

Thermodynamic Stability, Phase Formation, and Structural Evolution of Al-Zn-Cu Alloys: A Combined Theoretical and Experimental Investigation

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ARTICLE INF.

Article history:

Received: 24 FEB., 2025

Revised: 13 MAR., 2025

Accepted: 7 APR., 2025

Available Online: 28 JUN.
2025

Keywords:

Miedema model
solid solutions,
Enthalpy of formation

ABSTRACT

The thermodynamic characteristics are of significant importance for evaluating phase stability and understanding the relative stability of binary and ternary systems. This study investigates the thermodynamic and structural properties of Al-Zn-Cu alloys, with a particular focus on phase stability, enthalpy of formation. A semi-empirical model (Medema model) was used to estimate the enthalpies of these systems. The chemical enthalpy analysis of the Al-Cu, Zn-Cu, and Al-Zn binary systems reveals that Cu-Al and Cu-Zn exhibit negative enthalpy values, indicating a strong thermodynamic driving force for alloy formation, while the Al-Zn system displays positive enthalpy values, suggesting limited solubility. Elastic enthalpy calculations highlight significant lattice strain in the Al-Cu system due to atomic size mismatches, followed by Zn-Cu, while the Al-Zn system exhibits minimal elastic effects. Analysis of phase stability through enthalpy of formation calculations shows that intermediate compositions between Al and Cu along with Zn-rich areas achieve maximum thermodynamic stability. The empirical results show that after five hours of mechanical alloying of the Al₈₀Zn₁₀Cu₁₀ system yields a stable α -Al (Zn, Cu) solid solution with a face-centered cubic (FCC) structure formed and matches well with theoretical expectations. The nanoparticles exhibit irregularly shaped and a propensity to agglomerate together as a result of cold-welding during milling, according to FESEM (Field Emission Scanning Electron Microscopy) photos. The rod-like structures at the nanoscale indicate the formation of a secondary phase, which improves the hardness and wear resistance. The particle size distribution shows a successful decrease to an average of 33.112 nm with a consistent size spread, and EDX analysis validates the predicted elements composition.

DOI: <https://doi.org/10.31257/2018/JKP/2025/v17.i01.18863>

الخلاصة

الكلمات المفتاحية:

نموذج ميديما
المحاليل الصلبة
حرارة التكوين

الخصائص الديناميكية الحرارية لها أهمية كبيرة لتقييم استقرار الطور وفهم الاستقرار النسبي للأنظمة الثنائية والثلاثية. تبحث هذه الدراسة في الخصائص الديناميكية الحرارية والبنية لسبائك **Al-Zn-Cu**، مع التركيز بشكل خاص على استقرار الطور، وحرارة التكوين. تم استخدام نموذج شبه تجريبي (**Miedema's model**) لتقدير حرارة التكوين لهذه الأنظمة. يكشف تحليل الحرارة الكيميائية للأنظمة الثنائية **Al-Cu**، **Zn-Cu** و **Al-Zn** أن **Al-Cu** و **Zn-Cu** تظهر قيم حرارة سلبية، مما يشير إلى قوة دافعة حرارية قوية لتكوين السبائك، بينما يظهر نظام **Al-Zn** قيم حرارة موجبة، مما يشير إلى ذوبان محدود. تسلط حسابات الحرارة المرنة الضوء على إجهاد شبكي كبير في نظام **Al-Cu** بسبب عدم تطابق الحجم الذري، يليه **Zn-Cu**، بينما يظهر نظام **Al-Zn** تأثيرات مرنة ضئيلة. يُظهر تحليل استقرار الطور من خلال حسابات المحتوى الحراري للتكوين للنظام الثلاثي أن التركيبات الوسيطة بين **Al** و **Cu** إلى جانب المناطق الغنية بالزنك تحقق أقصى قدر من الاستقرار الديناميكي الحراري. تُظهر النتائج التجريبية أنه بعد خمس ساعات من المسابقة الميكانيكية لنظام **Al₈₀Zn₁₀Cu₁₀** ينتج محلول صلب مستقر **α-Al (Zn,Cu)** مع بنية مكعبية مركزية الوجه (**FCC**) ويتوافق جيدًا مع التوقعات النظرية. تُظهر الجسيمات النانوية شكلاً غير منتظم وميلاً للتكتل معاً نتيجة اللحام البارد أثناء الطحن، وفقاً لصور **FESEM**. تشير الهياكل الشبيهة بالقضبان على مقياس النانو إلى تكوين طور ثانوي، مما يحسن الصلابة ومقاومة التآكل. يُظهر توزيع حجم الجسيمات انخفاضاً ناجحاً بمعدل 33.112 نانومتر مع انتشار حجم ثابت، ويثبت تحليل **EDX** صحة تكوين العناصر المتوقعة.

