Revista de Metalurgia
January-March 2023, 59 (1), e233
ISSN-L: 0034-8570
https://doi.org/10.3989/revmetalm.233

Investigation of metallurgical properties of Al-Si-Mg casting alloys with integrated computational materials engineering for wheel production

Tuğçe Yağcı[a,*], Ümit Cöcen[b], Osman Çulha[a], Elvan Armakan[c]

[a] Manisa Celal Bayar University, Dept. of Metallurgical and Materials Engineering, Manisa, Turkey

[b] Dokuz Eylül University, Dept. of Metallurgical and Materials Engineering, İzmir, Turkey

[c] Cevher Alloy Wheels Company, İzmir, Turkey

(*Corresponding author: tugce.yagci@cbu.edu.tr)

Submitted: 6 May 2022; Accepted: 7 March 2023; Available On-line: 27 April 2023

ABSTRACT. In this study, integrated computational materials engineering, which is one of the new generation approaches in materials science, was used in the production of aluminum alloy wheels by low pressure die casting method. In casting alloys, the efficiency of grain refinement provided by master alloys added to the melt decreases with increasing silicon content of the alloy. In this context, as-cast properties of silicon reduced (Si: 5.0 wt.%) alloys with different Mg ratios (Mg: 3.0, 5.0, 7.0 wt.%) are discussed using integrated computational materials engineering approaches. It has been evaluated whether the examined alloys can be an alternative to the AlSi7Mg0.3 alloy, which is currently used traditionally in the production of aluminum-based wheels, with their microstructural and mechanical properties. The study consists of three stages which are computer-aided production, pilot production, testing and characterization studies. In computer-aided production, original sub-eutectic compositions were determined in types and amounts of alloying elements, alloy designs were realized and a database was created with a computational materials engineering software. Then, low pressure die casting analysis were performed in a virtual environment by transferring these data directly to the casting simulation software. Thus, the microstructural and mechanical properties of the wheel were obtained computationally on the basis of the varying alloy composition. In the second stage, the virtually designed alloy compositions were prepared and sample wheels were manufactured by the low pressure die casting method on an industrial scale. In the testing and characterization phase, spectral analyses, macro and microstructural examinations, hardness measurements and tensile tests were carried out. As a result of this study, it was determined that the studied alloys could be used in the production of wheels by the low pressure die casting method considering the metallurgical properties expected from the wheel. In addition, it is thought that the mathematical design of the material with integrated computational materials engineering approaches before casting simulations will play an active role in the competitiveness and sustainability of the aluminum industry in technological conditions.

KEYWORDS: Aluminum alloys; Integrated computational materials engineering; Low pressure die casting; Mechanical properties; Simulation

Citation/Citar como: Yağcı, T.; Cöcen, Ü.; Çulha, O.; Armakan, E. (2023). "Investigation of metallurgical properties of Al-Si-Mg casting alloys with integrated computational materials engineering for wheel production". *Rev. Metal.* 59(1): e233. https://doi.org/10.3989/revmetalm.233

RESUMEN: *Investigación de las propiedades metalúrgicas de las aleaciones coladas Al-Si-Mg para la producción de llantas utilizando ingeniería de materiales computacional integrada.* En este estudio, la ingeniería de materiales computacional integrada, que es uno de los nuevos enfoques en la ciencia de los materiales, se utilizó en la producción de llantas con aleaciones de aluminio por el método de fundición a baja presión. En la fundición de aleaciones, la eficiencia del refinamiento del grano proporcionado por las aleaciones maestras añadidas a la masa fundida disminuye con el aumento del contenido de silicio de la aleación. En este contexto, se discuten las propiedades de las aleaciones reducidas en silicio (Si: 5,0% en peso) con diferentes proporciones de Mg (Mg: 3,0, 5,0, 7,0% en peso) utilizando enfoques integrados de ingeniería computacional de materiales. Se ha evaluado si las aleaciones examinadas pueden ser una alternativa a la aleación AlSi7Mg0.3, que actualmente se utiliza tradicionalmente en la producción de llantas con base de aluminio, con sus propiedades microestructurales y mecánicas. El estudio consta de tres etapas que son la producción asistida por ordenador, la producción piloto, los ensayos y los estudios de caracterización. En la producción asistida por ordenador, se determinaron las composiciones subeutécticas originales en tipos y cantidades de elementos de aleación, se realizaron diseños de aleación y se creó una base de datos con un software de ingeniería de materiales computacional. A continuación, se realizaron análisis de fundición a baja presión en un entorno virtual transfiriendo estos datos directamente al software de simulación de fundición. De este modo, se obtuvieron computacionalmente las propiedades microestructurales y mecánicas de la rueda a partir de la composición variable de la aleación. En la segunda fase, se prepararon las composiciones de aleación diseñadas virtualmente y se fabricaron ruedas de muestra mediante el método de fundición a baja presión a escala industrial. En la fase de ensayo y caracterización, se llevaron a cabo análisis espectrales, exámenes macro y microestructurales, mediciones de dureza y ensayos de tracción. Como resultado de este estudio, se determinó que las aleaciones estudiadas podrían ser utilizadas en la producción de ruedas por el método de fundición a baja presión considerando las propiedades metalúrgicas esperadas de la rueda. Además, se cree que el diseño matemático del material con enfoques integrados de ingeniería computacional de materiales antes de las simulaciones de fundición desempeñará un papel activo en la competitividad y sostenibilidad de la industria del aluminio en condiciones tecnológicas.

PALABRAS CLAVE: Aleaciones de aluminio; Ingeniería de materiales computacional integrada; Fundición a baja presión; Propiedades mecánicas; Simulación.

ORCID ID: Tuğçe Yağcı (https://orcid.org/0000-0001-7478-9882); Ümit Cöcen (https://orcid.org/0000-0002-7776-2412); Osman Çulha (https://orcid.org/0000-0003-1611-8452); Elvan Armakan (https://orcid.org/0000-0001-6491-5451)

1. INTRODUCTION

Aluminum alloys are frequently preferred especially in the automotive industry, thanks to their recyclability, formability, high corrosion resistance and advanced mechanical properties. In this sector, silicon, magnesium, copper, iron, zinc, manganese, titanium, chromium and boron are the main alloying elements added to aluminum, although the type and amount of additives vary according to the desired metallurgical and mechanical properties (Stadler *et al.*, 2013; Fayomi *et al.*, 2017). On the other hand, aluminum parts (wheels, cylinder heads, travers, control arms, oil sumps, pistons etc.) are rapidly replacing steel components in vehicle weight reduction studies in order to meet the need for environmentally friendly processes and products as well as materials with more advanced properties (Mukund *et al.*, 2020; Eby *et al.*, 2022). The wheels are a safety element in a vehicle and are produced with aluminum alloys using the low pressure die casting (LPDC) method. In wheel production, silicon and magnesium (Si and Mg) are the basic elements added to the alloy. Si provides the fluidity of the alloy and improves the casting ability. Mg is added to improve its heat treatment properties and increase its strength (Kumar *et al.*, 2015; Şimşek and Özyürek, 2019).

In recent years, the use of computational materials engineering (CME) approaches, one of the new generation methods in alloy development studies, has been increasing in industrial and academic fields (Schäfer, 2006; Thornton *et al.*, 2009; Yağcı *et al.*, 2021). CME provides a great convenience for the simultaneous production, design and analysis of materials in a holistic and integrated system. In this way and thus playing an active role in the development of an alloy in the shortest time with the lowest cost. Thermodynamic and thermokinetic properties such as density, thermal and electrical conductivity, entropy, enthalpy, modulus of elasticity, free energy, viscosity, which vary depending on temperature and chemical composition of alloys, can be obtained with CME approaches based on the development of material models that quantitatively describe performance-structure-property relationships. In addition, yield-tensile strength, elongation, heat treatment properties, temperature-time-transformation (TTT) and continuous cooling-transformation (CCT) diagrams of alloys can also be obtained with these appraches (Ovrutsky *et al.*, 2004; Andersson *et al.*, 2002).

In integrated CME applications, the use of simulation softwares in aluminum casting processes minimizes time, labor, energy and cost elements in production. With casting simulations, solidification and filling analysis during casting, temperature gradient on the product and mold, material flow rates, macro and microporosity amounts and distributions, phase analysis, mechanical properties, etc. can be predicted before mass production. In other words, casting simulations play an important role in determining possible production problems in aluminum casting and taking precautions, determining the optimum process conditions, and revealing the effects of changes in process parameters on the product (Guofa *et al*., 2009; Jolly and Katgerman, 2022).

With the development of production technologies, CME and casting simulation softwares can be integrated with each other and data transfer can be provided between these two stations. In this way, it is possible to economically model the entire production chain from raw material to the final product. This new generation approach to product and manufacturing processes is called Integrated Computational Materials Engineering (ICME). ICME integration requires the execution of artificial intelligence, big data, multi-physics modeling and multi-scale modeling studies as a whole. This new approach is defined as an integration of material information, product performance analysis and production-process simulation. With ICME, the comparability of computational and real data in production processes has increased and the compatibility of simulation results with real data has been further increased (Allison *et al*., 2006; Wang *et al*., 2019; Thapliyal *et al*., 2020). This development also supports digitalization and digital twin, which have been popular all over the world in recent years.

In the literature, there are examples of industrial and academic research on aluminum alloys and the casting process, using CME and casting simulations. Guo and Sha (2005) focused on revealing the precipitation mechanism of Al_2Cu phase in Al-10Si-2Cu and Al-10Si-4Cu alloys. They used X-ray diffraction (XRD) method in their experimental studies and JMatPro, one of the CME software, in their computer-aided analysis. With JMatPro, the compositions of the phases formed in the alloys after different heat treatments were investigated. As a result of the XRD analysis, the precipitate fraction increased remarkably in the early stages of aging and then stabilized. In addition, the hardness of both alloys decreased somewhat, and it was thought that the decrease was caused by the coarsening of the precipitate that occurred when the precipitate fraction approached the equilibrium amount. After aging at 200 °C and 90 h, the amount of Al_2Cu formed in the alloys was determined to be 2.53% and 5.12 mol% for Al-10Si-2Cu and Al-10Si-4Cu alloys, respectively. Another study by Zou *et al*. (2022) is on the fluidity and hot tearing susceptibility of two different aluminum alloys, AlSi3.5Mg0.5Cu0.4 and A356 by using spiral and constrained-rod cast molds. Thermal analyzes and thermodynamic calculations of these alloys were carried out by using Thermo-Calc software. The fluidity of AlSi3.5Mg0.5Cu0.4 alloy is lower than A356 alloy due to its wide solidification range and high dendrite coherency point. In addition, a higher hot tearing susceptibility has been detected in AlSi3.5Mg0.5Cu0.4 alloy due to its wider sensitive hot tearing range. As a result of the calculations performed using Thermo-Calc software, the alloys with a sharper steepness during the solidification process have a high hot tearing susceptibility.

