MODELLING AND SIMULATION OF COMPOSITION AND MECHANICAL PROPERTIES OF HIGH ENTROPY MAGNESIUM-BASED MULTI COMPONENT ALLOY

Robert Kennedy Otieno[1], Edward V. Odhong[1] and James Mutua[2]

[1]Department of Mechanical and Mechatronic Engineering, Multimedia University of Kenya, Nairobi, Kenya
[2]Department of Mechanical Engineering, Jomo Kenyatta University of Agriculture and Technology, Nairobi, Kenya

ABSTRACT

Magnesium alloys are high potential materials for application in the aerospace and automotive industries due to their lightweight properties. They can help to lower dead weight and fuel consumption to contribute to sustainability and efficiency. It is possible to achieve high specific strength and high stiffness of the alloys by varying compositions of alloying elements. Applications of magnesium are limited due to its low strength and relatively low stiffness. This research focuses on a recipe of multi component alloys of magnesium with varied percentages of Mg, Al, Cu, Mn and Zn obtained from literature and optimizes the percentage compositions to obtain for high specific strength and specific stiffness. Relationships among percentage constituents of the alloy components are examined in Matlab R2022b using multiple linear regression. Optimization is achieved using genetic algorithm to determine the specific strengths and stiffness. The resulting optimal alloy component percentages by weight are used for microstructure simulation of thermodynamic properties, diffusion and phase transformations of proposed alloy is done in MatCalc software version 6.04. Results show potential for improved mechanical properties resulting from disordered structure in the high entropy magnesium alloy. Future research should focus on production and characterization of the proposed alloy.

KEYWORDS

High entropy alloys, multicomponent alloy, specific strength, specific modulus

1. INTRODUCTION

Sustainability of environment and reduction of carbon footprint can be ensured through reduction of weight in the automotive and aerospace sectors [1]. Currently, there is a shift from using high density materials to light-weight materials in order to increase payload and also achieve sustainability goals. However, existing light-weight metals have limited structural applications due to their low specific strength and undesirable specific stiffness coupled with high production costs [1]. To address this problem, continuous research efforts now focus on development of new types of low-cost, low-density alloys of light-weight metals to meet properties required for various engineering applications.

The main focus of researchers for many years has been to replace iron and steel with aluminum and magnesium alloys. Current research on light-weight metals focuses more on magnesium than aluminium because of its lower density [2]. Magnesium has specific gravity of 1.738 and is

known as the lightest structural material and next generation material. However, magnesium alloys have limited applications in critical engineering due to their low absolute strength, ductility and creep resistance [2].

Though many magnesium-base alloys have been developed, there is need for alloys with better strength and stiffness to meet material requirements in automotive and aerospace industries . Bulk metallic glasses (BMGs) and recently developed high entropy alloys (HEAs) of magnesium are promising and have very high compressive strength and hardness. However, they have poor ductility and no significant tensile responses for wide applications in the sectors [3]. The new approach of design of high entropy magnesium alloys with disordered structure achieves high specific strength and modulus for magnesium alloys containing Al, Cu, Mn and Zn in varied percentages [4]. For example, magnesium alloy containing Mg-80%wt-Al-10%wt-Cu-5%wt-Mn-5%wt-Zn-0%wt was found to have yield strength of 228Mpa, ultimate tensile strength of 328MPa and density of 1.68 g/cm3 but had Young's Modulus of 46.4GPa [5].

Based on previous research, lower densities of high entropy magnesium alloys can be achieved when percentage of Mg is above 80% by weight and that of copper is lower than 5% . For example Mg-91.2%wt-Al-8.3%wt-Cu-0%wt-Mn-0.15%wt-Zn-0.35%wt has a density of 1.85 g/cm3, but low yield strength of 145MPa and ultimate tensile strength of 270Mpa [4]. Also, Mg-95.34%wt-Al-4.4%wt-Cu-0%wt-Mn-0.26%wt-Zn-0%wt has density of 1.79 g/cm3, low yield strength of 125MPa and ultimate tensile strength of 210MPa. On the other hand, magnesium alloys with percentage of components higher than 5% have very high ultimate tensile strengths and yield strengths but are heavier [4]. Examples are Mg-45.6%wt-Al-13.6%wt-Cu-13.6%wt-Mn-13.6%wt-Zn-13.6%wt that has density of 2.53 g/cm3, yield strength of 265MPa and ultimate tensile strength of 454MPa and Mg-43%wt-Al-14.25%wt-Cu-14.25%wt-Mn-14.25%wt-Zn-14.25%wt having density of 2.71 g/cm3, yield strength of 284MPa and ultimate tensile strength of 486Mpa [4], [6].

The literature reviewed confirm that there has not been established clear component percentages relating to high specific strength and specific modulus of the studied multicomponent high entropy alloys of magnesium. Optimal percentage of alloying elements that can help attain high strength, greater stiffness and low density for aerospace and automobile applications is yet to be found. This research aims at finding optimal alloying constituent percentages for high performance multicomponent Mg alloy. The current research improves on [5]. It uses optimization of percentage compositions of alloying elements and does not restrict itself to near equal proportions. The approach uses the genetic algorithm with elitism to search for fit offspring that can achieve high specific strength and stiffness to cross to next generation.

2. LITERATURE REVIEW

Varying percentage composition of magnesium from 20% to 50% was used by [6] based on the principle of equiatomic ratio and high entropy of mixing to design microstructure and mechanical properties. They used induction melting technique followed by casting in a copper mould. The alloys had densities that ranged from 2.20 g/cm3 to 4.29 g/cm3. Compressive strengths were found to be between 400MPa and 500MPa at room temperature. However, the densities of these alloys were high and the percentages of aluminium were above 12% and could raise shrinkage and porosity as suggested in literature [7]. All the alloys proposed in the research had manganese content greater than 0.5% by weight therefore resulting into non-optimal alloy properties [8].