1. INTRODUCTION

Engineers have used aluminium-based alloys for machinery purposes since the 17th century because they offer good structural properties and mechanical performance with low production costs. The chemical composition of an alloy sets its characteristics through the ratio of alloying elements combined with base materials [1]. The aerospace and automotive industries extensively use aluminium-zinc alloys for their commercial applications. Heavy metals including bronze, brass, and cast iron feature prominently in many high-strength alloy compositions. These materials are widely used because they offer key benefits such as long-lasting durability coupled with corrosion resistance and easy shaping. Engineers show great interest in alloys that combine low density and high strength with excellent corrosion resistance and multi-phase microstructures while allowing easy fabrication and forming

due to their low melting points and ductility [2]. The process of melting metals is not always effective in enhancing interactions between metals to transform heterogeneous systems into homogeneous ones. This implies that melting does not always result in complete mixing of the constituent elements of an alloy, mainly when there are significant differences in the metals' physical and chemical characteristics. In this research, the traditional melting process was replaced with the method of mechanical alloying. This approach is recognized as one of the most efficient techniques for generating non-equilibrium phases in metallic systems [3, 4]. Therefore, the mechanical alloying (MA) process has been extensively utilized to create alloys within binary systems, facilitating the production of intermetallic compounds, supersaturated solid solutions, and amorphous alloys [5]. These alloys exhibit the unique ability to form nanostructures, which are anticipated to

enhance their physicochemical properties. However, the processing of ternary alloys through MA has received less attention compared to binary alloys. Therefore, investigating mechanical alloying within ternary systems is crucial to understand the alloying mechanisms and discover new alloys with improved physical properties. V.M.Lopez et al. showed that several phase transformations can be triggered by plastic deformation during tensile testing of a Zn-22 wt.% Al-2 wt.% Cu eutectoid alloy[6]. Consequently, mechanical milling (MM) of alloy powders presents a promising approach to monitoring the phase transformations induced by plastic deformation in the milling of Zn-Al-Cu alloys.

Three pure elemental powder mixtures of Zn-22%Al-18%Cu-60%, Zn-5%Al-11%Cu-84%, and Zn-27%Al-3%Cu-70% were mechanically alloyed by steel-ball milling processing, according to Zhu, Y. Perez et al. [7]. The outcome shown that mechanical alloying was used to create nanostructure Zn–Al-based alloys. The effects of adding Cu and Si to Zn-40Al alloy on its microstructural, mechanical, and machinability characteristics were examined by Senol Bayraktar et al. [8]. When Cu and Si were added to the Zn-40Al alloy, the alloy's hardness and TS increased while its EF (Fracture Elongation) decreased. The Si-added Zn-40Al-2Cu-2Si alloy had the highest hardness and TS values, whereas the Zn-40Al alloy had the lowest values. The solid precipitate hardened as a result of the addition of Cu. It was believed that Si particles made dislocation movement

challenging because they were more complicated than the matrix material. The current study examines the feasibility of creating binary and ternary alloys of Al-Zn-based systems with Cu by utilizing the Miedema model's computations. In order to supports the theoretical predictions made by the thermodynamic analysis, the article also presents experimental data on the materials' structural-phase state.