Patnaik *et al*. (2020) studied the development of the die design parameters for the crankcase part of a two-wheeler automobile to be produced by high pressure die casting from Al-Si-Cu alloy. In the simulation studies, variables such as the filling temperature and time, metal shrinks during solidification, air pressure and cooling system were evaluated with the Magmasoft software. The improved die model, which included extra cooling channels and central overflow, increased the efficiency in casting. With the new model, the filling time has been reduced by 8 ms and the air pressure in the mold cavity has improved. It was also stated that point cooling, which makes it possible to reach the minimum solidification time, provides better results compared to line cooling. Khan *et al*. (2020) studied the casting of the impeller with complex geometry without casting defects such as hot spots and porosity by using the Magmasoft simulation program. AlCu4TiMg alloy with high machinability was selected for the casting simulation of the impeller, which is exposed to high forces and rotates continuously, and the mechanism was modeled in Solidworks and transferred to Magmasoft. The total weight was ~10 kg, the casting time was 5 s, the initial temperature of the melt was 720 °C and the mold temperature was 20 °C. The casting mechanism was updated with simulations and the studies were repeated to minimize hot spots and porosity defects. The diameter of the riser has been increased and the porosity reduced to allow more metal during solidification. As a result of the study, casting was also carried out experimentally and it was observed that the results obtained were in harmony. The estimation and minimization of the defects has been ensured, high quality and performance impeller production with minimum defects has been realized. The number of published studies based on ICME approaches using a combination of CME and casting simulations for aluminum casting alloys is limited. In addition, alloy development studies in the aluminum casting industry continue with trial and error that greatly increases the research costs in alloy development, and computational materials engineering approaches are not utilized. Besides, the inadequacy of the modeling and simulation programs used in obtaining data from each other and the fact that this situation causes the current wheel production chain to fall behind the times in terms of competitiveness and sustainability in rapidly developing technological conditions are other factors that constitute the motivation of the study.

In this study, AlSi5 alloys with different Mg levels and AlSi7Mg0.3 alloy, which is currently used traditionally in wheel production, were modeled with JMatPro and ThermoCalc CME software, and the alloy data obtained were directly transferred to the Magmasoft casting simulation program. The usability of alloys in the production of wheels with ICME approaches is discussed in terms of the computationally and experimentally obtained microstructural and mechanical properties.

2. MATERIALS AND METHODS

In this study, modeling of alloys with CME, Magmasoft LPDC simulations, industrial scale sample wheel casting and test-characterization studies were carried out, respectively. Then, computational and actual production data were compared and the potential of AlSi5Mgx (x: 0.3, 0.5, 0.7) alloys as an alternative to AlSi7Mg0.3 alloy was evaluated based on ICME approaches. In CME activities, the databases for aluminum alloys of ThermoCalc (TCAL7) and JMatPro software were used and thermophysical and thermo-dynamic properties of the alloys were calculated. Then, the data files obtained with the CME of the studied alloys were directly transferred to the LPDC simulation module of the Magmasoft software. Virtual castings of the wheels, which are computer-aided modeled with the material data of the relevant alloys, were carried out under industrial production conditions with LPDC simulation. Then, the performance properties of the wheels were evaluated in accordance with the standards of the automotive industry, on the basis of metallurgy and material science, based on the structure-property-process-performance relationship. With Magmasoft simulations, phase analysis (α-Al, eutectic, Mg_2Si and AlFeSi compounds), the distribution and amounts of macro and micro porosities on the wheel, the dendrite arm spacing values in the wheel parts (spoke, hub and flange) and the change of mechanical properties (yield & tensile strength, elongation and hardness) were examined.

After the computer-aided production, industrial-scale wheel casting studies were carried out in Cevher Alloy Wheels Company located in İzmir Aegean Free Trade Zone. First of all, alloys were prepared by using AlSi7 and pure-Al ingots, master alloys and Mg tablets in a tilting type melting furnace with 750 kg Al capacity. The pure-Al ingot and appropriate amount of Mg tablets were added to AlSi7 melt to prepare AlSi5Mgx alloys. Also, AlTi5B1 and AlSr10 master alloys were added to the melt for grain refinement and modification of the microstructure. During the melting process, the composition was checked by optical spectrometry measurements on 5 samples of the liquid metal. After melting, the alloys were degassed for 15 min. This process is for removing dissolved hydrogen gas in the liquid metal and minimizing possible casting defects. After degassing, the melts were transferred to the LPDC unit with transfer crucibles and wheels castings were performed at 745 °C. The die made of H13 tool steel is also preheated to 470 °C before LPDC process. The die is subjected to pothole coating process with DYCOTE-30 before the casting process to control the heat transfer in the cast part, to have a better surface quality and to leave the mold without deformation. During the production, the same LPDC unit was used for each alloy and 30 sample wheels were cast in different compositions. Also, the cooling rate corresponds to ~2.08 $°C·s^{-1}$ when it is considered that the casting starts at 745 °C, ends at 25 °C and the cycle time is 5.45 min for the production of the one wheel. After casting, all of the wheels were subjected to X-Ray control. For the mechanical tests, at least 5 samples were obtained from the relevant parts of each wheel according to DIN EN ISO 6892-1 automotive standard. For tensile tests, the samples also were taken within the scope of DIN 50125 standard and the test was carried out with 50 N pre-load and 0.002 s^{-1} speed. Also, detailed macro and microscopic examinations were carried out in the spoke, hub and flange regions of the wheel samples based on ISO/IEC 17025 standard. In the metallographic sample preparation phase for microstructural examinations, after grinding with coarse to fine grained (240-2000 sands) abrasive paper, polishing was done with colloidal silica solution. NIKON SMZ1000 stereo microscope was used in macrostructural observations and NIKON LV100 optical microscope working with Clemex image analysis software was used in microstructural examinations.

3. RESULTS AND DISCUSSION

3.1. **Computational Materials Engineering (CME) Studies**

Computational, experimental and industrial scale studies were carried out for AlSi5Mg0.3, AlSi5Mg0.5, AlSi5Mg0.7 alloys as an alternative to AlSi7Mg0.3 alloy to be used in the wheel production by the low pressure die casting method. The detailed computational and experimental elemental compositions of the alloys are comparatively given in Table 1. As the main alloying elements that change in

Table 1. The subjected alloy compositions to CME and experimental studies (wt.%)

	Alloy	Si	Mg	Fe	Ti	B	Sr	Mn	Ni
CME alloy compositions	AlSi5Mg0.3	5	0.3	0.1	0.12	0.001	0.015	0.0025	0.005
	AlSi5Mg0.5	5	0.5	0.1	0.12	0.001	0.015	0.0025	0.005
	AlSi5Mg0.7	5	0.7	0.1	0.12	0.001	0.015	0.0025	0.005
	AlSi7Mg0.3	7	0.3	0.1	0.12	0.001	0.015	0.0025	0.005
Experimental alloy compositions	AlSi5Mg0.3	5.007	0.293	0.102	0.1084	0.0013	0.0121	0.0022	0.0053
	AlSi5Mg0.5	5.088	0.562	0.1096	0.1288	0.0025	0.0117	0.0023	0.0054
	AlSi5Mg0.7	5.100	0.731	0.1100	0.1168	0.0010	0.0122	0.0027	0.0054
	AlSi7Mg0.3	7.334	0.305	0.1008	0.1214	0.0004	0.0147	0.0026	0.0054

the alloy compositions, the ratios of Si and Mg, are the ones that directly affect the microstructural and mechanical properties in aluminum casting. The amounts of other alloying elements are the same as the content of the base AlSi7Mg0.3 alloy. As it can be seen from Table 1, there is overlapping between computational and experimental composition data. It shows that the compositions developed by CME studies can be obtained under industrial scale production conditions.

In the CME prediction studies performed with JMatPro and ThermoCalc software, solidification characteristics, mechanical (hardness, yield and tensile strengths) and thermophysical (density, liquid viscosity, thermal conductivity) properties related to temperature, which are critical data related to alloys, especially in the casting process, were studied. Figure 1a shows the variation of liquid viscosity from the casting temperature (700 °C) to temperatures (~550 °C) at which the liquid phase is consumed.

Accordingly, the studied alloys have similar viscosity values towards the temperatures where the liquid phase is depleted while AlSi5 alloys have relatively lower viscosity values at high temperatures. It is a fact that the fluidity generally increases as the composition of the alloy approaches the eutectic. On the subject, initial considerations were that changes in metal viscosity near the eutectic caused this (Flemings *et al*., 1976). However, it is now known that this increase is due only to the solidification characteristic. When the concept of fluidity is evaluated from many aspects, it should not be represented as viscosity. The viscosity of a liquid is physically related to the movements that occur in the liquid (Campbell, 2003). Therefore, it has a definite value at a specified temperature. The fluidity of the metal depends on two basic factors, the metal properties and the variables of the test performed. Metal-related factors include viscosity, surface tension, surface films, gas content, residues, inclusion, solidification and crys-

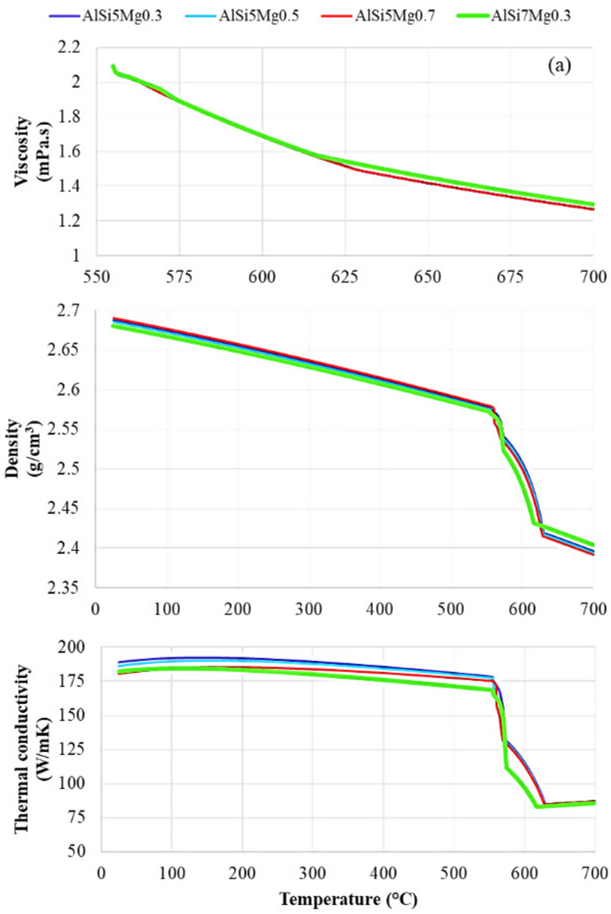

Figure 1. Temperature dependent graphs of (a) liquid viscosity, (b) density and (c) thermal conductivity values of alloys calculated by CME-JMatPro

tallization. There is a belief that liquid metals take quite different values in terms of viscosity and that poor and slow-flowing metal has high viscosity. In addition, it is an insignificant factor in castings as the fluid viscosity changes little with temperature (Atasoy, 1990). For this reason, as it is expected that the alloys used show close viscosity values, it can be said that the alloys will be an alternative to each other in terms of the casting process.

