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Computational Modelling for Phase Transformation Prediction in Super-Invar Alloys: Analytical and Experimental Data

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Abstract

The possibility of using computational modelling to predict phase transformation processes has been shown while examining super-invar samples. Due to the complicity of phase transformation processes in these alloys the correlation between modelling and experimental work has been described. Modelling allows basic background of composition behavior to be predicted but it doesn`t give the real structure components.

1 Introduction

Invar and super-invar alloys with cobalt are unique to design materials with low thermal expansion properties [1]. These alloys are divided into deformable and casting according to the manufacturing technology [2]. Various technologies enable mass diverse items to be obtained. Understanding the mechanism of structural units distribution is a key factor of final functional properties formation [3]. The present paper demonstrates how modern methods of modeling help to select the composition of experimental alloy. The modeled compositions are correlated with experimental compositions obtained by various research teams and our as well [4-6]. The application of modern computer analysis methods becomes essential due to cost-intensive production of experimental alloys with high composition of expensive alloying elements such as nickel and cobalt. The search of tailored composition for rational alloying can be carried out by modeling the composition and phase transformation as a result.

2 Experiment

2.1 Composition Modeling

The analyzed compositions are given in Table 1. The selection of these compositions is the consequence of practical applications of methods to compare the properties of alloys obtained by pressure metal treatment and foundry technologies (with carbon addition) [7]. The structure-formation of carbon alloys is of particular interest as there is no sufficient information to describe alloys provided in literature. The models have been implemented in computer software JMatPro at Materials Science Department, Missouri Science and Technology University, Missouri State, USA.

2.2 Experimental Compositions

All listed alloys were obtained from Ltd. First Foundry, Yekaterinburg, Ural region, Russia. Experimental alloys obtained were further analyzed applying metallography at Excellence center of Ural Federal University. The research was done in order to determine real composition of the experimental alloys.

Table 1: Analyzed compositions

Alloy	Composition			
	Fe (%)	Ni (%)	Co (%)	C (%)
Alloy 1	64	36	-	-
Alloy 2	64	32	4	-
Alloy 3	64	30	6	-
Alloy 4	63,4	32	4	0,6
Alloy 5	63,4	30	6	0,6

3 Results and Discussion

Distribution curves of corresponding phases in terms of variation in the concentration of components (nickel, cobalt, carbon) were obtained by composition modeling (Fig. 1, 2). The ranges of solid-solution and secondary phases can be defined on the resulting phase diagrams. It is obviously consistent with the theory [2-3]. Carbon-free alloys are excellent for calculations (Fig. 1 a, b, c and Fig. 2 a, b). Obtained temperature boundaries of phase genuinely correlate with literature data. In particular, it is true for liquidus and solidus curves. Moderately narrow interval of crystallization is observed in all alloys. It is confirmed by the results of experimental melting. Separation of structural components of carbon-free Fe-Co-Ni alloys applying metallography is complex. It seems possible to perform experiment by diffractometry including determination of metal lattice parameters. Although, this type of experiment was not conducted as it was not the purpose of research.

However there are significant differences between structural components modeled by JMatPro program and obtained by experimental melting. In particular, cementite can be found on phase diagrams of carbon-containing alloys (Fig. 1d, 2c). However, the formation of cementite in real alloys was not proved by metallography. It is suggested that cementite is formed due to cooling of alloy, but diffusion results in decomposition of this phase. The behavior of carbide phase largely determines final properties and applications of analyzed alloys. Taking into account the influence of such elements as nickel and cobalt, which form unstable carbides, it can be confirmed that the formation of iron carbide is also suppressed. In doing so, the classic theory of iron carbide formation is not denied. According to it, iron carbide is formed in certain temperature interval during crystallization of carbon-containing alloys based on iron. This carbide phase (cementite) was not fixed and determined by us.

The selection of compositions with cobalt content of 4% (alloys 2, 4) and 6% (alloys 3, 5) was not random. Highest thermal properties of experimental alloys (which were obtained by cast technologies) were observed in alloy with 4% cobalt composition. While alloy with 6% cobalt composition has a practical interest due to the expansion of invar interval. In superinvar alloys, the part of nickel atoms is actively substituted by cobalt. It is used for the improvement of thermal stability in wide range of temperature. We acted in a similar way, replacing the cobalt atoms for nickel atoms.

