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Research Article

Prediction of AlSi7MgLi Phases with Calphad methodology

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Abstract:

The introduction of lithium (Li) in AlSi7Mg alloys has significant implications for their mechanical properties and phase composition. This study investigates the effect of lithium on the phases present in an AlSi7MgLi alloy with the chemical composition of 7% Silicon, 0.36% Magnesium, and 0.80 Lithium using Thermo-Calc software with calphad methodology. Thermo-Calc, a powerful computational tool for thermodynamic and phase equilibrium analysis, allows for precise simulation of microstructural evolution and phase transformations. This research provides a detailed thermodynamic assessment of the specified alloy composition, focusing on the stability and distribution of phases such as primary silicon, magnesium silicide, and lithium-containing phases. The objective is to understand how lithium affects the phase behaviour and properties of the alloy, guiding the development of optimized compositions for enhanced performance. The results from Thermo-Calc simulations will be compared with available empirical and theoretical data to validate the predictions. This study highlights the importance of computational tools in advancing materials science, enabling precise phase predictions and offering insights into the role of lithium in aluminium alloys.

1. Introduction

The addition of lithium (Li) to aluminium (Al) offers significant potential for reducing the weight of alloys, as each 1 wt. % of Li decreases the density by 3% while increasing the elastic modulus. This study examines the effects of a 0.80 wt. % Li addition to the AlSi7Mg alloy (which contains 7.05 wt. % Si and 0.35 wt. % Mg). The alloy exhibited a reduced density and enhanced hardness after natural aging [1,2]. Experimental results demonstrated that the addition of Li led to changes in both the microstructure and mechanical properties of the alloy. Specifically, the introduction of 0.80 wt. % Li resulted in the formation of a new phase, AlLiSi, which significantly increased the hardness of the AlSi7Mg alloy. Thermo calc predicted the presence of distinct phases—α-Al, β-Si, and AlLiSi—induced by the Li addition [3,4].

2. Material and Methods

A new aluminium cast alloy, AlSi7MgLi, was investigated through experimental methods. Thermodynamic calculations were conducted using ThermoCalc software, utilizing the chemical compositions provided in Table 1 to generate phase diagrams for the alloy[3,4]. The samples were melted in an induction furnace with a graphite crucible and cast into a steel mold, where a simple thermal analysis was performed. Following data acquisition, the numerical results, cooling curves, and their derivatives were plotted to identify

Table 1. *Chemical composition of alloy in wt. %*

Alloy	Al	Si	Fe	Cu	Mg	Zn	Ti	Li
AlSi7MgLi	Rest	7.05	0.10	0.05	0.36	0.02	0.09	0.80

characteristic temperatures. ThermoCalc predictions indicated the phases expected based on the alloy's chemical composition [1-5].

3. Results and Discussions

The thermodynamic calculations of the AlSi7MgLi alloy provide critical insights into its phase behavior and solidification characteristics. Figure 1 illustrates the phase diagram for compositions ranging from 0-1% and 0-0.2% lithium, highlighting the equilibrium stability of phases across temperature and composition. The observed phases include AlLiSi, α-Al, β-Si, β-$Al_9Fe_2Si_2$, π-$Al_{18}Fe_2Mg_7Si_{10}$, and Mg_2Si.

Figure 2 presents the phase fractions, showing the relative stability and prevalence of each phase during solidification.

Figure 3 features the Scheil diagram under non-equilibrium conditions, revealing the progressive formation of these phases during cooling. The dominant phases, α-Al and β-Si, form the matrix, while intermetallics like β-$Al_9Fe_2Si_2$, π-$Al_{18}Fe_2Mg_7Si_{10}$, and Mg_2Si contribute to microstructural complexity and mechanical properties.

AlLiSi emerges as a lithium-containing phase, indicating the role of lithium in altering phase equilibria and enhancing material performance. These results emphasize the interplay between alloying elements and thermodynamic stability, guiding alloy design and processing optimization.