The graph in Fig. 1b shows the variation of the density of the alloys from the casting temperature (700 °C) to room temperature (25 °C). When metals melt, an increase in volume occurs. In this case, considering the density as the amount of mass per unit volume, it is possible to say that the density of the liquid is lower than that of the solid. In CME-JMatPro analysis, the density values of the alloys at 25 °C are 2.687, 2.685, 2.690, 2.680 g/cm^3 for the alloys AlSi5Mg0.3, AlSi5Mg0.5, AlSi5Mg0.7, AlSi7Mg0.3 respectively. In this case, it can be said that there is a small decrease in the density values due to the Si amount in the alloys. The reason why such a small amount of change occurs is because the density is a physical quantity and the predominant element in all alloys is Al, over 91%.

Another parameter that plays an effective role in the casting process is the thermal conductivity coefficient. Figure 1c shows the variation of thermal conductivity of alloys from the casting temperature (700 °C) to room temperature (25 °C). One of the most important factors affecting the service life of the product in Al alloys is the accumulation of thermal stresses in the product. For this reason, ensuring that the thermal gradient in the product is homogeneous during casting is extremely important for the efficiency of the process and product properties. When the studies investigating the effects of Al casting alloy composition on the thermal conductivity were examined, it was concluded that this was directly related to the microstructural properties of the alloy. Accordingly, while the thermal conductivity is lower in alloys with thinner dendritic network structure in aluminum casting alloys, the increase in the ratio of secondary phases in the structure decreases the conductivity. In alloys, a critical solidification rate must be determined in order to achieve the desired thermal conductivity value. According to Matthiessen's rule for thermal conductivity, increasing the concentration of elements in the solid solution increases the resistance of the overall alloy almost linearly (Yamashita and Hayakawa, 1976). In this context, Mülazimoğlu *et al.* (1989) in their study on the effect of silicon and magnesium amount on the thermal conductivity of the alloy in aluminum casting alloys, determined that the electrical and thermal conductivity decrease linearly with the increase of Si or Mg concentrations (Mulazimoglu *et al.*, 1989). When the microstructural properties of the alloys are examined, the lowest thermal conductivity is observed in the AlSi7Mg0.3 alloy, which has the thinnest aluminum dendrite network structure at the room temperature. As the amount of alloying element contained in the alloys decreases, the thermal conductivity values increase as expected. This trend shows parallelism at high and low temperatures.

Solidification analysis were obtained for AlSi5Mg0.3, AlSi5Mg0.5, AlSi5Mg0.7, AlSi7Mg0.3 alloys by defining all alloying elements to the Thermo-Calc system and by using the "one axis" command. The graphs showing the changes in the equilibrium phase fractions of the alloys with the temperature, obtained by cooling the alloy to the room temperature from the casting temperature are given in Fig. 2. When the temperature evolution of the different phases is examined, it can be said that the changes in the Si and Mg content of the alloys do not affect the eutectic transformation temperature values marked and it can be seen in Fig. 2. On the other hand, it is clearly seen that it significantly changes the solidification range, which is one of the parameters that are important in casting. The solidification range is the difference between the liquidus temperature at which the solidification process begins and the temperature at which solidification is completed. In alloys with a narrow solidification range, the tendency to form microsegregation in the cast structure is lower. Microsegregation is another consequence of the compositional differences occurring during the solidification of the alloys and is the change of concentration from the core outward in solidifying grains (Lumley, 2011). From the phase diagrams, the solidification process of the alloys is analyzed using to the solidus curve under equilibrium conditions. However, stable phase transformations do not occur since there are non-equilibrium cooling conditions during solidification in casting. Therefore, the problem of stratified solidification called microsegregation arises when the solidification range is large. For this reason, alloys with a narrow solidification range and close to eutectic composition are preferred in casting. The solidification ranges of the alloys were determined as 73.1, 58.4, 52.3, 66.0 °C, respectively. Accordingly, the lowest microsegregation tendency is seen in AlSi5Mg0.5 alloy.

3.2. Low Pressure Die Casting Simulation Studies

In materials, the microstructure and mechanical properties are closely linked. The possible phases in the microstructure affecting the mechanical properties of aluminum alloys were determined before casting with the Magmasoft software. The results of the phase distributions of α-Al, eutectic-Si, Mg_2Si and AlFeSi intermetallics in different regions of wheels, depending on alloy composition, are given in Fig. 3.

The numerical calculations of the colored data in Fig. 3 obtained from the Magmasoft casting simulation are given in Table 2 in detail. Accordingly, it

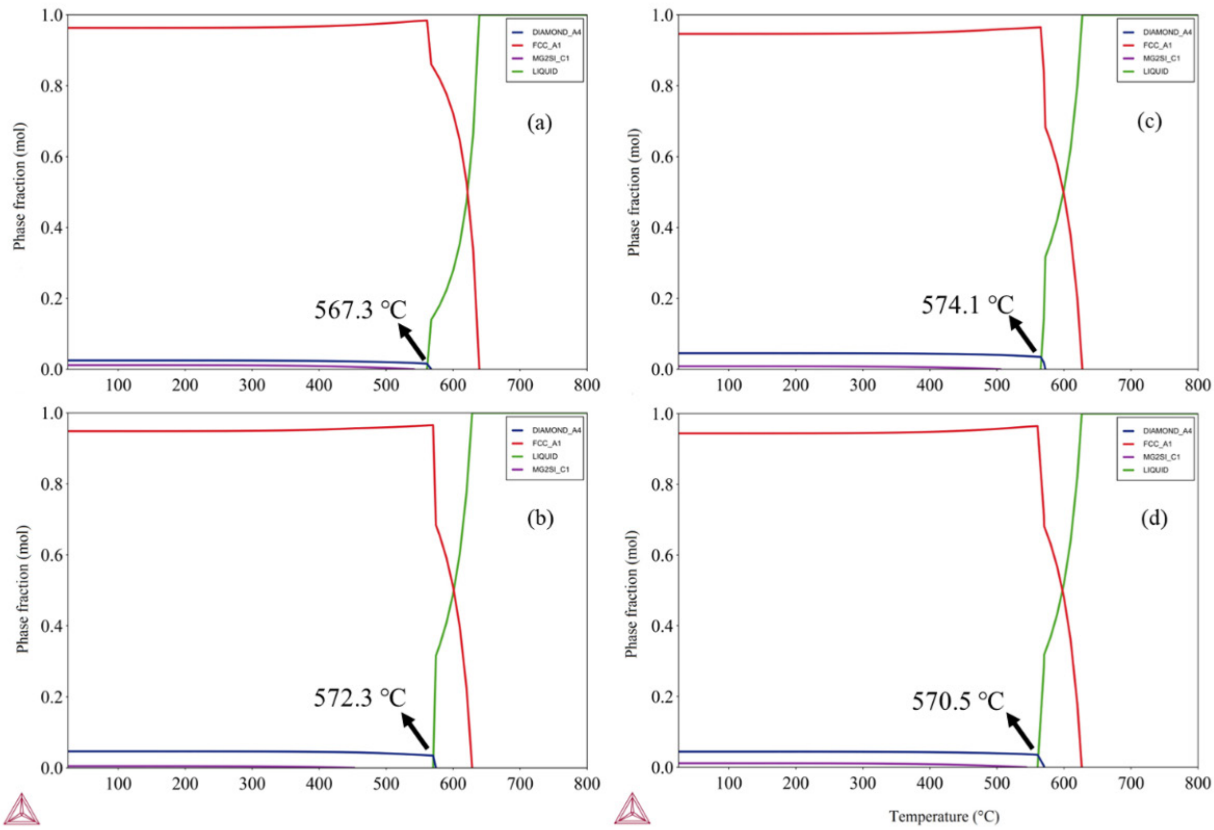

Figure 2. The graphs phase fractions changes of alloys with temperature under equilibrium conditions: (a) AlSi5Mg0.3, (b) AlSi5Mg0.5, (c) AlSi5Mg0.7, (d) AlSi7Mg0.3 obtained with CME-ThermoCalc. The marked points represent the eutectic transformation temperatures.

Table 2. Numerical results of Magmasoft phase analysis in wheel depending on composition (in %)

Phase	Wheels parts	Hub		Spoke		Flange	
	Alloys	min	max	min	max	min	max
α-Al	AlSi5Mg0.3	72.2	95.6	72.2	95.6	85.9	99.5
	AlSi5Mg0.5	72.2	95.6	72.2	95.6	87.8	99.5
	AlSi5Mg0.7	72.2	95.6	72.2	95.6	85.9	99.5
	AlSi7Mg0.3	55.9	68.3	55.9	68.3	55.9	68.3
Eutectic-Si	AlSi5Mg0.3	6.2	27.8	6.2	27.8	0.26	16.0
	AlSi5Mg0.5	6.1	27.8	6.1	27.8	0.21	16.0
	AlSi5Mg0.7	6.1	27.8	6.1	27.8	0.21	16.0
	AlSi7Mg0.3	37.9	44.1	10.0	44.1	28.6	44.1
Mg_2Si	AlSi5Mg0.3	0	0.18	0	0.29	0	0.02
	AlSi5Mg0.5	0	0.40	0.40	0.50	0	0.03
	AlSi5Mg0.7	0	0.39	0.60	0.78	0	0.05
	AlSi7Mg0.3	0	0.36	0	0.36	0	0.36
AlFeSi intermetallics	AlSi5Mg0.3	0	0.30	0.30	0.38	0.02	0.10
	AlSi5Mg0.5	0	0.30	0.30	0.80	0.02	0.10
	AlSi5Mg0.7	0	0.30	0.30	0.35	0.02	0.10
	AlSi7Mg0.3	0.34	0.45	0.10	0.45	0.41	0.45

