MG	AL	ZN
MG	96.0	3.0	1.0
Mu	-138.82	-9559.59	-24139.72
Activity	0.97	0.13	0.00631

Enthalpy H: 306.39422 J/g — Entropy S: 2.08060 J/(g K)
Total Gibb's Energy G: -886.10438 J/g — Heat Capacity Cp: 1.13698 J/(g K)

b)

Mg-6%Al-1%Zn

Summary of data at T= 300.0 C

Weight %	MG	AL	ZN
MG	93.33	5.7	0.97
MG17AL12	55.58	39.79	4.63
Mu	-234.26	-7161.07	-24112.92
Activity	0.95	0.22	0.00635

Enthalpy H: 313.26092 J/g — Entropy S: 2.09840 J/(g K)
Total Gibb's Energy G: -889.43756 J/g — Heat Capacity Cp: 1.31384 J/(g K)

c)

Mg-9%Al-1%Zn

Summary of data at T= 300.0 C

Weight %	MG	AL	ZN
MG	93.45	5.81	0.74
MG17AL12	55.98	40.45	3.57
Mu	-232.78	-7109.41	-25398.84
Activity	0.95	0.22	0.00484

Enthalpy H: 306.57792 J/g — Entropy S: 2.09059 J/(g K)
Total Gibb's Energy G: -891.64185 J/g — Heat Capacity Cp: 1.30690 J/(g K)

Figure 5 Effect of Aluminum Content on Phase Compositions, Chemical Potential, and Activity of Mg, Al, and Zn at 300 °C

Phase Compositions

From Figure 5, it is evident that increasing the Al content from 3 wt% to 9 wt% significantly influences the phase distribution and the composition of Mg, Al, and Zn in each phase:

Figure 5a (At 3 wt% Al): The alloy predominantly consists of the Mg phase (96.0 wt% Mg, 3.0 wt% Al, and 1.0 wt% Zn). The $Mg_{17}Al_{12}$ phase is not present at this Al concentration. Figure 5b (At 6 wt% Al): The Mg phase accounts for 93.33 wt% Mg, 5.7 wt% Al, and 0.97 wt% Zn, indicating that some Al has been partitioned into the intermetallic $Mg_{17}Al_{12}$ phase. The $Mg_{17}Al_{12}$ phase forms and contains 55.58 wt% Mg, 39.79 wt% Al, and 4.63 wt% Zn. This indicates that Al has become a significant constituent of the $Mg_{17}Al_{12}$ phase. Figure 5c (At 9 wt% Al): The Mg phase has a slightly increased Al content (5.81 wt% Al) but remains similar in Mg and Zn content (93.45 wt% Mg and 0.74 wt% Zn). The $Mg_{17}Al_{12}$ phase fraction increases, containing 55.98 wt% Mg, 40.45 wt% Al, and 3.57 wt% Zn. This trend highlights that as the Al content increases, more Al is incorporated into the $Mg_{17}Al_{12}$ phase, while Zn shows limited solubility.

Chemical Potential ($M\mu$)

The chemical potential ($M\mu$) values of Mg, Al, and Zn provide insights into the energy states and thermodynamic stability of these elements in the alloys.

Magnesium (Mg): The chemical potential of Mg decreases slightly with increasing Al content.

Table 1 Change in the Chemical Potential of Mg with Increasing Aluminum Content

Aluminum Content (wt.%)	3% Al	6% Al	9% Al
$M\mu_{Mg}$ (J/mol)	−138.82	−234.26	−232.78

This indicates that Mg becomes more stable (lower energy state) as Al content increases, which aligns with the formation of the intermetallic $Mg_{17}Al_{12}$ phase, consuming Al and stabilizing the Mg matrix.

Aluminum (Al): The chemical potential of Al remains significantly lower compared to Mg and Zn, reflecting its strong affinity to form intermetallic phases.

Table 2 Change in the Chemical Potential of Al with Increasing Aluminum Content

Aluminum Content (wt.%)	3% Al	6% Al	9% Al
$M\mu_{Al}$ (J/mol)	−9559.59	−7161.07	−7109.41

As the Al content increases, the magnitude of the chemical potential becomes less negative. This suggests that excess Al is less energetically favorable in the Mg phase and preferentially partitions into the intermetallic $Mg_{17}Al_{12}$ phase.

Zinc (Zn): The chemical potential of Zn remains largely unchanged across all compositions, indicating its minimal impact on the phase transformations.

Table 3 Change in the Chemical Potential of Zn with Increasing Aluminum Content

Aluminum Content (wt.%)	3% Al	6% Al	9% Al
$M\mu_{Zn}$ (J/mol)	−24139.72	−24112.92	−25398.84

This stability in the chemical potential of Zn suggests that Zn primarily remains in solid solution and does not significantly participate in intermetallic phase formation.

Activity (α)

The activity values of Mg, Al, and Zn reflect their deviation from ideal behavior and effective thermodynamic concentrations within the alloy.

Magnesium (Mg): The activity of Mg decreases slightly as Al content increases.