Casting technique and solution treatment followed by two-step aging treatment (S-T6) was used by [9] to propose magnesium alloy of composition by weight of Mg-80%wt-Al-10%wt-Cu-5%wt-Mn-5%wt-Zn-5%wt. The alloy had yield strength of 228MPa, ultimate tensile strength of

328MPa, Young's modulus of elasticity (E) of 46.4GPa, density of 1.68 g/cm3 and elongation of 16%. The researchers note that the mechanical properties of their proposed alloy were better than nearly all other high performance cast magnesium alloys. However, the alloy had low stiffness despite possessing attractive low density. High Mn content of above 0.5% in the alloy was not optimal and could cause high degradation rates [8].

Literature review approach was used to study tensile properties of commercial high strength cast alloys of magnesium [10]. It was found that magnesium alloys that are solution treated and peak aged (S-T6) such as Mg-91.2%wt-Al-8.3%wt-Cu-0%wt-Mn-0.15%wt-Zn-0.35%wt has density of 1.8 g/cm3, ultimate tensile strength of 270MPa, yield strength of 145 MPa and low Young's Modulus of 47.54Gpa. Another solution treated option of Mg-92.05%wt-Al-5.3%wt-Cu-0%wt-Mn-0.15%wt-Zn-2.5%wt has density of 1.81 g/cm3, ultimate tensile strength of 232MPa, yield strength of 122MPa and Young's Modulus of 102GPa [10]. The study also reviewed high entropy magnesium alloys produced through die casting (DC) and cast and solution treatment of the alloys such as AZ63 that had lower specific strength and stiffness compared to S-T6 and DC. Though this research achieved very high specific strengths, the problem of low stiffness was not addressed. It is noted that for high specific strength, percentage of Mg should be high, possibly above 90% by weight as demonstrated in this research. Further, this research only carried out tests on tensile properties but did not address behaviour under compression.

Magnesium-based multicomponent alloy with alloy composition as Mg-80%wt-Al-5%wt-Cu-5%wt-Mn-5%wt-Zn-5%wt [5]. The alloy was synthesized using disintegrated melt deposition (DMD) technique and then subjected it to hot extrusion. The yield strength in tension was 211MPa and ultimate tensile strength was 318MPa. Density of the alloy was 2.15 g/cm3 and ultimate compressive strength (UCS) was 616MPa. The modulus of elasticity, E, of the alloy was estimated as 49.35GPa under tension. Though this research achieved higher modulus of elasticity, it achieves lower strength compared to the alloy proposed in literature [9]. It therefore means reduction of aluminium from 10% to 5% and addition of zinc resulted into higher stiffness but slightly lower yield and ultimate tensile strengths.

An extensive literature review on high entropy magnesium alloys with Al, Cu, Mn, Zn and other alloying elements was carried out to determine properties [4]. They found out that ultra-high strength, corrosion resistance, good fracture toughness and ductility can be achieved by the alloys due to unusual combinations of elements. Another important finding in their research was that the mechanical behaviour of magnesium alloys was strongly affected by chemical ordering. These findings confirm those of previous researchers [5], [9]. However, the research does not address the problem of optimization of the alloy properties by changing percentage composition of alloying elements.

3. NUMERICAL ANALYSIS

Various approaches have been applied in numerical analysis of composition and mechanical properties of high entropy alloys. Numerical methods that have been used include modelling and simulation that are essential in exploring the relationships among the compositions, structures and properties the alloys. The existing models for predicting mechanical behaviour of the alloys are reviewed. The methods for simulating the microstructure evolution, deformation mechanisms, and mechanical behaviour are also reviewed.

Early approaches involved identification of mixtures of elements with potential of producing one solid solution bulk metallic glasses [11]. In this approach, it was suggested that atoms of different elements bring about disordered structure of multicomponent alloys. According to the research,

the disordered structure was relized on the basis of the atomic size mismatch. These combinations could produce high entropy alloys but were not efficient.
Later, thermodynamic approaches of modeling of alloys were proposed. These approaches are more credible and were based on μ or Ω, [12] electronegativity, valence electron concentration [13], bulk modulus and interatomic spacing mismatches [14]. It involves predicting thermodynamic behavior of alloys, and comparing the performance with to show how applicable they are. The performance of the thermodynamic approaches is difficult to measure since alloys that do not match database are discarded [15].

Reliance on databases for comparison of alloy properties led to statistics and machine learning techniques. The techniques combine the predictability of the search and comparison criteria and are able to produce more robust design ways for new high entropy alloys. The statistical methods based on Principal Component Analysis (PCAs) were proposed in literature to gather the maximum variance and to redefine areas with greatest correlations where solid solutions could occur [16]. The approach was also combined with clustering techniques of data processing that classify and show trends in databases for predicting properties [14].

More recently, researchers used neural networks (NNs) in combination with an optimization algorithms like genetic algorithm, to search the optimal alloy compositions. Use of such computational resources have contributed to exploration of much wider compositional spaces for high entropy alloys. Use of NNs in commercial alloys has been studied by researchers such as [17]. For example, density and solid solution hardening effects of high entropy alloys was predicted using multiobjective optimization to enhance mechanical properties [18]. Use of multi-objective optimization technique is necessary because some parameters and properties may be working in opposite directions [15], [18]. One challenge of the multiobjective technique is finding equilibrium to obtain high entropy alloy with interesting combination of properties since some may have inverse relationships [14]. observe that machine learning has demerit of high computational cost for each criteria and that the models are required to be small, to help provide predictions within reasonable time frame.

The use of CALPHAD and computational thermodynamics has been adopted to provide direct calculation of the Gibbs free energy for phase stability. The approach relies on databases as well as available data to researchers. The approaches have good prediction accuracy and have already been applied to successfully produce new high entropy alloys with good stability, including magnesium alloys [19], [20], [20], [21]. The issue of vacancies that is a problem with this kind of prediction can be addressed to take care of transformations due to diffusion.

