



CALPHAD: Computer Coupling of Phase Diagrams and Thermochemistry

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Thermodynamic modeling of Ti-Fe-Cr ternary system

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ABSTRACT

Previous work of the Ti-Fe-Cr ternary system and its related binary systems are reviewed. Based on the thermodynamic descriptions of the Ti-Fe, Ti-Cr and Fe-Cr systems available in the literature, and also the ternary experimental data previously reported, the Ti-Fe-Cr ternary system is reassessed in this work by means of the Calphad method. Isothermal sections at 923 K, 1073 K and 1273 K and three invariant reactions as well as the vertical section $\text{TiCr}_2\text{-TiFe}_2$ are calculated. It is shown that the present calculated results are in good agreement with most of the experimental data.

1. Introduction

The phase diagram of the Ti-Fe-Cr ternary system is fundamental to developing novel alloys containing the elements. Some high hydrogen storage capacity alloys are based on the Ti-Fe-Cr system, it was demonstrated that Fe can partially substitute V and in this way the cyclic durability of alloys will be improved [1–3]. The Ti-Fe-Cr system plays a significant role in performance improvement of Al-based nanocrystalline alloys, and a series of nanocrystalline alloys containing Ti, Fe, Cr were designed and researched [4–8]. In addition, titanium alloy design basing on the Ti-Fe-Cr system was also a hot topic recently. It is shown that after cooling at 25 K s^{-1} , the tensile strength and reduction area of a Ti-4.9Cr-2.9Fe alloy can reach 1200 MPa and 45%, respectively [9]. The addition of element Fe in Ti-Cr alloys can promote the material's toughness and corrosion resistance [10,11]. Meanwhile, the cubic C15 crystal structure is stabilized and the stability of the β phase can also be increased with the increasing Fe concentration, which results in higher toughness values. In addition, the elements Cr and Fe are common β -stabilizer for titanium alloys compared with other much cheaper elements like V, Mo, and Nb [12,13]. If Fe and Cr can substitute the expensive elements (such as V, Mo, Nb, etc), there will be a reduction in the cost of titanium alloys. Actually, several low-cost titanium alloys like Ti-4.3Fe-7.1Cr and Ti-4.2Fe-6.9Cr have already been developed [14,15]. Therefore, it is essential to study the Ti-Fe-Cr system and its phase diagram.

The earliest report on Ti-Fe-Cr ternary system was the liquidus

surface estimated by Vogel in 1940 s [16]. While the experimental phase diagram of this ternary system was first investigated by Thyne in 1950 s [17]. Now several sets of experimental data of this ternary system are available and some assessments and reviews are reported. However, no complete thermodynamic description has been published yet.

In this study, the available thermodynamic data for three binary systems (Ti-Cr, Ti-Fe and Fe-Cr) [18–20] is reviewed. Also, the thermodynamic parameters of the Ti-Fe-Cr system are optimized and ternary interaction parameters of phases BCC_A2, BCC_B2, HCP_A3, liquid, sigma, Laves phases (C14, C15 and C36), FCC_A1 and $\text{Ti}_5\text{Cr}_7\text{Fe}_{17}$ (the only ternary phase) are presented. Finally, three isothermal sections from 823 K to 1273 K and the invariant reaction temperatures are calculated.

2. Literature review

2.1. Binary systems

2.1.1. The Ti-Fe system

Several thermodynamic descriptions of the Ti-Fe binary system are available currently [19,21–24]. Jonsson [22] treated the FeTi phase as a stoichiometric phase and did not consider the solubility of Fe and Ti components. Besides, the order-disorder transition of BCC_A2/B2 wasn't taken into consideration in Jonsson's work. Kumar et al. [23] introduced a 3-sublattice model to describe the BCC_B2 phase and

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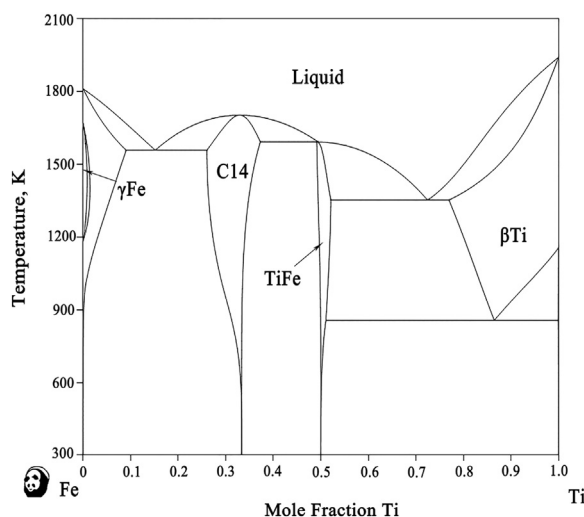


Fig. 1. The Ti-Fe phase diagram assessed by Hong et al. [19].

added the magnetic contribution to the Gibbs energy of the BCC_A2 phase. Yet, results showed that the calculated heat capacities of compounds Fe_2Ti and FeTi didn't match very well with the experimental ones. Keyzer et al. [24] modified the system based on Kumar's work and made two improvements, one was taking the 3-sublattice model to describe the C14 phase and the other was making the sign of the mixing enthalpy in the HCP_A3 phase the same with that of the FCC_A1 phase. Most recently, Bo et al. [19] re-optimized this system and the calculated phase diagram and thermochemical properties obtained by Bo et al. were almost identical to those obtained by Kumar et al. [23]. However, Bo et al.'s work paid special attention to the heat capacities of Fe_2Ti and FeTi and those experimental data were well reproduced. Thus Bo et al.'s work is accepted in the present work. Fig. 1 shows the phase diagram of Ti-Fe system.