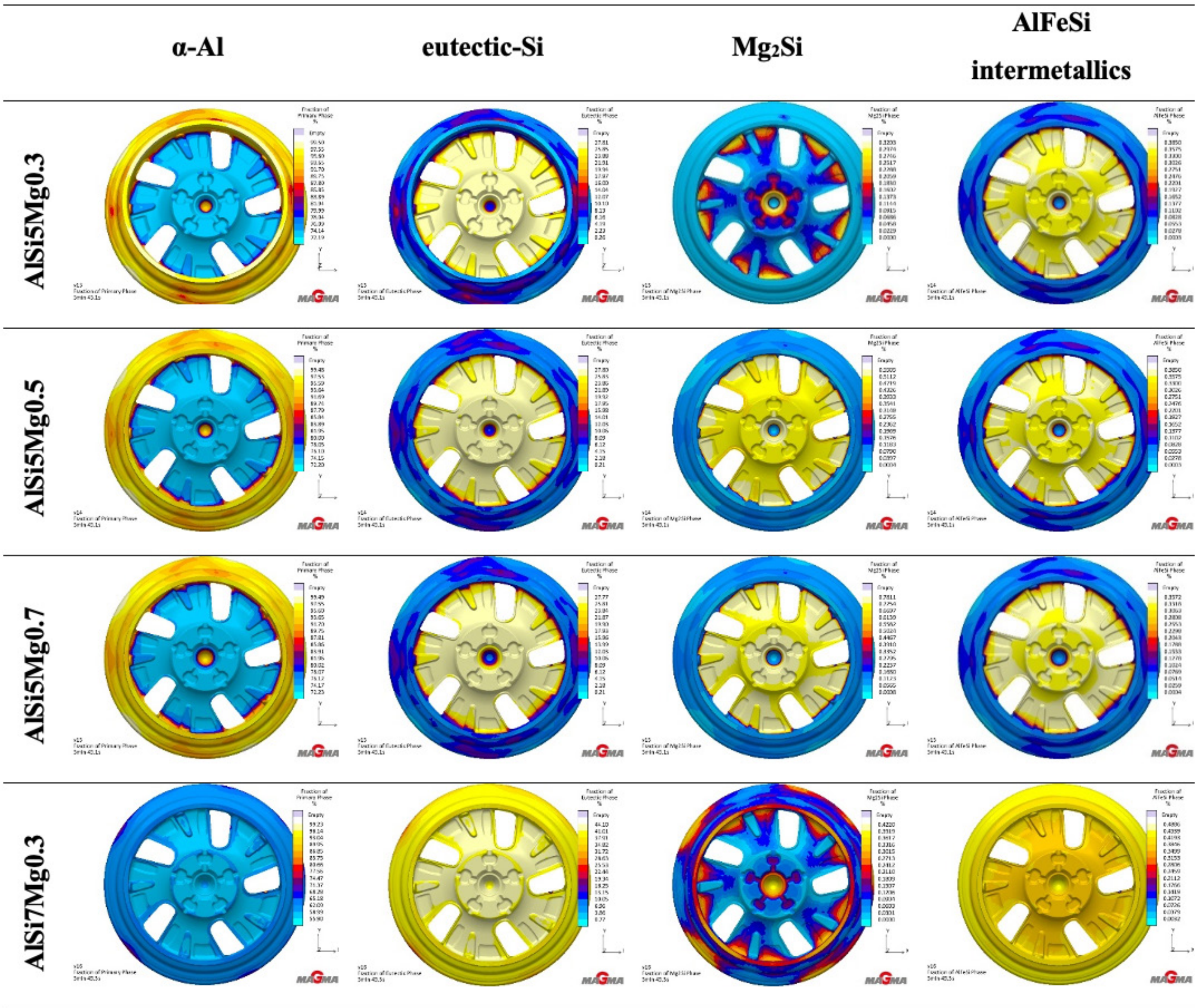

Figure 3. Phase distribution in wheels depending on alloy composition.

is possible to say that as the amount of Si increases, the amount of α-Al phase decreases in both the hub, spoke and flange regions of the alloys when the distribution of α-Al phase in the wheel is examined. This is an expected result as the eutectic composition is approached with increasing Si content and the solidification range is narrowed. On the other hand, the ratio of the eutectic phase increases with the increase of the Si content, inversely to the α-Al phase. Since the alloys are not heat-treated, it is an expected result that the Mg_2Si phase is close to zero in the hub, spoke or flange regions of the wheel. The amount of Mg_2Si phase is between 0 and 0.7%. Iron (Fe) is an undesirable element in Al alloys (Fortini *et al.*, 2016). The presence of iron compounds in the microstructure and their formation in needle-like morphologies adversely affect the mechanical properties (Narayanan *et al.*, 1994; Ji *et al.*, 2013). According to the casting simulation results, the amount of undesirable compounds formed by Fe with Al and Si in the microstructure is insignificant. In all regions of the wheel, the amount of AlFeSi intermetallic phases varies between 0 and 0.4%. These values are acceptable values to produce Al-Si based alloy wheels by the LPDC method.

The distributions and amounts of macro and micro porosities on the wheel were determined with the LPDC module of Magmasoft software. Also, the variation of the secondary dendrite arm spacing values along the wheel section, depending on the chemical composition, was analyzed as given in Fig. 4. In addition to the microstructural properties, the variation of the mechanical properties according to the regions of the wheel in alloys with different compositions was analyzed by the casting simulation. The visual and numerical results are given in Fig. 5 and Table 3, respectively. Depending on the directional solidification, the minimum and maximum

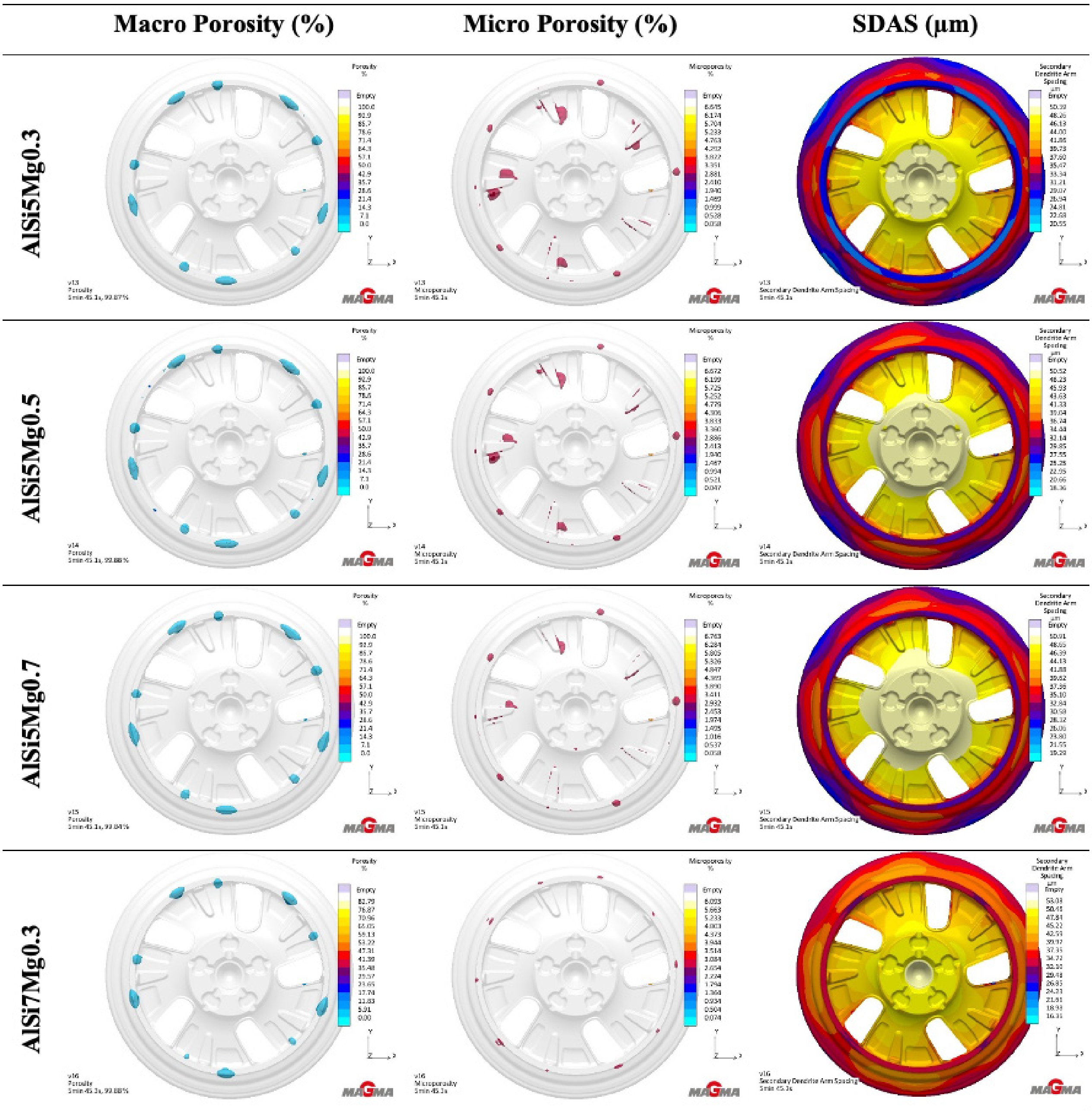

Figure 4. Magmasoft analysis results of the microstructural properties in wheels depending on chemical composition of the alloys.

values of the microstructural (macro, micro-porosity, SDAS values) and mechanical (tensile, yield strengths and elongation) properties are given in the hub, spoke and flange regions of the wheel. Accordingly, no macroporosity formation was observed in the hub and spoke region of the wheels in the alloys. On the other hand, the probability of macroporosity in the flange areas of the wheel is 0-7%. When the distribution of macroporosities in the flange region is examined (blue colored regions in Fig. 4), it is seen that it is similar to the AlSi7Mg0.3 alloy. The simulation results of the distribution and probabilities of the microporosities (regions marked in red) on the wheel are similar to the macroporosity results. In this case, there is no possibility of microporosity in the hub areas of the wheels in AlSi5 and AlSi7 alloys. For AlSi5Mg0.3, AlSi5Mg0.5, AlSi5Mg0.7 alloys, this probability is minimum 2.6% and maximum 3.1% in the spoke regions, On the other hand, there is no possibility of microporosity in the spoke of AlSi7Mg0.3 alloy according to the LPDC simulation results. For all alloys there is a possibility of