The current research uses a combination of multiobjective optimization and CALPHAD approaches. Optimization of percentage compositions of alloying elements is based on evolutionary computation and is not restricted itself to near equal proportions. The approach lets the genetic algorithm search for fit offspring using elitism within limits of alloying element compositions in literature.

3.1. Modelling Alloy Compositions and Mechanical Properties

Linear regression is applicable in establishing the mathematical relationship between density, yield strength, ultimate tensile strength and Young's modulus (E).The relationship can be established through log-linear regression model. We find relationship between natural log of E and that of yield strength (YS) as shown in Equation 1.

$$lnYS = \beta_0 + \beta_1 \ln E + \varepsilon \quad (1)$$

Where,

β_0= The regression constant;
β_1= Beta coefficient of log of E;
ε= Error term
Equation 1 becomes as shown in Equation 2

$$YS = e^{\beta_0} E^{\beta_1} \tag{2}$$

We replace e^{β_0} withk_1 and β_1 with tau_1 as follows

$$YS = k_1 E^{tau_1} \tag{3}$$

The log-linear relationship between density and Young's modulus can be found as shown in Equation 4.

$$\ln \rho_{alloy} = \beta_{0E} + \beta_E \ln E + \varepsilon$$
$$\rho_{alloy} = e^{\beta_{0E}} * E^{\beta_E} \tag{4}$$

Where,
β_{0E}= Regression constant for E.
β_E= Beta coefficient of ln E
ε= Error term
We replace $e^{\beta_{0E}}$ withk_2 and β_E with tau_2 as follows

$$\rho_{alloy} = k_2 * E^{tau_2} \tag{5}$$

Therefore we express Young's modulus as shown in Equation 6.

$$E = \left(\frac{\rho_{alloy}}{k_2}\right)^{\frac{1}{tau_2}} \tag{6}$$

Yield strength is found by substituting Equation 6 into Equation 3 as shown in Equation 7.

$$YS = k_1 \left(\frac{\rho_{alloy}}{k_2}\right)^{\frac{tau_1}{tau_2}} \tag{7}$$

The relationship between ln UTS and ln E using loglinear regression is given by Equation 8

$$\ln UTS = \beta_{0UTS} + \beta_{UTS} \ln E + \varepsilon$$
$$UTS = e^{\beta_0 UTS} * E^{\beta_{UTS}} \tag{8}$$

Which becomes:

$$UTS = k_3 * E^{tau_3} \tag{9}$$

And substituting for E we have Equation 10.

$$UTS = k_3 * \left(\frac{\rho_{alloy}}{k_2}\right)^{\frac{tau_3}{tau_2}} \tag{10}$$

Where,
$k_3 = e^{\beta 0_{UTS}}$;
β_{0UTS}= Regression constant for UTS
$\beta_{UTS} = tau_3$= Beta coefficient of E
Specific modulus becomes:

$$\frac{UTS}{\rho_{alloy}} = \frac{k_3}{k_2^{\frac{tau_3}{tau_2}}} * \left(\rho_{alloy}\right)^{\left(\frac{tau_3}{tau_2}-1\right)} \tag{11}$$

Optimal values of density, yield strength, ultimate tensile strength and stiffness are obtained from the optimal values of percentages generated from the objective functions. The specific strength at yield, $\frac{YS}{\rho_{alloy}}$, $\frac{UTS}{\rho_{alloy}}$ and specific modulus $\frac{E}{\rho_{alloy}}$become the objective functions for genetic algorithm implementation of multibojective optimization in Matlab R2022b. The aim is to maximize each as shown in Equation 12.

$$Maximize\begin{cases} \dfrac{YS}{\rho_{alloy}} = \dfrac{k_1}{(k_2)^{\frac{tau_1}{tau_2}}}\left(\rho_{alloy}\right)^{\left(\frac{tau_2}{tau_1}-1\right)} \\ \dfrac{UTS}{\rho_{alloy}} = \dfrac{k_3}{k_2^{\frac{tau_3}{tau_2}}} * \left(\rho_{alloy}\right)^{\left(\frac{tau_3}{tau_2}-1\right)} \\ \dfrac{E}{\rho_{alloy}} = \left(\dfrac{1}{k_2}\right)^{\frac{1}{tau_2}} * \left(\rho_{alloy}\right)^{\left(\frac{1}{tau_2}-1\right)} \end{cases} \quad (12)$$

Density is expressed as shown in Equation 13. Density of Mg is $\rho_{Mg} = 1.738$ g/cm^3, of Al is $\rho_{Al} = 2.7$ g/cm^3, Cu is $\rho_{Cu} = 8.96$ g/cm^3, Mn is $\rho_{Mn} = 7.26$ g/cm^3 and Zn is $\rho_{Zn} = 7.133$ g/cm^3. Masses of the components will be m_{Mg}, m_{Al}, m_{Cu}, m_{Mn} and m_{Zn} for magnesium, aluminium, copper, manganese and zinc. Density estimation is done using alloy formula based on density of components.

$$\rho_{alloy} = \frac{m}{v} \quad (13)$$

Where,

m=mass of alloy in grams; $m = m_{Mg} + m_{Al} + m_{Cu} + m_{Mn} + m_{Zn}$

v=volume of alloy, cm^3,.