2- Theoretical Study

2-1- Miedema's model

It serves as an effective method for estimating the enthalpy of a mixture. Initially, this model was developed for binary alloys; however, significant advancements have extended its application to ternary systems [9-11]. This hypothesis states that Wigner-Seitz cells make up a binary alloy. The boundaries of these Wigner-Seitz cells change as atoms of pure metal combine to produce alloys. The difference in electronegativity between the two components ($\Delta\Phi^*$) and the change in electron density ($(\Delta n_{ws}^{1/3})$) are two important elements that affect an alloy's mixing enthalpy. These elements affect the mixing enthalpy in opposite ways. The difference in electronegativity has contributes negatively, while the electron density variation contributes positively [12]. The overall enthalpy of a binary alloy in this model can be expressed as follows [13]:

$$\Delta H_{AB}^{total} = \Delta H_{AB}^{chemical} + \Delta H_{AB}^{elastic} + \Delta H_{AB}^{structural} \quad (1)$$

Where $\Delta H^{chemical}$ refers to the chemical contribution, $\Delta H^{elastic}$ represents the elastic enthalpy. The structural enthalpy resulting from the binary system's crystal structure variations is referred to as $\Delta H^{Structural}$. The structural enthalpy may be disregarded in this context because of its negligible effect. [14].

The difference between the atoms' binding energies in their initially states and the mixed state is what causes the chemical enthalpy. For every binary system, the chemical enthalpy term may be determined using the following formula [13]:

$$\Delta H_{A \text{ in } B}^{Chemical} = 2k X_A^S X_B^S C(x) \frac{(X_A V_A^{2/3} + X_B V_B^{2/3})}{(n_{ws}^A)^{-1/3} + (n_{ws}^B)^{-1/3}} \times [-(\Delta\phi^*)^2 + Q/P (\Delta n_{ws}^{1/3})^2 - R^*/P] \quad (2)$$

Where,

$$X_A^S = \frac{X_A V_A^{2/3}}{X_A V_A^{2/3} + X_B V_B^{2/3}} \quad (3)$$

$$X_B^S = \frac{X_B V_B^{2/3}}{X_A V_A^{2/3} + X_B V_B^{2/3}} \quad (4)$$

To resolve the discrepancies between the mixing enthalpy predicted by this model and the experimental data, Wang et al. [15] proposed a correction factor, $C(x)$. This factor considers the atomic sizes of both the solute and solvent atoms.

$$C(x) = 1 - S \frac{X_A X_B |V_A - V_B|}{X_A^2 V_A + X_B^2 V_B} \quad (5)$$

where the impact of atomic size differences is explained by the semi-quantitative empirical variable S . This

variable is assigned a value of 1.0 for a disordered solid solution, 0.5 for a liquid alloy, and 2.0 for an ordered compound. [16].

The molar volumes of A and B are shown by V_A and V_B , respectively, while the molar fractions of A and B are indicated by X_A and X_B . The electron density is denoted by n_{ws} , whereas the work function of the component elements is represented by ϕ^* . Constants are P , Q , and R^* .

Depending on whether the metal is a transition or non-transition type, the constant P has two values: 14.2 and 10.7. Additionally, a P/Q ratio of 9.4 was identified. R^* is an extra parameter that accounts for the enthalpy of metals, both transition and non-transition.

The elastic enthalpy $\Delta H^{elastic}$, caused by atom-size mismatch, can be expressed as [17,18]:

$$\Delta H_{AB}^{elastic} = K_B G_A (X_A \Delta H_{B \text{ in } A} + X_B \Delta H_{A \text{ in } B}) \quad (6)$$

where the bulk modulus is denoted by K and the shear modulus by G .