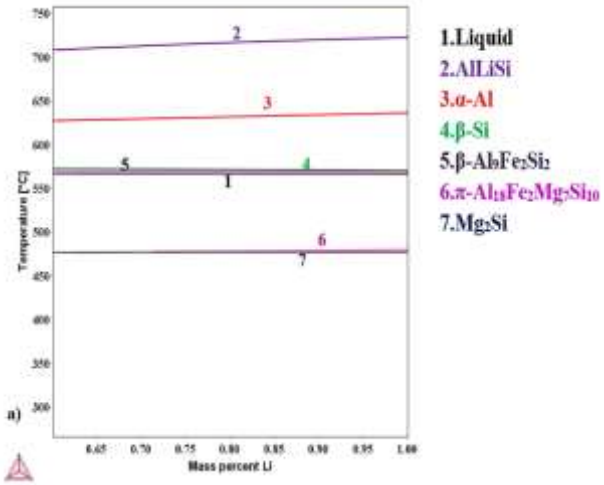

Figure 1. *Thermodynamic calculation of phase diagram (0-1% and 0-0,2%) of AlSi7MgLi alloy*

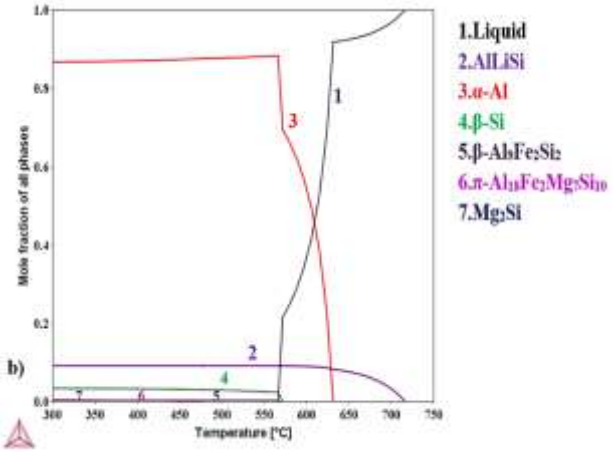

Figure 2. *Thermodynamic calculation of phase fraction*

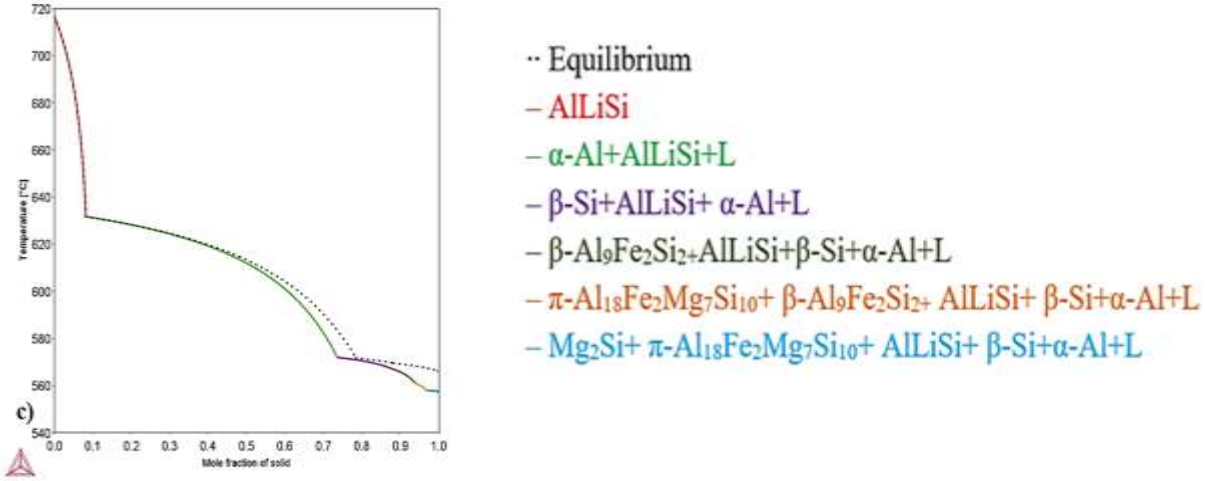

Figure 3. *Thermodynamic calculation of Scheil diagram equilibrium.*

4. Conclusions

New alloy with Li addition to AlSi7Mg alloy was studied. For this purpose, 0.80 wt. % Li was added to designed AlSi7MgLi alloy containing 0.36 wt. % Mg and 7.05 wt. % Si. It was found that Li combination with AlSi7Mg resulted on different solidification, development of new microstructure and creation of new phase AlLiSi. Li has influence to increase the mechanical properties in as cast state to AlSi7Mg. Thermo calc predicted and analysis revealed that the addition of Li promotes the formation of main phases: AlLiSi, α-Al, β-Si, β-$Al_9Fe_2Si_2$, π-$Al_{18}Fe_2Mg7Si10$ and Mg_2Si.

Author Statements:

- **Ethical approval:** The conducted research is not related to either human or animal use.
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