But v is the sum of volumes of the components of the alloy. Meaning volume of magnesium, $v_{Mg} = \frac{m_{Mg}}{\rho_{Mg}}$, aluminium, $v_{Al} = \frac{m_{Al}}{\rho_{Al}}$, copper, $v_{Cu} = \frac{m_{Cu}}{\rho_{Cu}}$, manganese, $v_{Mn} = \frac{m_{Mn}}{\rho_{Mn}}$ and $v_{Zn} = \frac{m_{Zn}}{\rho_{Zn}}$.

$$\rho_{alloy} = \frac{m}{v_{Mg} + v_{Al} + v_{Cu} + v_{Mn} + v_{Zn}} = \frac{m}{\left(\frac{m_{Mg}}{\rho_{Mg}} + \frac{m_{Al}}{\rho_{Al}} + \frac{m_{Cu}}{\rho_{Cu}} + \frac{m_{Mn}}{\rho_{Mn}} + \frac{m_{Zn}}{\rho_{Zn}}\right)} \quad (14)$$

Since the density of magnesium is the lowest of the alloy components, low optimal density is found by establishing the highest amount of magnesium that can provide optimal strength and stiffness. Mass of alloying element divided by alloy mass gives percentage composition of each alloying element. Percentage composition by weight of the components is p_{Mg}, p_{Al}, p_{Cu}, p_{Mn} and p_{Zn} for magnesium, aluminium, copper, manganese and zinc. Alloy density is therefore expressed in terms of percentage composition as shown in Equation 15.

$$\rho_{alloy} = \frac{1}{\left(\frac{p_{Mg}}{\rho_{Mg}} + \frac{p_{Al}}{\rho_{Al}} + \frac{p_{Cu}}{\rho_{Cu}} + \frac{p_{Mn}}{\rho_{Mn}} + \frac{p_{Zn}}{\rho_{Zn}}\right)} \quad (15)$$

Substituting for alloy density in Equation 12, we have objective functions as presented in Equation 16. Percentage composition is therefore varied to maximize specific strengths and modulus.

$$Maximize\begin{cases} \dfrac{YS}{\rho_{alloy}} = \dfrac{k_1}{(k_2)^{\frac{tau_1}{tau_2}}}\left(\dfrac{p_{Mg}}{\rho_{Mg}}+\dfrac{p_{Al}}{\rho_{Al}}+\dfrac{p_{Cu}}{\rho_{Cu}}+\dfrac{p_{Mn}}{\rho_{Mn}}+\dfrac{p_{Zn}}{\rho_{Zn}}\right)^{\left(1-\frac{tau_2}{tau_1}\right)} \\ \dfrac{UTS}{\rho_{alloy}} = \dfrac{k_3}{k_2^{\frac{tau_3}{tau_2}}} * \left(\dfrac{p_{Mg}}{\rho_{Mg}}+\dfrac{p_{Al}}{\rho_{Al}}+\dfrac{p_{Cu}}{\rho_{Cu}}+\dfrac{p_{Mn}}{\rho_{Mn}}+\dfrac{p_{Zn}}{\rho_{Zn}}\right)^{\left(1-\frac{tau_3}{tau_2}\right)} \\ \dfrac{E}{\rho_{alloy}} = \left(\dfrac{1}{k_2}\right)^{\frac{1}{tau_2}} * \left(\dfrac{p_{Mg}}{\rho_{Mg}}+\dfrac{p_{Al}}{\rho_{Al}}+\dfrac{p_{Cu}}{\rho_{Cu}}+\dfrac{p_{Mn}}{\rho_{Mn}}+\dfrac{p_{Zn}}{\rho_{Zn}}\right)^{\left(1-\frac{1}{tau_2}\right)} \end{cases} \quad (16)$$

In this research, genetic algorithm iterations are set at 600 generations. Population size is set to 500 and elitism at 25. Offspring in each iteration replaces some individuals from the population. Elitism means that the most fit 25 individuals are guaranteed placement in the next generation. Cross-over probability is set at 0.8 and mutation set at 0.1, which are defaults for genetic algorithm. Crossover probability refers to the selection probability of an individual from a generation. Search domain for genetic is set as Mg, Al, Cu, Mn and Zn and lower and upper bound defined based on percentages that give better properties.

For aluminium, the genetic algorith searches within limits of 5-8% and for zinc it is in the range of 0.5-2% so that total composition of Al and Zn does not exceeds 10% as recommended in literature to achieve high specific strength, corrosion resistance and address the problem of porosity at alloy freezing point [7], [22]. Manganese is within the limits of 0.15 and 0.5% that is found to be optimal for ensuring corrosion resistance when it forms aluminium-manganese phases that address the issue of impurities becoming cathodes [8][23]. Composition of copper is optimized between the ranges of 0.1 and 0.5% to help in enhancing strength, solderability, plateability and modulus of elasticity of the alloy [7], [24]. Copper will also enhance fluidity of magnesium alloys during alloy preparation process [24]. Table 1 illustrates lower and upper bounds for the elements and density.

Table 1. Lower and upper bounds of composition of alloying elements

	Mg (wt%)	Al (wt%)	Cu (wt%)	Mn (wt%)	Zn (wt%)	ρ_{alloy} g/cm^3
Lower bound	80	8	0.1	0.15	0.5	1.74
Upper bound	94.25	9	0.5	0.5	2	2.15

Data for optimization in Matlab is as shown in Table 2. There are five variables, three nonlinear inequality constraints and one nonlinear equality constraint. Options for creation is uniform, crossover is intermediate, selection function is tournament and mutation function is on positive basis.

Table 2. Data for optimization of composition and mechanical properties

Mg (wt%)	Al (wt%)	Cu (wt%)	Mn (wt%)	Zn (wt%)	Density (g/cm^3)	UTS (MPa)	Yield (MPa)	E* (GPa)	Method used	Method used and Source Citation
91.2	8.3	0	0.15	0.35	1.8	270	145	47.54	S-T6	[10], [25]
91.2	8.3	0	0.15	0.35	1.8	270	90	35.51	S-T4	[10], [25]
91.2	8.3	0	0.15	0.35	1.8	230	150	49.18	DC	[10], [25]
92.05	5.3	0	0.15	2.5	1.81	254	94	101	S-T4	[10], [25]
92.05	5.3	0	0.15	2.5	1.81	232	122	102	S-T6	[10], [25]
92.1	0	2.4	0	5.5	1.85	210	125	104	S-T6	[10], [25]
92.9	6.5	0	0.6	0	1.79	225	130	100	DC	[10], [25]
93	6	0	0	1	1.78	260	129	99.5	DC	[10], [25]
95.34	4.4	0	0.26	0	1.77	210	125	99	DC	[10], [25]
20	20	20	20	20	4.3	717	450	150	IM	[6]
45	13.75	13.75	13.75	13.75	2.71	486	284	151	IM	[6]
45.6	13.6	13.6	13.6	13.6	2.53	454	265	141	IM	[6]
50	12.5	12.5	12.5	12.5	2.2	394	230	123	IM	[6]
80	10	5	5	0	1.68	328	228	46.4	S-T6	[9]
80	5	5	5	5	2.15	318	211	49.35	DMD	[5]