The binary system's crystal structure variations are the source of the structural enthalpy. Based mostly on the number of valence electrons (Z), $\Delta H^{Structural}$ describes the propensity of transition metals to preferentially crystallize in one of three crystallographic phases: bcc, fcc, or hcp. Bakker et al. first out a formula for the structural enthalpy in 1979. [19,20]:

$$\Delta H_{A \text{ in } B}^{struct} = (E_B^{struct} - E_A^{struct}) + (Z_A - Z_B) \frac{\partial E^{struct}(B)}{\partial Z} \quad (7)$$

E_B^{struct} and E_A^{struct} denote the lattice stability of each crystal structure (bcc, fcc, and hcp), Z_A and Z_B stand for the valence electrons of each of the A and B atoms. The smallest amount that might be disregarded when calculating the mixing enthalpy is the structural enthalpy.

3- Experimental Procedures.

Using stainless steel balls and hardened steel vials, mechanical alloying of $Al_{80}Zn_{10}Cu_{10}$ was carried out at 300 rpm in Benech-Top Planetary Automatic Ball Mills (MTI). To allow the balls and powder particles to easily move about in the milling container, approximately 50% of the vial's area was left vacant. In order to maintain a ball-to-powder weight ratio of 10:1 throughout milling, 100 g of stainless steel balls and 10 g of the blended elemental powder mix were placed into the milling container for each experiment. In this investigation, balls of two different diameters (6.3 and 4.7 mm) were employed. In order to prevent excessive cold welding of the powder particles to the grinding tools and to each other, stearic acid ($CH_3(CH_2)_{16}COOH$), which made up around 3 weight percent of the powder charge, was utilized as a process control agent during milling. Depending on the system being studied, milling was done at various periods. The Al-Zn system was milled for 1, 3, and 5 hours, whereas the Al-Zn-Cu system was milled for 5 hours. To lessen the powder's temperature rise, milling was stopped for ten minutes every fifteen minutes.

A tiny amount of the powder was taken for structural analysis following each 2-hour run. It was discovered that, particularly in the early phases of milling, the powder had a tendency to adhere to the vial walls. This could interfere with the particles' alloying kinetics. Consequently, the vial was opened often, the powder was scraped from the vial walls, and milling was restarted in order to reduce this impact. At different milling stages, the XRD patterns were obtained using an Al-2700B X-ray diffractometer.

4- Results and Discussions

The phase stability diagram based on the energy above the hull for the ternary system Al-Zn-Cu can be shown in Figure 1. The most stable compositions are shown in the green dots, which represent the ideal alloys. The mechanical casting was optimized by carefully weighing the proportions of Al, Zn and Cu to obtain stable phases so that the dynamic stability and thermal structural cohesion are good. It is clear that the phases close to the green dots have low energy above the hull and are relatively stable [21]. While the red dots indicate mechanical instability, representing compositions with high energy above the hull. Through these stages and understanding the stability trends are important during the design of the desired alloys in terms of thermal and mechanical properties.

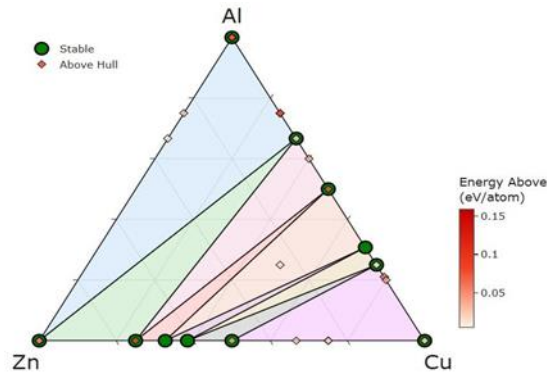


Figure 1: The Al-Zn-Cu system Phase diagram [21].

Chemical enthalpy ($\Delta H^{\text{chemical}}$) of intermetallic compounds and solid solution of the binary systems Al-Cu, Zn-Cu, and Al-Zn as a function of composition can be seen in Figure 2. The mixing process is clearly exothermic because the chemical enthalpy values are negative in the Cu-Al system. When the enthalpy reaches high negative values at about 5-6% for Al, the formation of the solid solution is more stable. The intermetallic compounds also have negative enthalpy values, but to a lesser extent than for the solid solution, which means that the formation of the solid solution is thermodynamically more favorable in this system. The strong atomic interactions in the Cu-Al system contribute to the stability of both phases. For the Cu-Zn system, the enthalpy values follow a similar trend, with the solid solutions showing more negative values than the intermetallic compounds while the $\Delta H^{\text{chemical}}$ values are lower compared to the Cu-Al system, indicating weaker atomic interactions. The enthalpy reaches its lowest point at about 5-6% for Zn, indicating that this composition is ideal for the stability of the solid solution.

