Thermodynamic Analysis and Calculations of (Fe-Co) Alloy by Modeling and Simulation using Thermo-Calc Software

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Abstract
In this paper Thermodynamic calculation is shown. We have found simulation for phase diagram, Gibbs free energy and Activity curve at different temperatures (1200 K, 1225 K and 1250 K). Phase diagrams, Gibbs free-energy and the component activities of (Fe-Co) alloys system were calculated by Calphad method. Results show that the values of Gibbs energy were negative, which shows the stability of (Fe-Co). Negative deviation had occurred from Raoult’s Law in activities, which indicates that there is strong interaction between Fe and Co in (Fe-Co) alloy. By increasing the temperature the activity increases and deviation in activity decreases. For all the thermodynamic calculations the Thermo-Calc software, databases and Calphad method have used.

Keywords: CALPHAD, (Fe-Co) binary alloys; Thermo-Calc software; Phase diagram; Activity curve; Gibbs curve, Thermodynamic calculation.

Introduction
The study on Experimental measurement of thermodynamic properties and phase equilibrium for some systems is very difficult since these systems may be costly. For these systems using modeling and simulation is of great interest. This modeling and simulation reduces the time and to find equilibrium conditions for binary and multi-component systems. J.W. Gibbs established the relationship between thermodynamics and phase equilibria [1]. Iron-cobalt alloy has magnetic properties, with high Curie temperatures, the highest saturation magnetizations and high permeability etc. Elmen discovered these alloys in 1929 [2]. Also (Fe-Co) alloy has been studied by Ellis and Greiner [3], Normanton et al [4]. In 2002 by Ohnuma et al [5]. This alloy has applications in electric engine, which contain magnetic materials [6]. And it is now a good thermodynamic explanation of it. Thermo-Calc is powerful and flexible software to performing various kinds of thermodynamic and phase diagram calculations. This software can helpful to solve difficult problems interaction of many elements and phases that shows highly non ideal behavior [7]. The first version of thermo-calc was shown in 1981. In 2002 modern version of thermo-calc was present. The first description on thermo-calc was in 1985 [8].

Calphad method
Calphad stands for calculation of phase diagram. The Calphad method is used to find the thermodynamic properties of different materials system. The CALPHAD method was established as tool for phase equilibria of different multicomponent systems and for treating thermodynamics. For the calculations, the modules reported are used [9]. CALPHAD method has been employed for the material properties [10]. Recently the Calphad approach has been applied to a systems having more phase-based properties, as reported molar volume, elastic moduli and the database for processing these functions have been developed [11]. For materials the Calphad method can be used to describing the composition, temperature of optical activity, thermo-electric and acoustic properties [12]. All the calculations have been done by Calphad method.

Results and Discussion
A thermodynamic calculation in Fe-Co has been done using Thermo-Calc Software and Databases. The results of calculated activities in (Fe-Co) at 1200 K, 1225 K and 1250 K are presented in fig1. Gibbs energy for the investigated binary system is shown in figure2. In this paper the reaction, equilibria, phase diagram and figures modules were used.

In liquid (Fe-Co) alloy there negative deviation can occur in activities. The activities increase proportionally with increasing of the temperature and deviation decreases in activity according to the Raoult’s law [13].

Figure 1: Activity of Fe-Co alloy at different temperatures (a) 1200 K (b) 1225 K (c) 1250 K.

Figure 2: Gibbs energy Curve of Fe-Co alloy at different temperatures (a) 1200 K (b) 1225 K (c) 1250 K.
Raoult’s law in Fe-Co binary system, which is important for engineering technology and metallurgy. A phase diagram for the investigated binary system is calculated by the use of Thermo-Calc software and database. Obtained results presented one good base for the further thermodynamic analysis and developing in this group of innovative Fe base alloys. The obtained and shown results for the (Fe-Co) system provide complete thermodynamic optimization of this system.

References

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