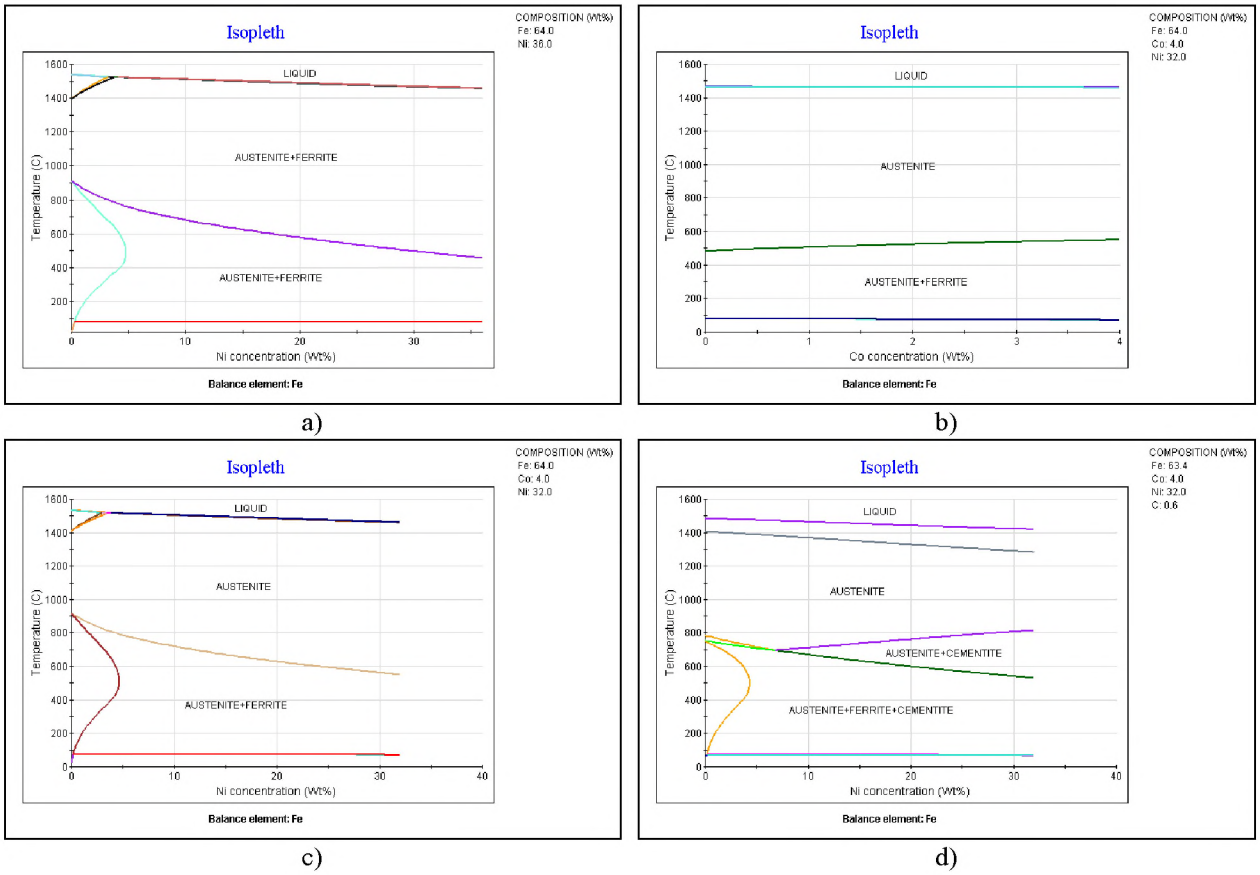

Figure 1: Calculated phase diagrams for a) classic invar alloy 64%Fe-32% (alloy 1) b) and c) 64%Fe-32%Ni-4%Co (alloy 2); d) 63,4%Fe-32%Ni-4%Co-0,6%C (alloy 4)

It is obvious that cobalt actively forms solid solutions based on austenite which maintains final functional properties of alloys (fig. 1b and 2a). But the appearance of cementite in the interval between 600 - 800 °C (Fig. 1d and 2c) and the existence of this phase in structure at room temperature generate questions. Phase diagrams do not indicate the phase of graphite. In our experimental alloys obtained by cast technologies (alloys 3, 5) graphite has always been one of the major structural components [6]. Unfortunately none of the diagrams has shown the presence of graphite at room temperature. On the other hand, cementite which had not been observed in experimental alloys obtained by cast technologies, was traced in all diagrams of carbon-containing alloys (alloys 3, 5) (Fig. 1 and 2). Real liquidus and solidus lines are found within the range of calculated lines. The data reported here have shown good agreement with results. Based on the presented results, the following model of structure formation has been proposed. Cementite is formed at high temperature; this phase decays into metal and graphite during the cooling of alloy. Products of decay are not shown on phase diagrams (Fig. 1 and 2). It has been proved above that graphite is formed in carbon-containing alloys during cooling [6]. Graphite exists in structure of alloys at room temperature. Calculated curves partly confirmed the hypothesis of existence and following decay of non-stable metal carbides in researched alloys. But full understanding of structure formation at room temperature is not achieved because of cementite presence and simultaneously absence of graphite on phase diagrams.