Conversely, the chemical enthalpy values of the Zn-Al system are listed which suggests an endothermic mixing process. These positive enthalpy values indicate a low solid-state solubility of Zn and Al, resulting in a smaller driving force for alloy formation compared to Cu alloys. The results indicate that both Cu-Al and Cu-Zn systems demonstrate a high tendency towards alloy formation due to their negative enthalpy values, while the Zn-Al system exhibits weaker thermodynamic advantages for solid solution formation.

In contrast, the Zn-Al system exhibits positive chemical enthalpy values, signifying an endothermic mixing process. The positive enthalpy values suggest limited solubility between Zn and Al in the solid state, leading to a lower tendency for alloy formation compared to the Cu-based systems. Overall, the results suggest that Cu-Al and Cu-Zn systems favor alloy formation due to their negative enthalpy values, while the Zn-Al system shows a lower thermodynamic driving force for solid solution formation. These results are important in the context of alloy design for practical applications as they identify the compositions which enhance stability and mechanical properties across the various binary alloy systems.

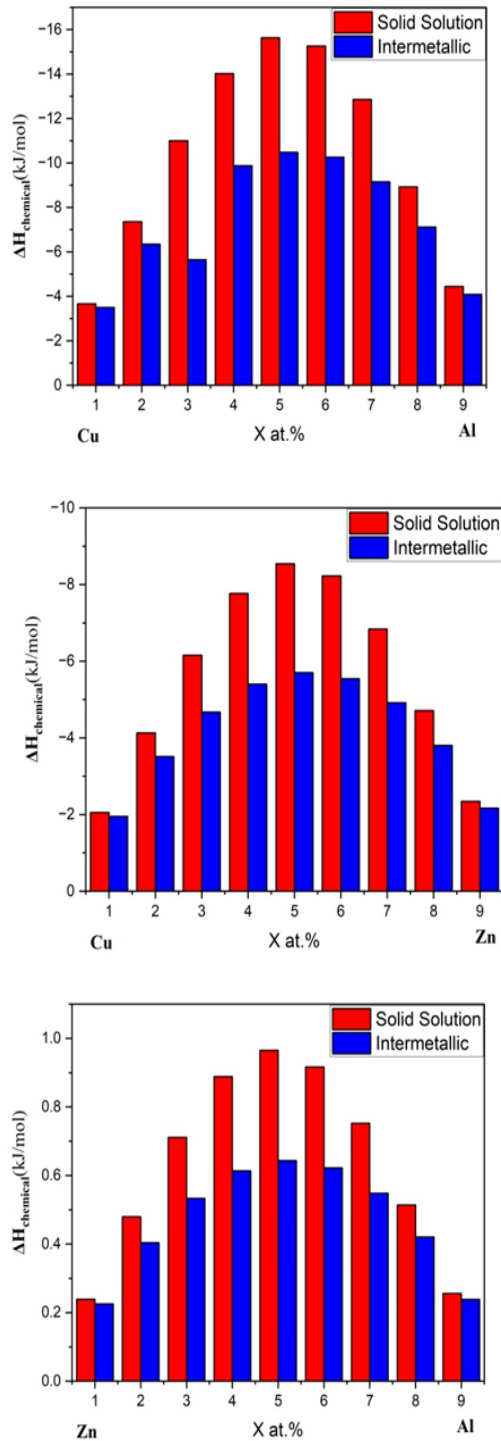


Figure 2: The chemical enthalpy of binary systems Al-Cu, Zn-Cu, and Al-Zn as a function of composition.