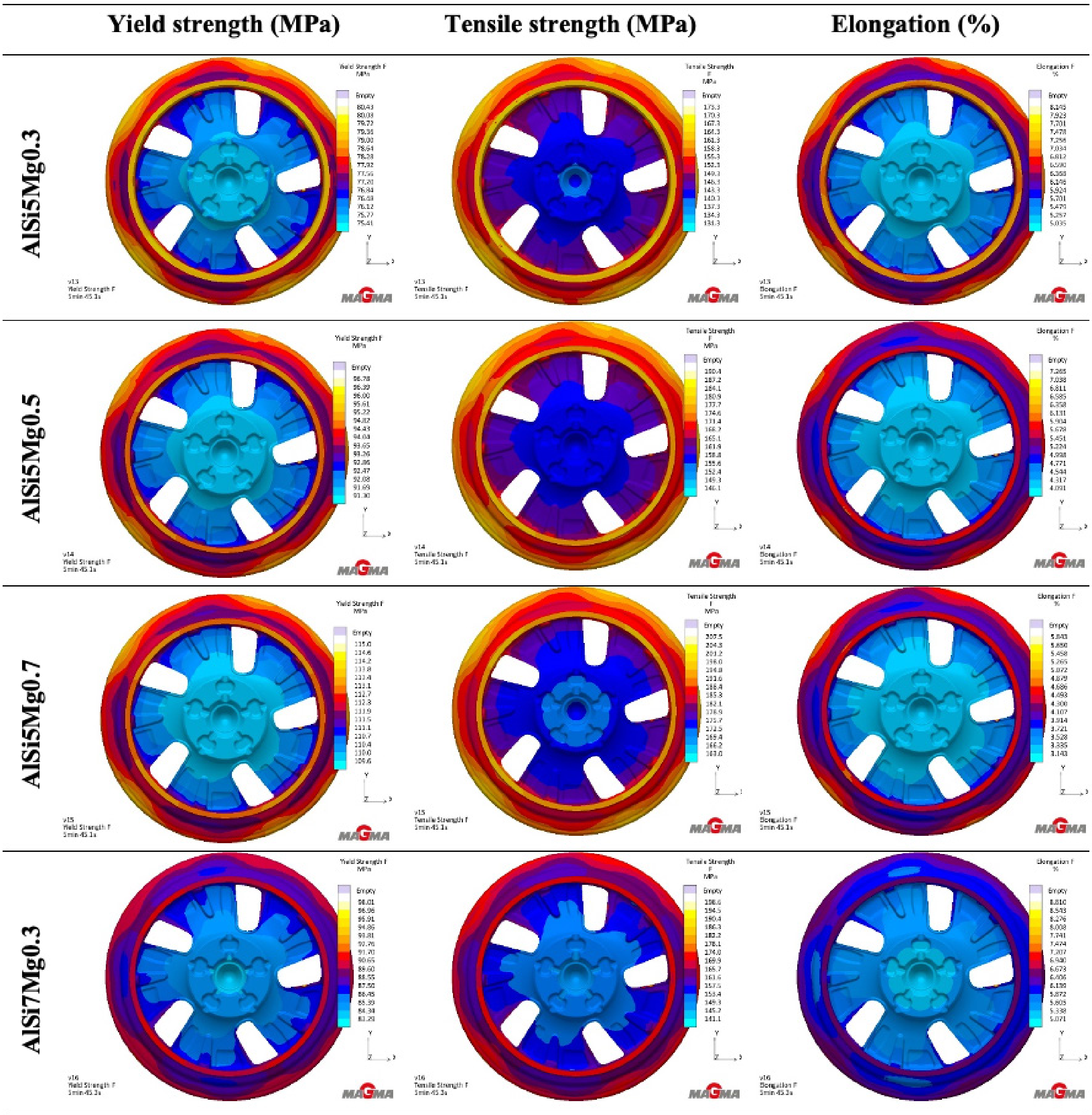

FIGURE 5. Magmasoft analysis results of the mechanical properties in wheels depending on chemical composition of the alloys.

microporosity in the flange regions, but it is very low and can be neglected.

Another factor affecting the microstructure and thus the properties in Al casting alloys is the secondary dendrite arm spacing (SDAS) values. As this value decreases, it is expected that the mechanical properties of the alloys will improve. When the analysis results given in Fig. 4 are examined, the SDAS value decreases from the hub to the flange for the alloys. The section thickness of the wheel decreases from the hub to the flange. Accordingly, the cooling rate increases and a microstructure with fine grains emerges in the flange region.

In the automotive industry, tensile tests are carried out in 3 different regions, namely the spoke, inner and outer flanges. According to the automotive standards, the minimum yield strength value required for a wheel that has not been heat treated in the spoke, inner and outer flange is 80 MPa. According to the Magmasoft analysis results (Table 3), it is clearly seen that this value is exceeded in all parts of the wheel, except for AlSi5Mg0.3 alloy. In Al-

Table 3. Numerical results of the microstructural and mechanical properties obtained from Magmasoft analysis

Property	Wheels parts	Hub		Spoke		Flange	
	Alloys	min	max	min	max	min	max
Macroporosity (%)	AlSi5Mg0.3	0	0	0	0	0	7.0
	AlSi5Mg0.5	0	0	0	0	0	7.0
	AlSi5Mg0.7	0	0	0	0	0	7.0
	AlSi7Mg0.3	0	0	0	0	0	7.0
Microporosity (%)	AlSi5Mg0.3	0	0	2.8	3.3	2.8	3.3
	AlSi5Mg0.5	0	0	2.8	3.3	2.8	3.3
	AlSi5Mg0.7	0	0	2.9	3.4	2.9	3.4
	AlSi7Mg0.3	0	0	0	0	2.6	3.1
SDAS (μm)	AlSi5Mg0.3	41.9	50.4	37.6	46.1	26.8	35.5
	AlSi5Mg0.5	41.3	50.5	36.7	48.2	25.2	36.7
	AlSi5Mg0.7	48.6	50.9	37.4	48.6	21.2	35.1
	AlSi7Mg0.3	45.2	53.1	37.3	54.2	36.8	37.3
Yield strength (MPa)	AlSi5Mg0.3	75.4	76.1	76.1	76.8	77.6	80.9
	AlSi5Mg0.5	91.3	91.7	91.7	92.9	93.6	95.2
	AlSi5Mg0.7	109.6	110.4	110.4	111.5	111.9	113.8
	AlSi7Mg0.3	83.3	85.4	85.4	87.5	88.5	90.6
Tensile strength (MPa)	AlSi5Mg0.3	131.3	143.3	143.3	149.3	152.3	167.3
	AlSi5Mg0.5	155.6	158.8	158.8	165.1	171.4	180.9
	AlSi5Mg0.7	166.2	172.5	172.5	182.1	185.3	198.0
	AlSi7Mg0.3	145.2	149.3	149.3	161.6	165.7	174.0
Elongation (%)	AlSi5Mg0.3	5.0	5.2	5.2	5.9	6.1	7.0
	AlSi5Mg0.5	4.0	4.3	4.3	4.7	4.9	5.9
	AlSi5Mg0.7	3.1	3.3	3.3	3.7	4.1	4.8
	AlSi7Mg0.3	5.0	5.3	5.3	5.8	6.1	6.6
Hardness (HB)	AlSi5Mg0.3	41.5		43.3		48.5	
	AlSi5Mg0.5	46.0		47.8		52.4	
	AlSi5Mg0.7	50.0		52.8		57.4	
	AlSi7Mg0.3	43.3		46.8		50.4	

Si5Mg0.3 alloy, this yield strength value is ~75 MPa in the hub, ~76 MPa in the spoke and ~78 MPa in the flange. The casting process is a difficult process to keep under control and it is possible to say that this alloy has achieved the standard value. The yield strength values after the heat treatment should also be considered since the heat treatment has not been applied yet.

When the alloys are evaluated according to the increasing Mg amount, the improving effect of the Mg element on the mechanical properties is clearly noticeable. For example, while the yield strength value obtained in the spoke of the AlSi5Mg0.3 alloy is ~76 MPa, this value is ~110 MPa in the same region for the AlSi5Mg0.7 alloy. Tensile strength values are similar to the tendency of yield strength ones. As it is seen in the virtual simulation results, the highest yield strength was recorded in the flange of the AlSi5Mg0.7 alloy. Another important mechanical property tested on wheels in the automotive industry is the elongation. From the computational elongation data, it can be said that increasing the Mg amount affects the elongation in alloys negatively. In addition, the elongation closest to the AlSi7Mg0.3 alloy was observed in the AlSi5Mg0.3 alloy in both hub, spoke and flange.

Since it is not possible to obtain color visual results related to the hardness analysis from the Magmasoft casting simulation, the hardness values in different parts of the wheel were calculated using the "UTS (MPa)=3.45xHB" relationship between the ultimate tensile strength (UTS) and Brinell

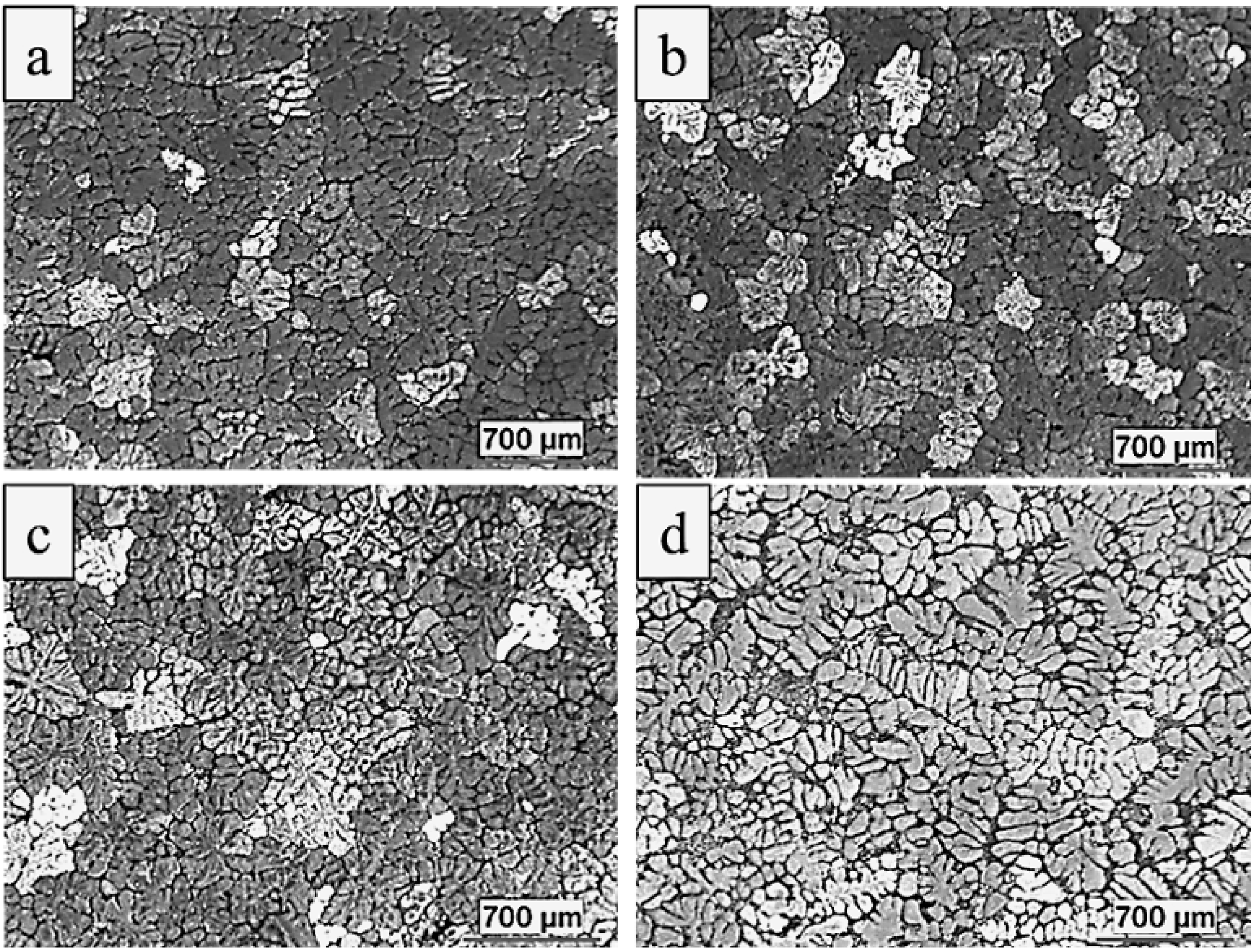

Figure 6. Stereo microscope images from the hub of the samples (30x), a) AlSi5Mg0.3, b) AlSi5Mg0.5, c) AlSi5Mg0.7, d) AlSi7Mg0.3.

hardness (HB). In the calculations, a single value was obtained instead of the minimum and maximum values, since the computationally reached maximum tensile strength value in the relevant region was used. When the hardness data obtained by the ICME studies were examined, an increase was observed in hardness values from AlSi5Mg0.3 alloy to AlSi5Mg0.7 alloy, depending on the increasing amount of Mg. For example, while the AlSi5Mg0.3 alloy obtained a hardness value of ~43 HB in the spoke, a hardness of ~53 HB was achieved in the same region in AlSi5Mg0.7 alloy.