2.1.2. The Ti-Cr system

Recently, the Ti-Cr binary system was assessed by Ghosh [18], Zhuang et al. [25], Pavlů et al. [26], Lee et al. [27] and Cupid et al. [28], respectively. Lee et al. [27] assessed the Ti-Cr system with the consideration of the $\gamma\text{-TiCr}_2$ and identified the three different types (C14, C15 and C36) of the TiCr_2 Laves phases. Ghosh's work [18] paid particular attention to the $\beta/(\beta+\alpha)$ and $\beta+\text{Cr}_2\text{Ti}$ boundaries and took the consideration of the activity of Cr at 1653 K in BCC_A2 phase. Pavlů et al. [26] calculated the ab initio data of three Laves phases and used it in the parameters' optimization of the Gibbs energies. Cupid et al. [28] re-assessed this binary system according to the latest thermodynamic data and besides, the calculated results were in very good agreement with the experimental data in the three Laves phases' homogeneity ranges. Since Ghosh's work was employed in our previous ternary system [29,33], the current work just adopted Ghosh's parameters to be extrapolated into ternary system. The phase diagram of Ti-Cr system is shown in Fig. 2.

2.1.3. The Fe-Cr system

The Fe-Cr binary system has been assessed by Andersson and Sunderman [20]. Later, Lee [30] revised the thermodynamic description for the purpose of getting a better agreement between the calculation and experimental data concerning the BCC_A2/liquid tie-lines and the liquidus temperatures in the Fe-rich region of three ternary systems Fe-Cr-C, Fe-Cr-Ni and Fe-Cr-Mn. Recently, the system was re-assessed by Xiong et al. [31]. In their work, a new description of pure Fe from Chen and Sunderman [32] was used and a new sublattice model $(\text{A,B})_{10}(\text{A,B})_{20}$ was chosen for sigma phase. To be compatible with our previous calculations [33], we decided to select the thermodynamic parameters from SGTE for pure Fe and the sublattice model

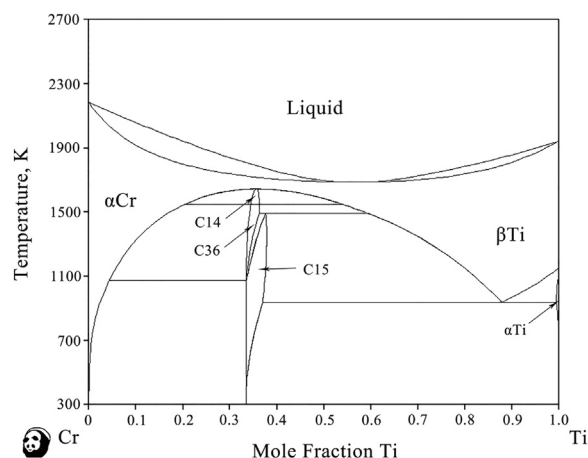


Fig. 2. The Ti-Cr diagram assessed by Ghosh [18].

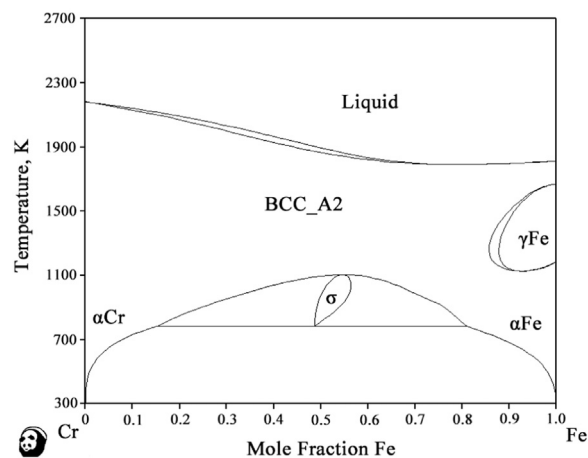


Fig. 3. The Fe-Cr diagram assessed by Andersson and Sunderman [20].

$(\text{A})_8(\text{B})_4(\text{A,B})_{18}$ for sigma phase. Therefore, the Fe-Cr descriptions from Andersson and Sunderman [20], and Lee [30] were considered in the present work. Fig. 3 shows the phase diagram of Fe-Cr system.

2.2. Ti-Fe-Cr ternary system

The phase diagram of Ti-rich portion of the Ti-Fe-Cr system was early investigated by Thyne et al. [33] and several isothermal sections between 827 and 1173 K, as well as some isopleths were constructed. Later, a series of studies on this ternary system were carried out by Boriskina and Kornilov [36–39], including isothermal sections at 823, 1073, 1273 K, and a projection of the liquidus surface and the $\text{TiFe}_2\text{-TiCr}_2$ quasibinary system. All the experimental results mentioned above were the basis of the review of Raghavan [40].

Isothermal sections at 1273 and 823 K for the Fe- $\text{Fe}_2\text{Ti-Cr}_2\text{Ti-Cr}$ part of the triangle were experimentally constructed by Boriskina and Kornilov [37] with the annealing time of 100 h and 500 h, respectively. Then, the whole region of isothermal sections at 823, 1073 and 1273 K were investigated [39] by light microscopy and X-ray diffraction methods, the annealing time for the experimental samples were 100 h for 1273 K, 300 h for 1073 K and 1000 h for 823 K, respectively. Those experimental data were generally consistent with earlier results reported by Thyne et al. [35], and were accepted by the following reviews [40,41]. Kaufman and Nesor [42] computed isotherms at 1700, 1500 and 1273 K. Even though the calculated isotherms at 1500 K showed a good agreement compared with the experiment results, a major deficiency still exists that the new ternary phase $\text{Ti}_5\text{Cr}_7\text{Fe}_{17}$ was not taken into account. To obtain an indication of the γ Fe region with

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