Elastic enthalpy arises from the size difference between solute atoms. Figure (3) illustrates the elastic enthalpy ($\Delta H^{\text{elastic}}$) as a function of composition for the Al-Zn, Al-Cu, and Zn-Cu binary

systems. Among these, the Al-Cu system exhibited the highest elastic enthalpy values (3.5 kJ/mol). It manifests that substantial lattice strain arises from lattice mismatch (atomic size difference) between Al and Cu as well, which leads to high elastic energy. For the Zn-Cu system, the elastic enthalpy was found to be lower, peaking at approximately 2.0 kJ/mol. This indicates that Zn and Cu have a moderate atomic size mismatch, which allows them to have lower elastic strain energy than Al-Cu system. On the contrary, in the Al-Zn system, the minimum values of elastic enthalpy was conserved, which is still close to zero across all compositions. This indicates a small lattice strain and indicates Al and Zn atomic sizes was compatible leading to small elastic energy contributions. In general, Al-Cu produces the highest elastic strain energy, followed by Zn-Cu, and Al-Zn that shows little elastic effects. This can be attributed to the differences in atomic size, which plays a major role in determining the elastic strain energy of binary alloys and can therefore be used as a guide to adjust their mechanical properties and phase stability.

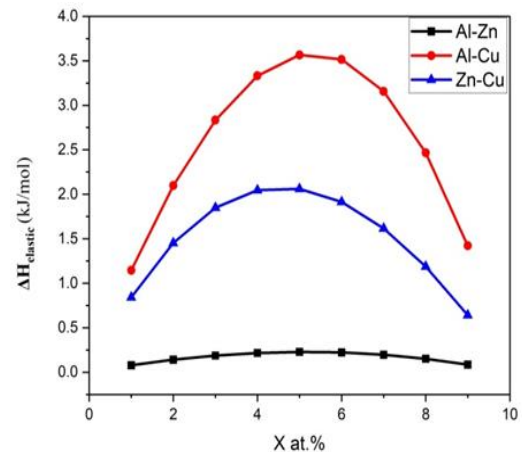


Figure 3: The elastic enthalpy of binary systems Al-Zn, Al-Cu, and Zn-Cu as a function of composition.

The enthalpy of formation of the Al-Zn-Cu system is shown in Figure 4 as a composition function. The lowest enthalpy values were observed in some places between Al and Cu as well as in some Zn richer regions, indicating that the stability in these compositions is very strong thermodynamically. The presence of negative enthalpy values suggests the formation of stable intermetallic phases, which can enhance the mechanical and structural properties of the alloy. Conversely, regions with enthalpy values close to zero correspond to compositions where atomic interactions are relatively weak. This behavior may be attributed to atomic size mismatches. Overall, the enthalpy of formation analysis reveals that Al-Zn-Cu alloys exhibit varying degrees of thermodynamic stability depending on their composition. The strong interactions between Cu and Al, as well as between Zn and Al, promote the formation of energetically favorable phases, which play a crucial role in tailoring the properties of these alloys for practical applications.

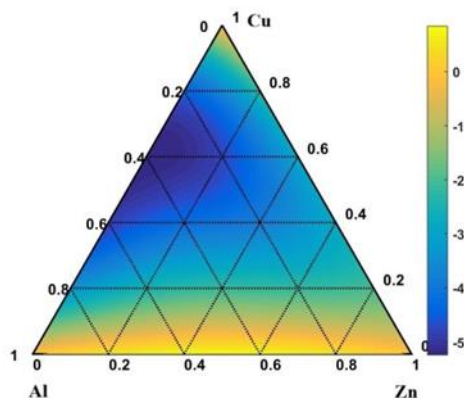


Figure 4: The enthalpy of formation as a function of composition for Al-Zn-Cu ternary system.