3.3. Test and Characterization Studies

In this section, the material data obtained from ICME and the data obtained from laboratory-scale testing and characterization studies are given comparatively. For macrostructural examinations, images were taken from the hub of the sample with a stereo microscope for each alloy composition. Figure 6 shows stereo microscope images of the studied alloys. In Magmasoft casting analysis carried out before the industrial-scale studies, the probability of macro porosity was 0% in the hub and spoke, while this probability was predicted as 7% in the flange. It is possible to say that the results at the laboratory scale macrostructural studies are in parallel with Magmasoft analysis. Accordingly, while casting defects such as micro-level and acceptable amounts of porosity were observed in the samples of the alloys in macrostructure examinations, no macrostructural defects were found.

After the macrostructural evaluations, detailed microstructural studies were carried out with the image analysis systems in an optical microscope. Microstructure images, given in Fig. 7, were recorded from the hub, spoke and flange regions of each sample. In addition, phase analyzes were performed from the hub and the results are given in Fig. 8. From the optical microscope images, it is clear that the microstructure of the alloys consists of two main phases, α-Al and eutectic represented in light and dark gray, respectively. The eutectic phase is lo-

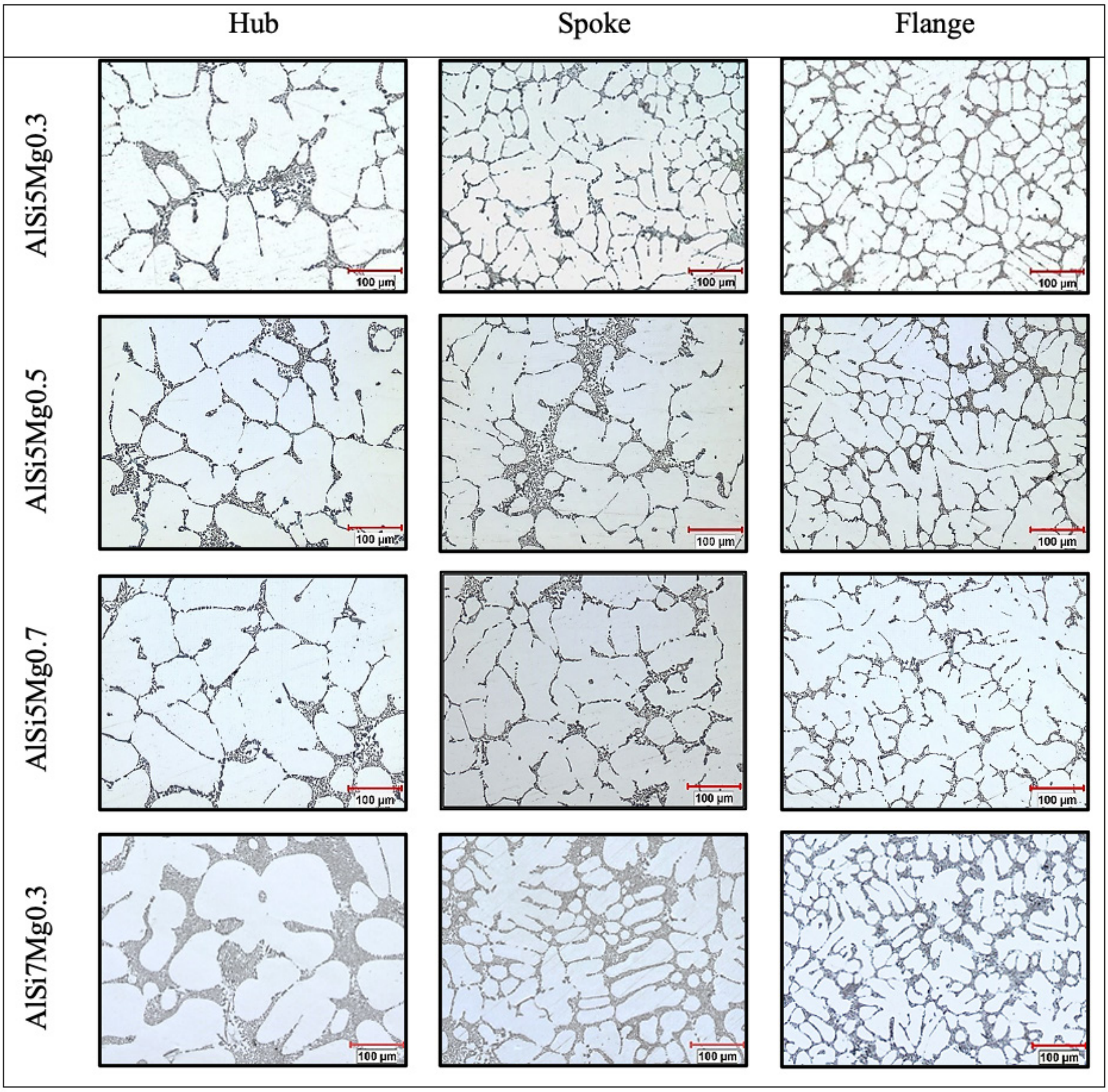

Figure 7. Optical microscope images from different parts of the wheel (200x).

cated between the primary α-Al dendrites. This is the microstructure of hypoeutectic (Si< 12.6 wt.%) Al-Si alloys. For the alloys, the microstructure is refined from the hub to the flange and the size of the main phase, α-Al dendrites, is reduced. In addition, as the Si amount of the alloys increases, the amount of the eutectic phase increases, while the amount of the α-Al phase decreases. Moreover, it is concluded that the grain refinement and modification processes applied respectively to the alloys before the casting process by using AlTi5B1 and AlSr10 master alloys are successful when the microstructures are examined. With the modification process, the morphology of the eutectic phase was transformed from a needle-like structure to a fibrous structure (Timpel *et al.*, 2012).

The phase analysis given in Fig. 8 are based on the representation of different phases with different colors in the optical microscope and the determination of the phase percentages in the relevant area. In the analysis, green color was chosen for the α-Al and dark blue color was selected for the eutectic phase and measurements were taken 5 times from the hub for each alloy. The data in Fig. 8 are the average values obtained from 5 measurements. Accordingly, α-Al phase was determined as 93.6%, 94.8%, 92.7% and 91.3% in AlSi5Mg0.3, AlSi5Mg0.5, AlSi5Mg0.7, AlSi7Mg0.3 alloys, respectively. The eutectic phase

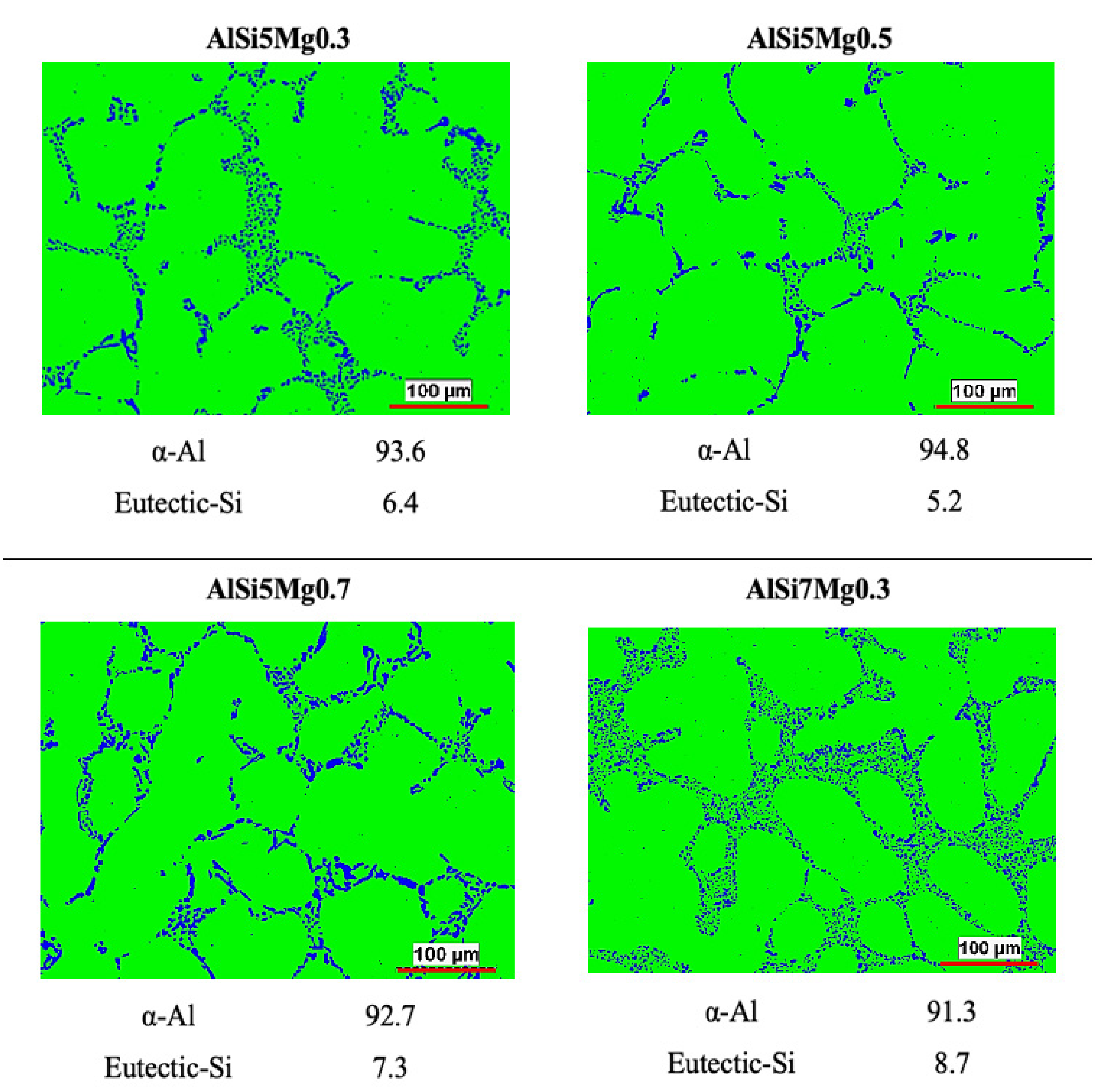

Figure 8. The results of phase analysis (in %).