Table 4 Change in the Activity of Mg with Increasing Aluminum Content

Aluminum Content (wt.%)	3% Al	6% Al	9% Al
Activity of Mg (α_{Mg})	0.97	0.95	0.95

Since all values are close to 1, it is observed that Mg behaves nearly ideally within the Mg matrix phase but shows slight deviations with increasing Al content due to the formation of the $Mg_{17}Al_{12}$ phase.

Aluminum (Al): The activity of Al increases with higher Al content but remains significantly lower than Mg.

Table 5 Change in the Activity of Al with Increasing Aluminum Content

Aluminum Content (wt.%)	3% Al	6% Al	9% Al
Activity of Al (α_{Al})	0.13	0.22	0.22

The low activity values (values much lower than 1) indicate that Al strongly deviates from ideal behavior due to its incorporation into the intermetallic phase, where it exhibits lower thermodynamic freedom.

Zinc (Zn): The activity of Zn remains very low across all compositions.

Table 6 Change in the Activity of Zn with Increasing Aluminum Content

Aluminum Content (wt.%)	3% Al	6% Al	9% Al
Activity of Zn (α_{Zn})	0.00631	0.00635	0.00484

This further supports the observation that Zn has minimal interaction with other phases and remains as a dilute solute.

In conclusion, the single temperature calculations at 300 °C demonstrate that increasing Al content leads to:

- A greater partitioning of Al into the $Mg_{17}Al_{12}$ phase, reducing its presence in the Mg phase.
- A stabilization of the Mg phase, reflected by a slight decrease in Mg's chemical potential.
- Lower chemical potential and activity values for Al, emphasizing its strong tendency to form intermetallic phases.
- Minimal changes in the chemical potential and activity of Zn, indicating its limited role in the phase transformations.

These results align with the trends observed in phase fraction diagrams and highlight the critical role of Al in determining the phase stability and thermodynamic properties of Mg-Al-Zn alloys.

CONCLUSION

In this study, the effect of increasing aluminum (Al) content (3 wt%, 6 wt%, and 9 wt%) on the phase stability and thermodynamic properties of Mg-Al-Zn alloys was investigated using JMatPro computational materials science software. Zinc (Zn) content was held constant at 1 wt%, and the remaining balance was magnesium (Mg). Key findings from the phase fraction diagrams, single-temperature thermodynamic calculations, and chemical potential and activity analyses at 300 °C are summarized as follows:

- Phase Evolution: The phase fraction diagrams revealed that increasing Al content promotes the formation of the intermetallic $Mg_{17}Al_{12}$ phase. At 3 wt% Al, the alloy is dominated by the primary Mg phase, with negligible $Mg_{17}Al_{12}$ formation. As Al content increases to 6 wt% and 9 wt%, the volume fraction of $Mg_{17}Al_{12}$ grows significantly, highlighting the critical role of Al in phase transformation behavior.
- Thermodynamic Properties: The chemical potential ($M\mu$) of magnesium decreases slightly with increasing Al content, reflecting enhanced stabilization of the Mg phase due to Al partitioning. In contrast, the chemical potential of Al becomes less negative as it preferentially forms the $Mg_{17}Al_{12}$ phase, while the chemical potential of Zn remains relatively unchanged across all compositions.
- Activity of Elements: The activity of Mg decreases marginally with rising Al content, indicating near-ideal behavior with slight deviation due to phase interactions. Aluminum exhibits low activity, particularly at higher Al contents, emphasizing its thermodynamic preference to form intermetallic phases. Zinc maintains very low activity values, confirming its limited participation in phase transformations and its role as a dilute solute in the alloy system.
- Mechanical Properties: The formation and increased volume fraction of the $Mg_{17}Al_{12}$ intermetallic phase have notable implications for the mechanical performance of Mg-Al-Zn alloys. As a relatively hard and thermally stable phase, $Mg_{17}Al_{12}$ contributes positively to the alloy's hardness and high-temperature strength by hindering dislocation motion and improving creep resistance. However, due to its brittle nature and limited deformability, excessive formation of this

phase can detrimentally affect the alloy's ductility and impact resistance, particularly under dynamic or cyclic loading conditions. Therefore, the thermodynamically predicted increase in $Mg_{17}Al_{12}$ content with higher aluminum additions must be carefully balanced in alloy design to achieve an optimal combination of strength and toughness for structural applications. This underscores the importance of correlating phase evolution with mechanical behavior in the development of advanced Mg-based materials.

Overall, this study demonstrates that increasing Al content in Mg-Al-Zn alloys significantly influences phase stability, particularly through the formation of $Mg_{17}Al_{12}$, while stabilizing the Mg phase. These insights provide a deeper understanding of the thermodynamic behavior of Mg-Al-Zn alloys and offer a systematic framework for optimizing alloy compositions to enhance their structural performance. Future studies may explore the mechanical properties and microstructural evolution of these alloys to further validate the findings and facilitate their practical applications in lightweight structural materials.

Ethical standard

The author has no relevant financial or non-financial interests to disclose.