*Where E was not stated by authors, the researcher estimated from stress-strain curves in the respective publications; DC – die casting, IM-induction melting, DMD-Disintegrated melt deposition, S-T4 solution heat treatment followed by tempering, S-T6 solution heat treatment followed by quenching and precipitation hardening

3.2. Simulation of Thermodynamic and Phase Transformations

MatCalc version 6.04 software is used to simulate the thermodynamics, diffusion and phase transformations of the alloy. Equilibrium and precipitate kinetics which consist of the stages of heat treatment is determined for the alloy. The software uses classical nucleation theory in calculating growth and coarseness of alloy precipitates as side products of the Svoboda–Fischer–Fratzl–Kozeschnik (SFFK) model [26]. The model is based on Onsager's extremum principle and accounts for the energy dissipated from diffusion in the matrix, diffusion in the precipitates and that in the moving interfaces[26], [27]. Moreover, interfacial energies are calculated automatically based on generalized broken-bond model [28].

Chemical composition of the alloy is defined in terms of percentage of alloying elements Mg, Al, Cu, Mn and Zn by weight based on output of simulation in the genetic algorithm from Matlab R2022b. Precipitate phases are chosen from the alloying elements. The phases include MgZn, MgZn2, Mg2Zn11, Mg2Cu, MgCu2, MnAl, MnAl2 Mn5Al8 and Mg17Al12, CuMg1 and CuMg0 co-clusters. Precipitation kinetic simulations requires additional input parameters that include microstructural information and nucleation settings. The parameters for kinetic simulation include heat treatment and definition of grain sizes and dislocation density. Formation of alloy is done at 1300oC and normalization at 400oC for a period of one hour for.

Precipitation domains are set in MatCalc version 6.04 to trap solutes of Mg, Al, Cu, Mn and Zn and trapping enthalpy is defined. Thermo-mechanical treatments are defined and include melt deposition at 1300oC set as segment-start-temperature and cooling of the alloy to temperature of 400oC as segment-end-temperature after about 20 minutes. The resulting temperature gradient is -0.75oC per second. This is followed by homogenization at the same temperature of 400oC that is done for one hour to ensure uniform particle sizes and composition. After homogenization, the alloy is quenched to room temperature of 25oC with temperature gradient of -100oC per second to improve strength and then maintained at room temperature for 30 minutes. The alloy is reheated to 400oC during hot-rolling process for about 10 minutes and kept at that temperature for about 15 minutes during rolling. It is then quenched to 25oC for one hour at cooling rate of of -100oC per second. After that, natural aging in air occurs on the alloy for seven days. Precipitation simulation is set to capture changes in temperature, number density, phase fractions and mean radii of precipitates. Number density, phase fractions and precipitate mean radii are known to affect coarsening behaviour of alloys and influence strength [29], [30].

4. RESULTS AND DISCUSSIONS

ANOVA is carried out as one of exploratory data analysis to find whether variation of compositions significantly influence density, UTS, YS and E. Results of ANOVA in Table 3 show that variations of columns and rows of data were significant at α=0.05. This means that changes in percentage composition of the alloys as well as alloying elements are significant. Interactions are insignificant meaning that there are no significant differences among groups across different alloy compositions.

Table 3. Results of ANOVA on data

Source	SS	df	MS	F	Prob>F
Columns	744578.9	3	248193	34.51	0
Rows	62152.4	2	31076.2	4.32	0.0208
Interactions	57912.9	6	9652.1	1.34	0.2643
Error	258904.2	36	7191.8		
Total	1123548.4	47			

Variation between yield strength and density of the alloy is shown in Figure 1. The regression line of the variation is green. Non-parametric mean is represented by dashed red line while the degree of spread or variance is indicated using blue line. The ellipses show regions within 90% and 95% confidence. The smaller ellipse confirm that it is possible to vary density from 1.75 to 2.5 g/cm^3 as yield strength increases from 174MPa to 260MPa within 95% confidence interval. At 90% confidence, with the larger ellipse, it is possible to achieve yield strength of between 220MPa and 324MPa. The box-plots in each of the Figures 1 and 2 indicate mean values of strengths and density.

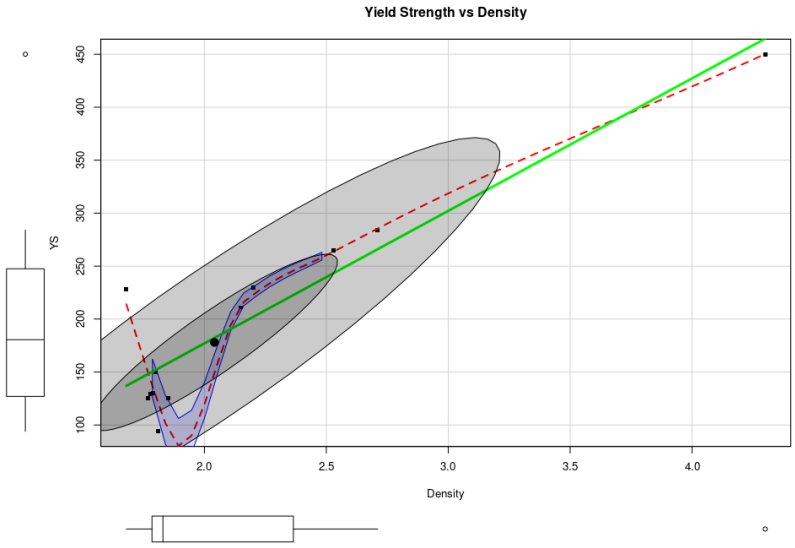

Figure 1. Variation of yield strength and density

Figure 2 illustrates that as density of the alloy varies from 1.75 to 2.5 g/cm^3, it is possible to have alloy of ultimate tensile strength with the range of 242MPa to 424MPa within the 95% confidence interval and 305MPa to 530MPa within 90% confidence interval.