content was recorded as 6.4%, 5.2%, 7.3%, 8.7% in AlSi5Mg0.3, AlSi5Mg0.5, AlSi5Mg0.7, AlSi7Mg0.3 alloys, respectively. The phase percentages do not differ according to the hub, spoke or flange on a wheel. It is only the percent of the phases that varies by region. In these analyzes, only the areal percentage of the phases represented by different colors in the relevant image area is calculated. For this reason, the samples were analyzed only from the hub. When the results obtained from the Magmasoft casting simulation and phase analysis using optical microscope image analysis techniques are compared with the experimental data, it is seen that the trends are similar. In both computational and industrial scale evaluations, the amount of eutectic phase increases and the amount of α-Al phase decreases from AlSi5Mg0.3 to AlSi7Mg0.3 alloy.

Another important result derived from the microstructure evaluations is related to Mg element. Since the alloys are still in as-cast condition, the Mg element is dissolved in the microstructure. When heat treatment is applied to the alloys, Mg and Si elements will react at the appropriate temperatures and conditions to form the Mg_2Si phase in the microstructure which contributes to the increase in strength. Therefore, Mg_2Si phase was not found in the microstructure, as seen in the computational and experimental results.

The yield strength values obtained from the tensile test and ICME studies results are given in Fig. 9. The tensile test was carried out on the spoke, outer and inner flange specimens in accordance with automotive industry standards. The minimum yield strength values required for the base alloy AlSi7Mg0.3 in the

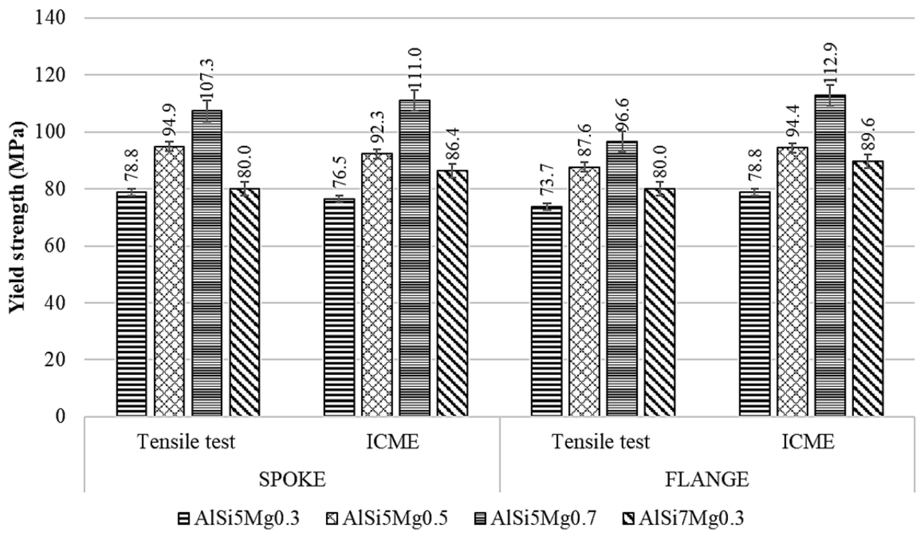

Figure 9. Comparative plot of yield strength values for the spoke and flange calculated with the ICME and obtained from the tensile test results.

spoke and flanges is 80 MPa. In the tests and analyzes, the yield strength of both the spoke and flange for AlSi5Mg0.3 alloy remained below 80 MPa. On the other hand, other alloy compositions showed a yield strength above the limit value of 80 MPa in both the spoke and flange regions, and exhibited a character that could be an alternative to AlSi7Mg0.3 alloy in terms of strength. Among the studied alloys, the highest yield strength was recorded in AlSi5Mg0.7. When the results are interpreted numerically, the yield strength value in the spoke is 94.9 MPa in the tensile tests for the AlSi5Mg0.5 alloy, while this value is 92.3 MPa in the virtual data obtained with the Magmasoft casting simulation. In the case of a traditional and dynamic method such as casting, a very low difference of 2.8% was recorded between the numerical and experimental yield strength values. Furthermore, there is no outer and inner flange distinction for these regions in terms of yield strength in a wheel. Since these regions are very close to each other in terms of cross-section, the values recorded separately for the outer and inner flange regions from the tensile tests were averaged and compared with the simulation values. Similarly, when the yield strength values of the flange region are examined, the yield strength value obtained as a result of the tensile test at the flange for AlSi5Mg0.7 alloy is ~100 MPa, while the virtual result is ~111 MPa. In this case, the difference between experimental and computational data is again extremely low.

Another important result of the tensile test is the elongation. The elongation values obtained for the

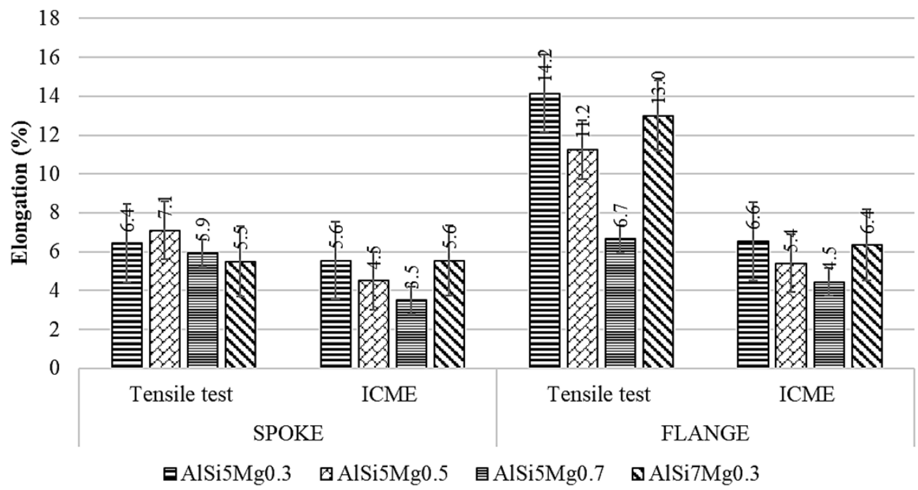

Figure 10. Comparative plot of elongation values for the spoke and flange calculated with the ICME and obtained from tensile test results

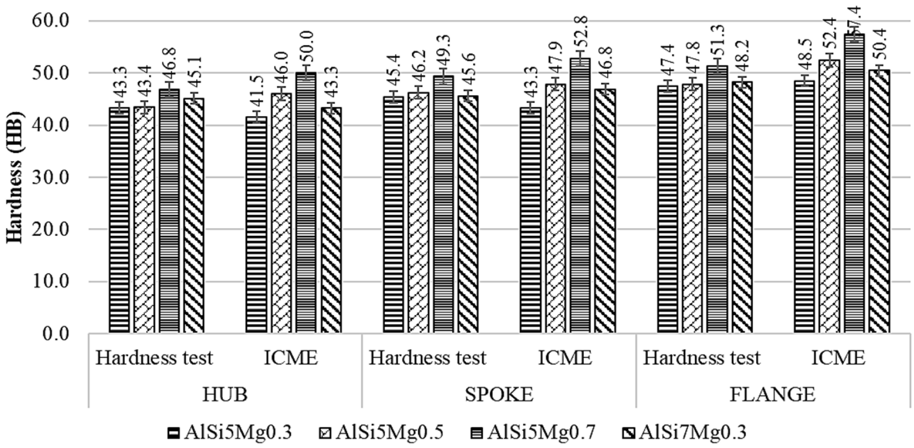

Figure 11. Comparative plot of hardness values for the hub, spoke and flange calculated with the ICME and obtained from the tensile test results

spoke, inner and outer flange regions of an unheated wheel produced from AlSi7Mg0.3 alloy in the automotive sector were determined as 5.5%, 14.0% and 12.0%, respectively. Figure 10 shows the elongation values of the related alloys. Since a large elongation was recorded in the different regions of the rim with the simulation studies, the average of these values recorded for the hub, spoke and flange regions was taken as the basis to compare with experimental data. According to this, the results above the required value of 5.5% were obtained in AlSi5Mg0.3, AlSi5Mg0.5, AlSi5Mg0.7 alloys, 6.4%, 7.1% and 5.9%, respectively, on the spoke. In AlSi5Mg0.3, AlSi5Mg0.5, AlSi5Mg0.7 alloys, results were obtained above the required value of 5.5%, 6.4%, 7.1% and 5.9%, respectively, on the spoke. On the other hand, higher values were recorded for the outer and inner flanges, with only 15.2% and 13.1% for the AlSi5Mg0.3 alloy, respectively, compared to the base alloy AlSi7Mg0.3 alloy. However, the desired elongation value could not be reached in the outer and inner flange regions of other alloy compositions.

When the tensile test results calculated with the ICME are examined, the values obtained in the simulated environment vary between 3% and 7%, regardless of the wheel region, while the actual data varies between 4% and 15%. In this case, it is not correct to compare virtual and real data in terms of elongation. The reason for this is that the Magmasoft casting simulation software, which can calculate the elongation, is not yet efficient enough for low pressure die casting process design.

After performing the tensile tests of the alloys, the results of the hardness measurements carried out to evaluate the mechanical properties are given in Fig. 11. As it was stated in the "Materials and Method" section, the hardness values of the visualized regional of the wheel cannot be reached with the Magmasoft casting simulation software. For this reason, the equation of ultimate tensile strength and Brinell hardness "UTS (MPa)=3.45xHB" in metallic materials was used. As it is seen in Fig. 11, the results of computational and physical comparison data with very low standard deviation value show the usability and efficiency of ICME approaches in terms of low pressure die casting process efficiency in aluminum alloys. For example, while the virtual calculations for the base alloy AlSi7Mg0.3 has a hardness of ~50 HB in the flange region, this value is ~49 HB at the same point according to the experimental hardness test results. To give another example, while the hardness value of 41.5 HB was reached in the hub of AlSi5Mg0.3 alloy with the computer aided calculations, a value of 43.3 HB was obtained from the experimental hardness measurements. The difference between the computational and experimental values is 4%, which is extremely low and negligible for the casting process. It is predicted that the alloys can be an alternative to AlSi7Mg0.3 alloy by utilizing ICME approaches in terms of hardness values obtained in all the regions of a wheel.