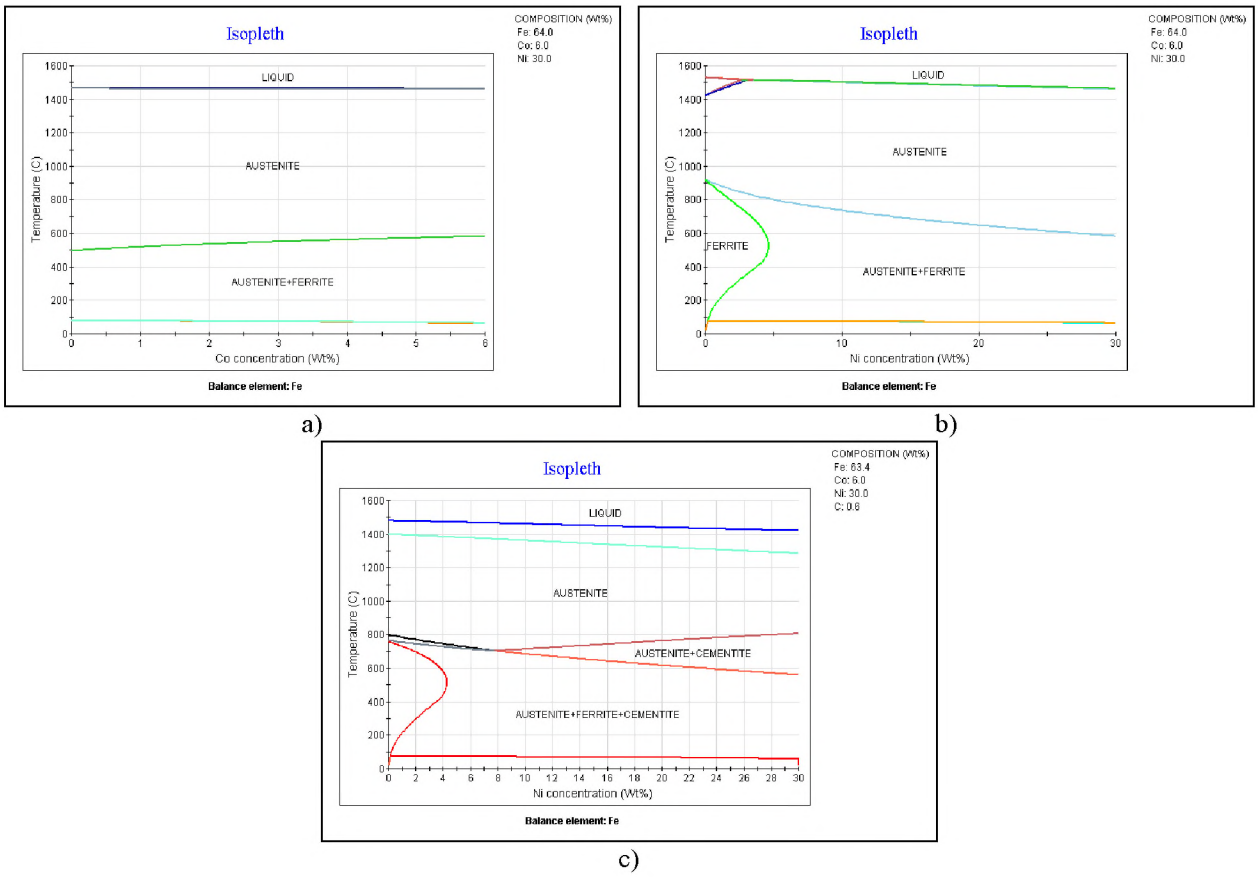

Figure 2: Calculated phase diagrams for a) and b) 64%Fe-30%Ni-6%Co (alloy 3); c) 63,4%Fe-30%Ni-6%Co-0,6%C (alloy 5)

Obtained model of phase equilibriums (Fig. 1 and 2) is useful for experimental alloys casting. It gives the understanding of beginning and ending of crystallization. In consequence it allows us to set right parameters for not only experimental but industrial castings.

Thus it is shown that modern methods of modeling make it possible to get reasonable representing of phase distribution of alloys components in high temperature field. On the base of simulated phase diagrams, correct parameters of industrial casting can be chosen. However incorrect data of secondary phase (for example cementite) are observed in calculated curves. In addition, phase of graphite common in carbon-containing alloys at room temperature is not indicated in phase diagrams. Formation of cementite is not proved by metallography. The motivation for further researches arises. The process responsible for disappearance of cementite phase is to be determined next.

Acknowledgment

Paper is dedicated to cherished memory of emeritus professor of UrFU S.V. Grachev.

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