Computational Modelling for Phase Transformation Prediction in Cast Aluminum-Iron-Silicon Alloys

Modern IT technologies for Materials Science applications

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Abstract

The present work shows how it is possible to use computational modelling for the prediction of phase transformation processes in cast aluminum-iron-silicon alloys. Correlation between experimental and modelling data is also discussed. Modelling of alloys phases doesn`t give the actual structure components information, however it allows for prediction of phase transformations during structure formation process under cooling.

1 Introduction

Aluminum-silicon alloys are materials which are widely used in large amounts in industrial fields [1]. Aluminum-silicon alloys are casting alloys according to their manufacturing technology [2]. In the focus of the present work, these alloys are the subject of investigation because the design of advanced properties material may be only made by taking into account deep understanding of structural phase distribution and its influence on properties [3]. The present paper demonstrates how modelling may help in searching among compositions of experimental alloys which will be evaluated for further work by metallurgical methods. All modeled compositions contain iron. This addition is necessary to input for making the alloys better suited for die casting technologies [4]. These technologies allow for the production of large final product volumes daily at industrial facilities [5].

2 Experiment

The analyzed compositions are given in table 1. The selection of these compositions is based on the fact that iron improves complete filling of the mold when the alloy is produced by casting technologies [6]. That is why it is necessary to know what phases iron will form during the manufacturing process. The variation of silicon is also required for better understanding of crystallization intervals for every composition. The models have been implemented using the computer software “ThermoCalc 9.0” at Department of Materials Science in the Missouri University of Science and Technology, Missouri State, USA.

Table 1. Analyzed compositions

Alloy	Composition		
	Al (%)	***Si (%)***	***Fe (%)***
Alloy 1	92%	6%	2%
Alloy 2	94%	4%	2%
Alloy 3	96%	2%	2%
Alloy 4	93,5%	6%	0,5%
Alloy 5	95,5%	4%	0,5%
Alloy 6	97,5%	2%	0,5%

3 Results and Discussion

Distribution curves of phases in terms of variation in the concentration of silicon were obtained by composition modeling (fig. 1, 2). The regions of solid-solutions existence, secondary phases crystallization and liquid-solid equilibrium curves can be defined on the resulting phase diagrams. The modelled results correspond to the theory [2-3]. Iron additions influences the stability of iron-containing phases in "liquid + solid = solid" transformations as well as increasing the number of these transformations. The obtained temperature boundaries of each phase show how the concentration of silicon changes: it is reducing during cooling in all phases. Moderately narrow intervals of crystallization are observed in all alloys. In future papers it will be discussed how reducing of silicon concentration in every phase influences on final structure components distribution in experimental alloys which operate at room temperature. The major goal of the work is to find how the final properties of experimental alloys correlate with predicted properties as well as what is the use of modern modelling in understanding of real structure formation process.

Obviously, more silicon addition into the alloy results in differences in starting and finishing of crystallization, scale of temperature crystallization intervals and positions of the "liquid + solid = solid" transformations. Of course, the presence of these high temperature calculated phases in actual alloys was not proved by metallography; however, during crystallization at low cooling rates the liquid phase might have zones with abnormal chemical composition which was formed by a decrease in the content of alloying elements in the liquid phase situated among solid solution crystals. While crystals of solid solution or chemical phase grow, the content of alloying elements in the liquid phase decreases significantly. This leads to the formation of these zones with an unequal distribution of alloying elements in liquid phase.