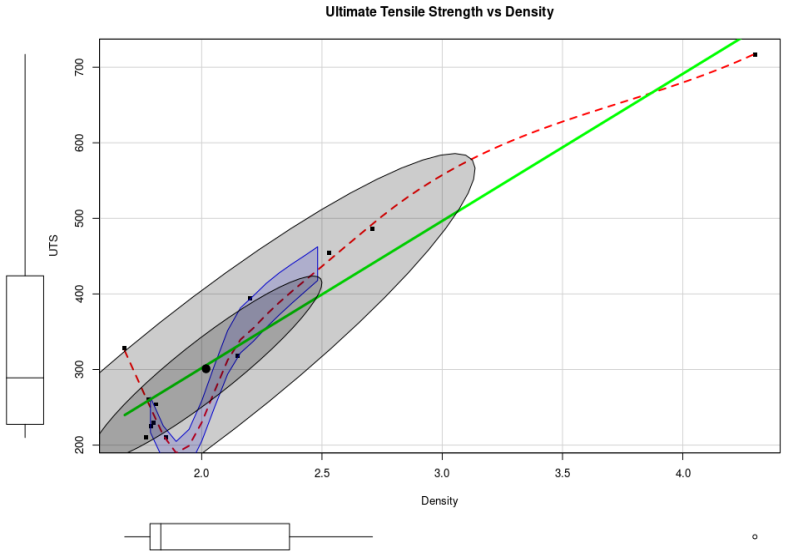

Figure 2. Variation of ultimate tensile strength and density

Figure 3 illustrates that as density of the alloy varies from 1.75 to 2.5 g/cm^3, it is possible to have alloy of Young's Modulus within the range of 55.55GPa to 72.45GPa within the 95% confidence interval and 66.72GPa to 95.09GPa within 90% confidence interval.

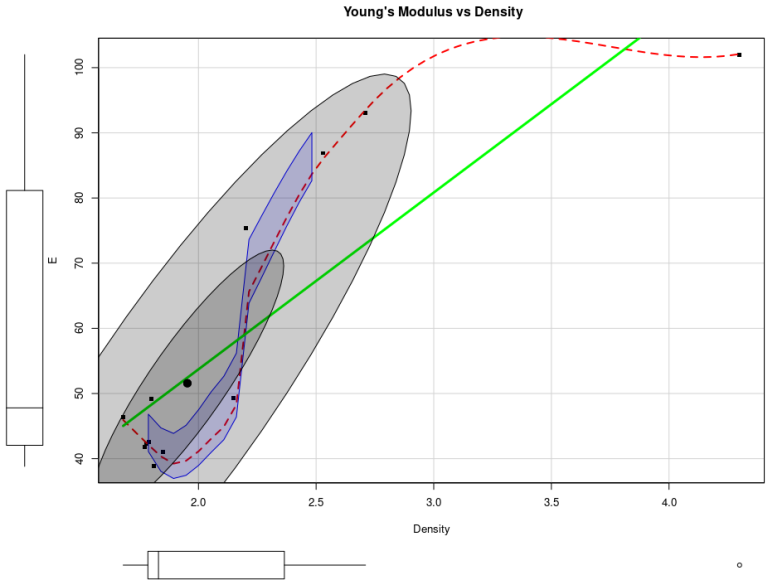

Figure 3. Graph of Variation of Young's Modulus with density

Results of optimization using constrained multi-objective optimization in Matlab R2022b show that the alloying elements have these percentage compositions by weight: 89.429% for magnesium, 8.159% for aluminium, 0.344% for copper, 0.255% for manganese and 1.814% for zinc. Optimal specific strength is 142.6045kPam3/kg for yield strength, 282.7679 kPam3/kg for ultimate tensile strength and specific modulus is 80.0959 MPam3/kg. Optimal density is obtained as1.8247 g/cm^3.

Results of multi-objective optimization are that optimal value of yield strength is 260.21MPa, optimal ultimate tensile strength is 515.96MPa and optimal value of Young's Modulus is 146.15GPa. Results of optimal yield strength are within the 95% confidence limit predicted in plots in Figure 1 and those of ultimate tensile strength are within the 90% confidence limit predicted in Figure 2.

Figure 4 illustrates heat treatment in MatCalc version 6.04. The simulation is performed from temperature of 400oC to room temperature followed by hot rolling and quenching back to room temperature. Mechanical properties depend on heat treatment. Quenching is important in preserving the suitable properties and fine grains to enhance strengthening [31].