4. CONCLUSIONS

In this study, integrated computational materials engineering approaches, which have been developed in the recent past and which are gaining momentum in the development of innovative materials, process advancement and innovation studies in the field of metallurgy and materials science, are used in the production of aluminum-based wheels with low pressure die casting as a new application area. The findings are given below:

- Three different aluminum-based alloys, AlSi5Mg0.3, AlSi5Mg0.5, AlSi5Mg0.7, which are the subject of the study, meet the targeted properties for the wheel production.
- In the ICME examinations, there is no macro-size porosity in the hubs of the wheels pro-

duced with the developed alloy compositions. In this context, no macroporosity defects were found in the macrostructural evaluations as a result of the macrostructural evaluations of the hub regions. Similarly, in the microstructural evaluations, in parallel with the computational and industrial production results, there is a 3% probability of microporosity occurring only in the flange.

- When the three-dimensional phase distributions obtained in the wheel are examined in the alloys as a result of the ICME studies, they show that the amount of α-Al phase decreases gradually as the amount of Si increases. The amount of Mg_2Si phase varies between 0 and 0.5% in the samples. In addition, the amount of AlFeSi intermetallic phases in the alloys varies between 0 and 0.4%. These data are acceptable values for the production of Al-Si based alloy wheels by the LPDC. Optical microscopy examinations yielded similar trend results with the data obtained from computer-aided manufacturing studies. Also, Mg_2Si compounds were not found in the cast Al-Si alloys, as expected in the analysis.
- Considering the distribution of the mechanical properties obtained from the casting simulations of the different regions of the wheel, the strength above the 80 MPa yield strength value, which should be reached according to automotive standards, was obtained in all parts of the wheel of the alloys except for the AlSi5Mg0.3 alloy. Yield strength values increased due to the increased amount of Si and Mg in the alloys.
- The elongation value obtained from the tensile test results cannot be used with today's technology in the comparison of computational and experimental data, since the low pressure die casting simulation program works with a high deviation for this value. In the future, with the development of the capabilities of the casting simulation software and the computational theories, it will be possible to carry out the elongation analysis.
- It has been proven that the data for the mechanical and microstructural properties of the alloys obtained in the virtual environment with the ICME approaches can be compared with the real data obtained as a result of a series of tests and characterization of the samples taken from the wheels cast under industrial conditions, and the result can be used in alloy design and process optimization studies before mass production.

ACKNOWLEDGEMENTS

This study was supported by the Manisa Celal Bayar University Scientific Research Projects Coordination Unit. Project Number: 2018-182. Also, the authors would like to thank Cevher Alloy Wheels Company for their contribution to the realization of the casting activities of the alloys in this study on an industrial scale. In addition, we would like to thank ONATUS Company for supporting the realization of computational materials engineering studies with the use of ThermoCalc and JMatPro software.

REFERENCES

Allison, J., Backman, D., Christodoulou, L. (2006). Integrated computational materials engineering: A new paradigm for the global materials profession. *JOM* 58, 25-27. https://doi.org/10.1007/s11837-006-0223-5.

Andersson, J.O., Helander, T., Höglund, L., Shi, P., Sundman, B. (2002). Thermo-Calc & DICTRA, computational tools for materials science. *CALPHAD* 26 (2), 273–312. https://doi.org/10.1016/S0364-5916(02)00037-8.

Atasoy, Ö.A. (1990). *Eutectic Alloys: Solidification Mechanisms and Applications*. Istanbul Technical University, Istanbul.

Campbell, J. (2003). *Castings*. 2nd Edition, Londra: Butterworth-Heinemann.

Eby, F.J., Narayanan, S.A., Abhiram, R., Navaneeth, M.V., Manu, K., Shankar, K.V., Nidhin, A.R. (2022). Influence of solutionising time on the dendrite morphology and mechanical behaviour of Al-Si-Mg-Ni hypoeutectic alloy. *Silicon* 14 (12), 6749-6760. https://doi.org/10.1007/s12633-021-01401-z.

Fayomi. O.S.I., Popoola. A.P.I., Udoye. N.E. (2017). *Effect of alloying element on the integrity and functionality of aluminium-based alloy. In Aluminium Alloys - Recent Trends in Processing, Characterization, Mechanical Behavior and Applications.* 13, pp. 243-262. https://doi.org/10.5772/intechopen.71399.

Flemings, M.C., Riek, R.G., Young, K.P. (1976). Rheocasting. *Mater. Sci. Eng.* 25, 103-117. https://doi.org/10.1016/0025-5416(76)90057-4.

Fortini. A., Merlin. M., Fabbri. E., Pirletti. S., Garagnani. G.L. (2016). On the influence of Mn and Mg additions on tensile properties. microstructure and quality index of the A356 aluminum foundry alloy. *Procedia Struct. Integr.* 2, 2238-2245. https://doi.org/10.1016/j.prostr.2016.06.280.

Guo, Z., Sha, W. (2005). Quantification of precipitate fraction in Al–Si–Cu alloys. *Mater. Sci. Eng.* A. 392 (1-2). 449–452. https://doi.org/10.1016/j.msea.2004.09.020.

Guofa, M., Xiangyu, L., Kuangfei, W., Hengzhi, F. (2009). Numerical simulation of low pressure Die-Casting aluminum wheel. *China Foundry* 6 (1), 48-52.

Ji, S., Yang, W., Gao, F., Watson, D., Fan, Z. (2013). Effect of iron on the microstructure and mechanical property of Al–Mg–Si–Mn and Al–Mg–Si diecast alloys. *Mater. Sci. Eng.* A. 564, 130-139. https://doi.org/10.1016/J.MSEA.2012.11.095.

Jolly, M., Katgerman, L. (2022). Modelling of defects in aluminium cast products. *Prog. Mater. Sci.* 123, 100824. https://doi.org/10.1016/j.pmatsci.2021.100824.

Khan, M.A.A., Sheikh, A.K., Asad, M. (2020). Mold design and casting of an impeller using MAGMASoft. *Int. J. Mech. Eng. Robot. Res.* 9 (12), 1579-1583. https://doi.org/10.18178/ijmerr.9.12.1579-1583.

Kumar, V., Mehdi, H., Kumar, A. (2015). Effect of silicon content on the mechanical properties of aluminum alloy. *Int. J. Eng. Technol.* (IRJET) 2 (4), 1326-1330.

Lumley. R. (2011). *Fundamentals of aluminium metallurgy*. Wood Publishing Limited, Oxford.

Mukund, A., Nair, A.S., Nived, S., Raagavendran, R., Premkumar, A., Raj, A.N., Shankar, K.V. (2020). Impact of solutionising temperature on the microstructure, hardness and tensile strength of Al-6.6Si-0.3Mg-3Ni alloys. *Mater. Today: Proc.* 38 (5), 2117-2122. https://doi.org/10.1016/j.matpr.2020.04.725.

Mulazimoglu, M.H., Drew, R.A.L., Gruzleski, J.E. (1989). The electrical conductivity of cast Al−Si alloys in the range 2

to 12.6 wt pct silicon. *Metall. Mater. Trans. A* 20, 383–389. https://doi.org/10.1007/BF02653917.
Narayanan, L.A., Samuel, F.H., Gruzleski, J.E. (1994). Crystallization behavior of iron containing intermetallics compounds in 319 aluminum alloy. *Metall. Mater. Trans. A* 25, 1761-1773. https://doi.org/10.1007/BF02668540.
Ovrutsky, A.M. Prokhoda, A.S., Rasshchupkyna, M.S. (2014). *Computational Materials Science, Computer Modeling of Physical Phenomena and Processes*. Elsevier.
Patnaik, L., Saravanan, I., Kumar, S. (2020). Die casting parameters and simulations for crankcase of automobile using MAGMASoft. *Mater. Today: Proc.* 22 (3), 563-571. https://doi.org/10.1016/j.matpr.2019.08.208.
Schäfer, M. (2006). *Computational engineering-introduction to numerical methods*. Berlin, Springer-Verlag.
Stadler, F., Antrekowitsch. H., Fragner. W., Kaufmann. H., Pinatel. E.R., Uggowitzer. P.J. (2013). The effect of main alloying elements on the physical properties of Al–Si foundry alloys. *Mater. Sci. Eng. A* 560, 481-491. https://doi.org/10.1016/j.msea.2012.09.093.
Şimşek, İ., Özyürek, D. (2019). Investigation of the effects of Mg amount on microstructure and wear behavior of Al-Si-Mg alloys. *Eng. Sci. Technol. Int. J.* 22 (1), 370-375. https://doi.org/10.1016/j.jestch.2018.08.016.
Thapliyal, S., Komarasamy, M., Shukla, S., Zhou, L., Hyer, H., Park, S., Sohn, Y., Mishra, R.S. (2020). An integrated computational materials engineering-anchored closed-loop method for design of aluminum alloys for additive manufacturing. *Materialia* 9, 100574. https://doi.org/10.1016/j.mtla.2019.100574.
Thornton, K., Nola, S., Edwin Garcia, R., Asta, M., Olso, G.B. (2009). Computational materials science and engineering education: A survey of trends and needs. *JOM* 61, 12-17. https://doi.org/10.1007/s11837-009-0142-3.
Timpel, M., Wanderka, N., Schlesiger, R., Yamamoto, T., Lazarev, N., Isheim, D., Schmitz, G., Matsumura, S., Banhart, J. (2012). The role of strontium in modifying aluminium-silicon alloys. *Acta Mater.* 60 (9), 3920-3928. https://doi.org/10.1016/j.actamat.2012.03.031.
Wang, W.Y., Li, J., Liu, W., Liu, Z. (2019). Integrated computational materials engineering for advanced materials: A brief review. *Comput. Mater. Sci.* 158, 42-48. https://doi.org/10.1016/j.commatsci.2018.11.001.
Yağcı, T., Töcen, Ü., Çulha, O. (2021). Aluminum alloy development for wheel production by low pressure die casting with new generation computational materials engineering approaches. *Arch. Foundry Eng.* 21 (4), 35-46. https://doi.org/10.24425/afe.2021.138677.
Yamashita, J., Hayakawa, H. (1976). Deviations from Matthiessen's rule in electrical resistivity of nickel-based alloys. *Prog. Theor. Phys.* 56 (2), 361-374. https://doi.org/10.1143/PTP.56.361.
Zou, G., Chai, Y., Shen, Q., Cheng, T., Zhang, H. (2022). Analysis of the fluidity and hot tearing susceptibility of AlSi3.5Mg0.5Cu0.4 and A356 aluminum alloys. *Inter. Metalcast.* 16, 909–923, https://doi.org/10.1007/s40962-021-00649-w.