Availability of data and material

Not applicable.

Conflicts of interest

The author declares that there is no conflict of interest regarding the publication of this paper.

LITERATURE CITED

Alaca, Y., Y. Uzunoğlu, and B. Emin, 2025 Investigation of the effect of alloying elements on the density of titanium-based biomedical materials using explainable artificial intelligence. Computers and Electronics in Medicine **2**: 15–19.

Alidoust, M., D. Kleiven, and J. Akola, 2020 Density functional simulations of pressurized mg-zn and al-zn alloys. Physical Review Materials **4**.

Avedesian, M. and H. Baker, 1999 *Magnesium and Magnesium Alloys*. ASM International.

Brubaker, C. O. and Z.-K. Liu, 2004 A computational thermodynamic model of the ca–mg–zn system. Journal of Alloys and Compounds **370**: 114–122.

Chen, L. Q., 2019 Chemical potential and gibbs free energy. MRS Bulletin **44**: 520–523.

Dai, J. H., X. Wu, and Y. Song, 2013 Influence of alloying elements on phase stability and elastic properties of aluminum and magnesium studied by first principles. Computational Materials Science **74**: 86–91.

David, M., R. Foley, J. Griffin, *et al.*, 2016 Microstructural characterization and thermodynamic simulation of cast al–zn–mg–cu alloys. International Journal of Metalcasting **10**: 2–20.

Emin, B., Y. Uzunoğlu, and Y. Alaca, 2025 Investigation of the impact of alloying elements on the mechanical properties of superalloys using explainable artificial intelligence. Chaos and Fractals **2**: 20–27.

Hayashi, N., K. Nakashima, M. Enoki, and H. Ohtani, 2020 Thermodynamic analysis of the al-mg-zn ternary system. Journal of the Japan Institute of Metals and Materials **84**: 141–150.

Huang, X. *et al.*, 2023 Influence of aluminum content on microstructure and performance of mg-zn-ca-al-mn magnesium alloys. Journal of Alloys and Compounds **948**: 169719.

JMatPro Sense Software, Accessed in 2024 Modelling of phase transformations in magnesium alloys. https://www.sentesoftware.co.uk/site-media/mg-alloys-kinetics, [Online].

Kaya, A. A., 2020 A review on developments in magnesium alloys. Front. Mater. **7**: 198.

Li, Q., Y. Zhao, Q. Luo, S. Chen, J. Zhang, *et al.*, 2010 Experimental study and phase diagram calculation in al–zn–mg–si quaternary system. Journal of Alloys and Compounds **501**: 282–290.

Liang, H., S.-L. Chen, and Y. A. Chang, 1997 A thermodynamic description of the al-mg-zn system. Metallurgical and Materials Transactions A **28**: 1725–1734.

Luo, A. A. *et al.*, 2012 Magnesium alloy development for automotive applications. Materials Science Forum **706–709**: 69–82.

Matsushita, T. and K. Mukai, 2018 *Chemical Potential and Activity*. Springer, Singapore.

Sahoo, S. K., M. Kumar, and S. K. Karak, 2024 *Fugacity, Activity, Equilibrium Constant and Ellingham Diagram*. Springer, Singapore.

Silva, A., J. Cao, T. Polcar, and D. Kramer, 2022 Design guidelines for two-dimensional transition metal dichalcogenide alloys. Chemistry of Materials **34**: 10279–10290.

Uzunoğlu, Y. and Y. Alaca, 2025a High-accuracy prediction of the thermo-physical properties of 6xxx series aluminum alloys using explainable artificial intelligence. International Journal of Computational Materials Science and Engineering **0**: 2550010, [In Press].

Uzunoğlu, Y. and Y. Alaca, 2025b Inverse prediction of the calphad-modeled physical properties of superalloys using explainable artificial intelligence and artificial neural networks. Bitlis Eren Üniversitesi Fen Bilimleri Dergisi **14**: 331–347.

Uzunoğlu, Y., B. Emin, and Y. Alaca, 2025 High-accuracy prediction of mechanical properties of ni-cr-fe alloys using machine learning. ADBA Computer Science **2**: 7–14.

Yu, J. and X. Li, 2011 Modelling of the precipitated phases and properties of al-zn-mg-cu alloys. Journal of Phase Equilibria and Diffusion **32**: 350–360.

Yuzbekova, D., J. Borisova, and A. Mogucheva, 2019 Influence of the phase composition of al-mg alloys on the propagation of deformation bands. In *AIP Conference Proceedings*, volume 2167, p. 020395.

Zhang, Z., J. Zhang, X. Zhao, X. Cheng, X. Liu, *et al.*, 2024 Thermodynamic simulation calculations of phase transformations in low-aluminum zn-al-mg coatings. Materials **17**: 2719.

How to cite this article: Uzunoğlu, Y. Computational Study of the Effect of Aluminum Content on the Thermodynamic Properties and Phase Stability of Mg-Al-Zn Alloys. *ADBA Computer Science*, 2(2), 36-42, 2025.