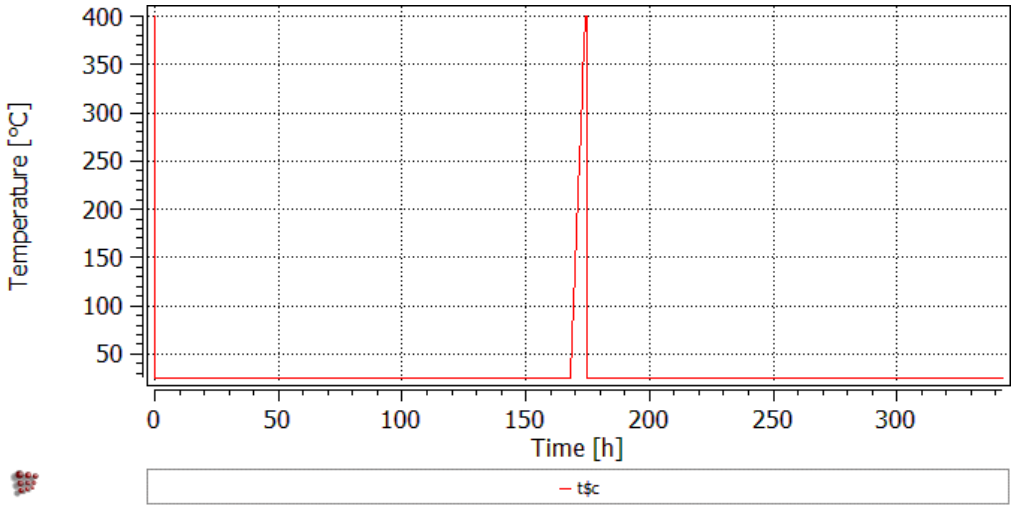

Figure 4. Heat treatment of the alloy

Figure 5 illustrates variation of number density with time in hours. Number density of CuMg1 and CuMg0 co-clusters are about 7.9916×10^{22}m^{-3} and 5.3213×10^{22}m^{-3}, respectively, during the process and zero during hot rolling since co-clusters disappear when temperatures rise to 400^{o}C. After hot rolling, a number of precipitates occur as temperatures reduce from 400^{o}C to room temperature. gamma $Al_{12}Mg_{17}$ with number density of 4.5861×10^{15}m^{-3}, AlCuZn_T precipitate with number density of 2.0448×10^{18}m^{-3} and AlCu_Eta precipitates has number density ranging from $6.84688 \times 10^{12}m^{-3}$ between 182 and 250 hours and 1.7623×10^{11}m^{-3} after 250 hours. MgAlCuZn_T precipitates maintain number density of 1.7623×10^{11}m^{-3} after hot rolling. The number densities of the precipitates decrease with thermal exposure during heat treatment then stabilizes as a result of isothermal aging processes at room temperature. This corroborates findings of [29]who studied coarsening behaviour in phases of Ni-Al binary model and found that number density and phase fraction of gamma phases decrease with the increase in thermal exposure.

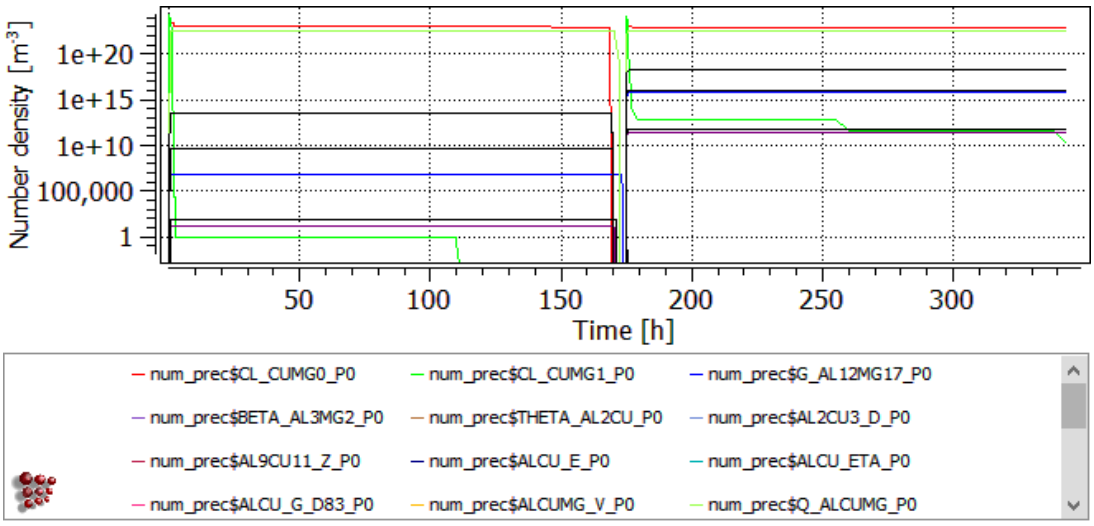

Figure 5. Variation of number density with time

Figure 6 illustrates variation of phase fractions with time. The highest phase fraction is illustrated by CuMg1 co-clusters at 0.007 before and after hot rolling. Stable phase fraction of CuMg0 co-clusters is 1.9358×10^{-4}. The co-clusters represent parent sites for precipitation. Presence co-clusters indicates strengthening effect that is the main strengthening mechanism in the alloy that contributes to high specific strengths and modulus. This finding confirms that there is direct relationship between strength and the amount of co-clusters formed [32].