The X-ray diffraction (XRD) patterns of the $\text{Al}_{80}\text{Zn}_{10}\text{Cu}_{10}$ alloy were plotted against milling time (1, 3, and 5 hours) as seen in Figure 5. Severe powder adherence on balls and vial surfaces was noticed after an hour of milling. This can hamper the amorphization reaction by limiting the impact energy of colliding balls and drastically lowering the milling efficiency. From the Figure 5, it was noticed that after 3 hours of mechanical alloying, all the peaks were prominent with a slight decrease in intensity and an increase in the width of the peaks. This indicates that as the grinding time increased, the particle size decreased. No amorphous phase was developed during five hours of mechanical alloying. Rather, an α -Al solid solution with a face-centered cubic (FCC) crystalline structure that contained Zn and Cu formed. The dissolution of copper and zinc in the aluminum lattice may cause a minor change in position, resulting in lattice distortion and the production of a fcc α -Al(Zn,Cu) solid solution. The intensity of the diffraction peaks decreases as they get broader. The reduction in particle size and the microstrain brought about by milling that are linked to the broadening. Mechanically, the ternary alloy Al Zn Cu is a single-phase material with a nanocrystalline (15-88 nm) and a high degree of micro-distortion, according to the X-ray analysis results. Overall, the XRD analysis highlights that mechanical alloying leads to the progressive dissolution of Zn and Cu

into the Al matrix, promoting solid solution strengthening. The formation of a homogenous α -Al phase at extended milling times suggests enhanced alloy uniformity, which can positively influence the material's mechanical properties.

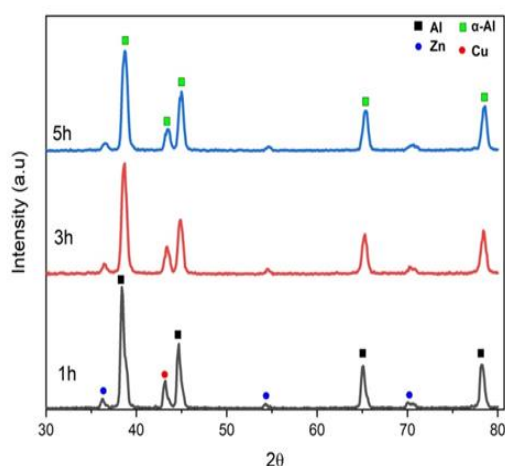


Figure 5: X-ray diffraction patterns of $\text{Al}_{80}\text{Zn}_{10}\text{Cu}_{10}$

The microstructure of the $\text{Al}_{80}\text{Zn}_{10}\text{Cu}_{10}$ nanoparticles synthesized by mechanical alloying is clearly visible in the FESEM pictures (Figure 6). According to the micrographs, the particles exhibit irregular morphology and a noticeable propensity to aggregate, which is a common characteristic of powders that have been mechanically milled. The cold welding effect, in which particles stick together as a result of frequent high-energy collisions during milling, is responsible for this agglomeration. Furthermore, tiny particles seem affixed to the surfaces of bigger ones, suggesting a combination of welding and fragmentation processes taking place at the same time. The existence of nanoscale rod-like structures is seen in the photos at higher magnifications;

these structures may be related to the development of secondary phases, intermetallic complexes, or oxide precipitates. The material's mechanical and thermal characteristics may be greatly influenced by these nanostructures, which might improve the material's strength and resistance to wear. Their development implies that a uniform distribution of elements at the nanoscale was made possible by the alloying process, which enhanced hardness and refined the grain.

These results are confirmed by the particle size distribution histogram, which displays a mean particle size of 33.112 nm. The near-Gaussian distribution of the particle sizes, which range from 15.41 nm to 88.04 nm, indicates that the milling operation successfully decreased particle size while preserving a comparatively uniform size distribution. Large particles in the distribution, however, suggest that some agglomeration and re-welding had place during milling; this might be avoided by modifying the ball-to-powder ratio, milling time, and process control agents.

The EDX spectrum displays clear peaks for Al, Zn and Cu. The most prominent peak in the spectrum corresponds to aluminum, confirming that the primary matrix of the alloy is predominantly composed of aluminum. The zinc and copper peaks, which appears with lower intensity, reflects its smaller quantity compared to aluminum, consistent with the intended chemical composition of the alloy.