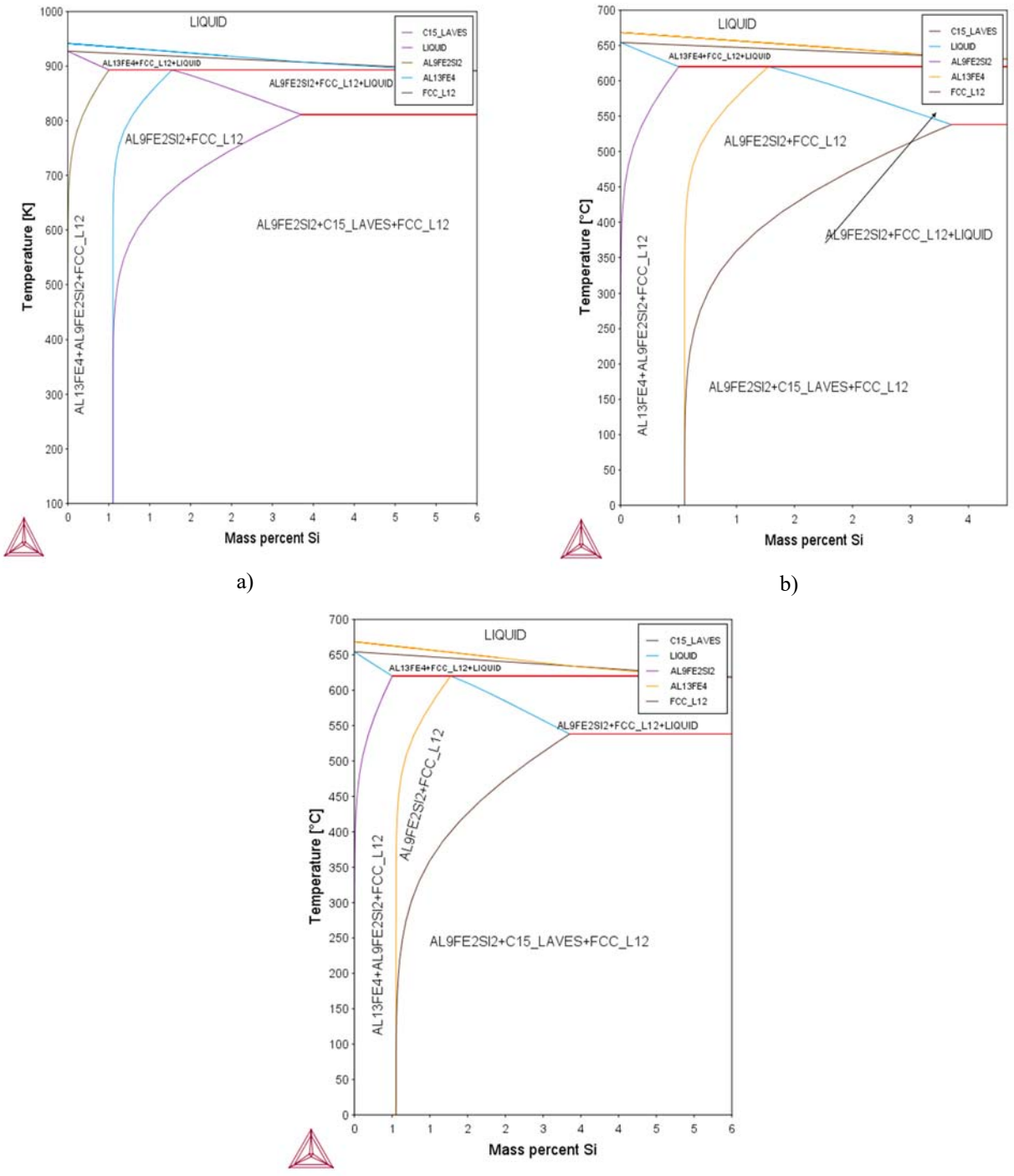
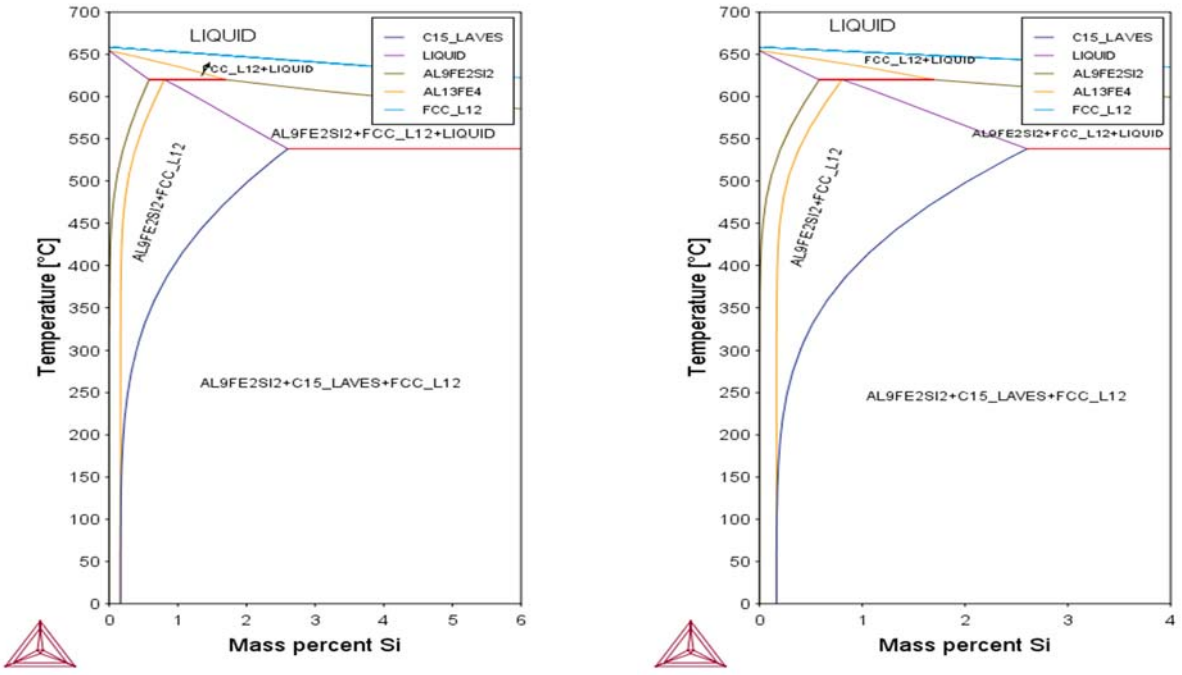
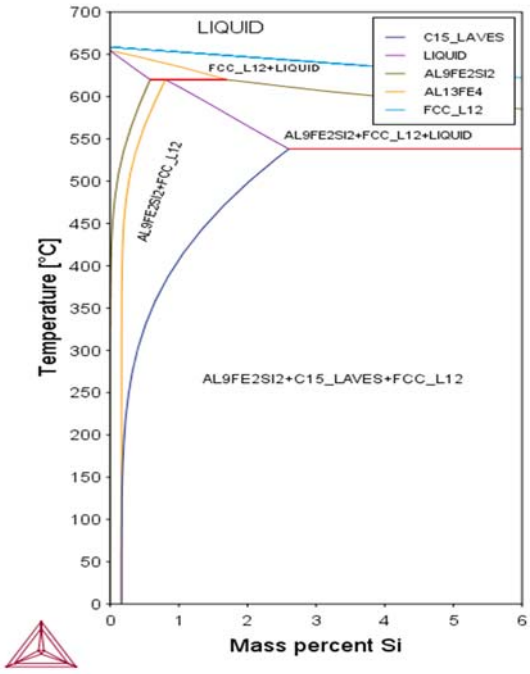


Figure 1 – Calculated phase diagrams for alloys: a) 92%Al-6%Si-2%Fe; b) 94%Al-4%Si-2%Fe;c) 96%Al-2%Si-2%Fe



a) b)



c)

Figure 2 – Calculated phase diagrams for a) 93,5%Al-6%Si-0,5%Fe; b) 95,5%Al-4%Si-0,5%Fea) 97,5%Al-2%Si-0,5%Fe

It is suggested that iron containing phases at high temperature are saturated by silicon. This results in diffusion of silicon from iron containing phases during further cooling down to 250 °C.

Thus, modeling allows getting reasonable representations of the phase composition information in the high temperature region and expected temperatures of phase transformation areas as well as values of changing of elements percentage in phases during crystallization at low cooling rates. On the basis of simulated diagrams, it becomes possible to choose alloy compositions and technologies for experimental alloys manufacturing which will be the next step of current work in searching of advanced thermally conductive cast aluminum alloys compositions.

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