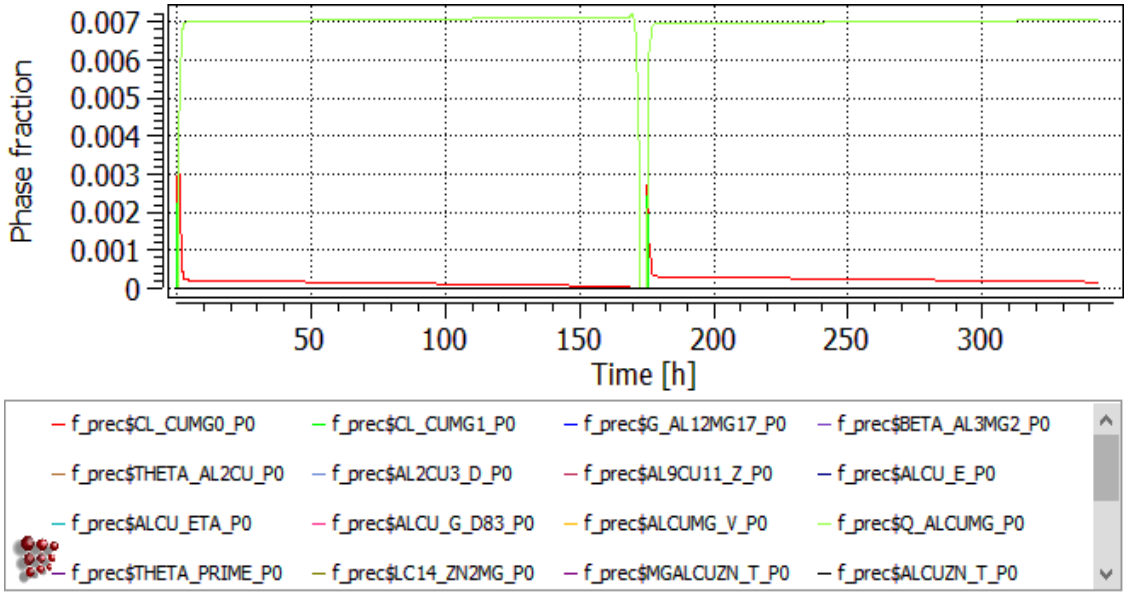

Figure 6. Variations of phase fractions with time

Mean radius of precipitates formed are shown in Figure 7. Mean radius of gamma Al12Mg17 precipitates is stable at 28.14nm before hot rolling and rises to 4µm during hot rolling then stabilizes at 27.628nm after hot rolling. Mean radius of AlCuZn_T precipitates at 20.959nm after hot rolling while that of CuMg1 co-clusters are stable at 3.26nm. All the other precipitates have mean radius of less than 3.26nm. From Figures 6 and 7, the graphs show that precipitate mean radius of phases decreases with increasing phase fractions and vice versa, which corroborates findings in literature [30].

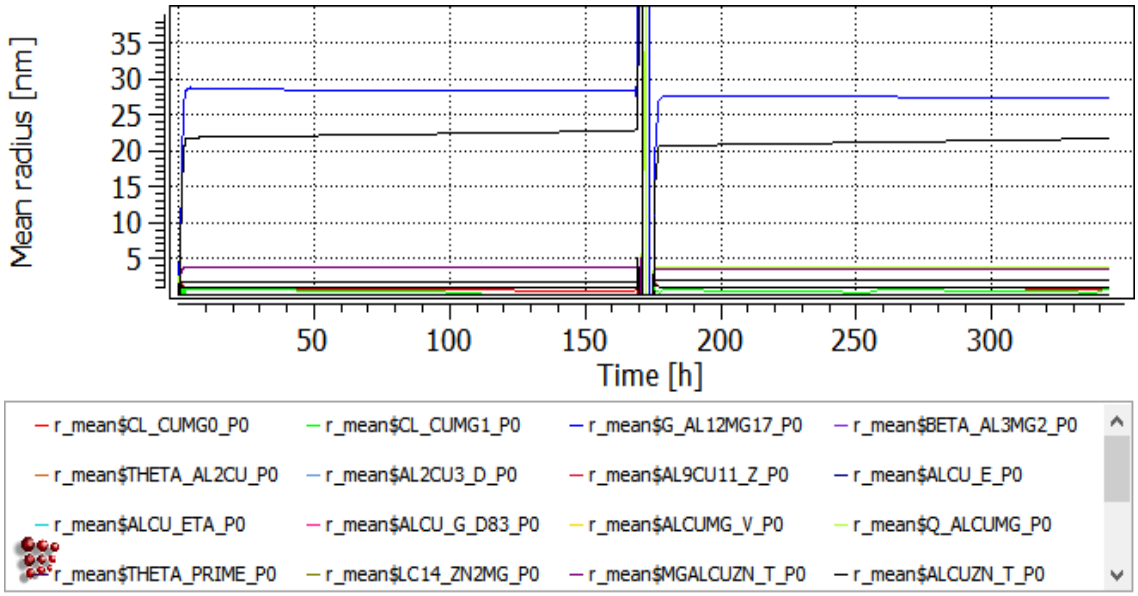

Figure 7. Variations of mean radius with time

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5. CONCLUSIONS

In this research, we applied constrained multi-objective optimization to design magnesium alloys with improved mechanical properties for aerospace and vehicle applications. We used a genetic algorithm to optimize the composition and microstructure of the alloys, subject to various constraints such as density, ductility, and corrosion resistance. We compared our optimized alloys with equiatomic magnesium alloys, which have been widely studied in the literature. We found that our optimized alloys have higher specific strengths and specific modulus than the equiatomic alloys, meaning that they can withstand higher loads and deformations per unit mass. This is beneficial for reducing the weight and fuel consumption of aerospace and vehicle components. Our results demonstrate that constrained multi-objective optimization is a powerful tool for designing magnesium alloys with superior performance.

The results show that the optimal value of yield strength was 260.21 MPa, the optimal ultimate tensile strength was 515.96 MPa and the optimal value of Young's modulus was 146.15 GPa with the following alloy composition by weight: 89.429% for magnesium, 8.159% for aluminium, 0.344% for copper, 0.255% for manganese and 1.814% for zinc. The optimal alloy composition had a low density of 1.79 g/cm^3 and a high specific strength of 288.22 MPa/g/cm^3. The microstructure simulation suggests that the optimal alloy has a fine-grained structure with uniform distribution of intermetallic phases. The optimal alloy composition can be used for lightweight and high-performance applications in aerospace and automotive industries.

The results of simulation show that non-isothermal treatments cause precipitation strengthening as a result of microstructural and strength evolutions through variation of mean radii and number density of precipitates. Aging at room temperature allows further precipitation. The highest phase fraction is of CuMg1 co-clusters at 0.007 followed by that of CuMg0 co-clusters at 0.00019358.The high specific strength and stiffness is believed to result from the fine and dense distribution of CuMg1 and CuMg0co-clusters that act as effective obstacles to dislocation motion.

Possible applications of the proposed high entropy alloy of magnesium in the automotive industry include light engine blocks, power transmission cases, vehicle steering wheels, instrumentation panels, seat frames and wheels. We suggest that the proposed alloy can be used in various structural and non-structural aerospace vehicle components such as brackets, housings, covers, frames, and connectors. It is believed that the alloy has good electrical conductivity and electromagnetic shielding characteristics, that are useful aerospace electronics. Further research and development are needed to produce the alloy and test the properties and compare with these results of simulation.

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