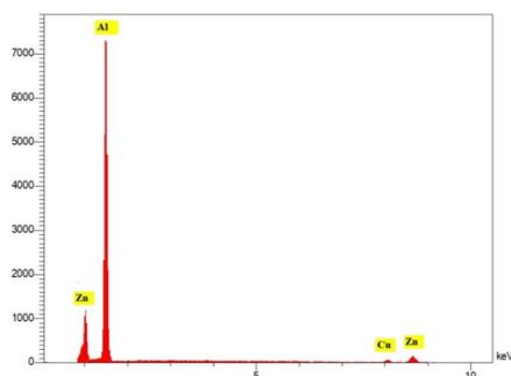
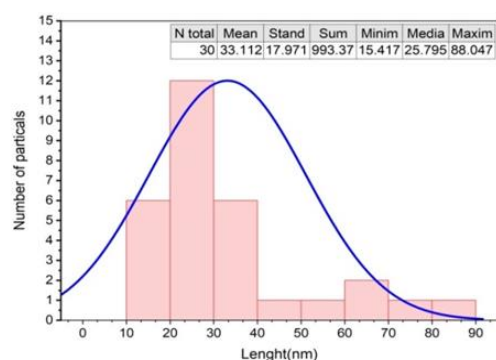
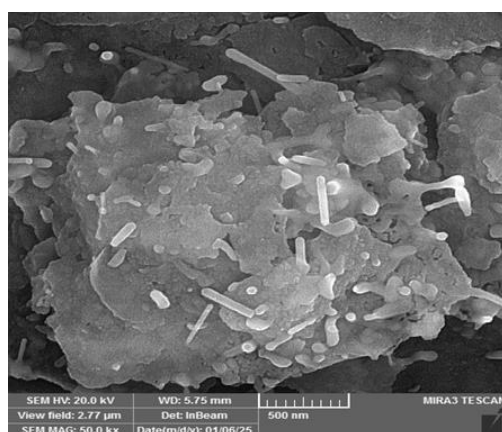
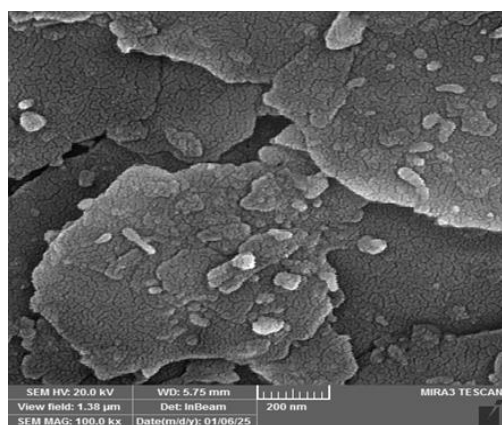


Figure 6: FESEM images, size distribution histogram and EDX spectra of $\text{Al}_{80}\text{Zn}_{10}\text{Cu}_{10}$ nanoparticles prepared by mechanical alloying.

5- Conclusions

One of the most important factors in defining the alloy system's capacity for phase stability is the enthalpy of formation. The presence of negative enthalpy values in the Al-Zn-Cu system signifies a strong thermodynamic driving force favoring alloy formation and stability. Moreover, the successful application of the Miedema model in this study highlights its robustness in predicting the behavior of ternary and multicomponent systems. The mechanical alloying process successfully facilitated the formation of Al-Zn-Cu ternary alloys with a nanostructured morphology, demonstrating the viability of mechanosynthesis in producing homogeneous multicomponent alloys. FESEM images show the microstructure of $\text{Al}_{80}\text{Zn}_{10}\text{Cu}_{10}$ nanoparticles, which exhibit irregular morphology and a tendency to agglomerate due to cold welding during grinding. The nanorod-like structures indicate the formation of secondary phases, which enhance the hardness and wear resistance. The particle size distribution indicates that the size was successfully reduced to an average of 33.112 nm with a quasi-Gaussian distribution. The experimental results align closely with the predictions made using the Miedema model, reinforcing its reliability as a predictive tool in materials science.

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