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CALPHAD-type thermodynamic assessment of the Ti–Mo–Cr–V quaternary system

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ABSTRACT

Based on the thermodynamic descriptions of six constitutive binary systems (Ti–Mo, Ti–Cr, Ti–V, Mo–Cr, Mo–V and Cr–V) as well as the experimental phase equilibria data of the ternary and quaternary systems available in the literature, the Ti–Mo–Cr–V quaternary system has been evaluated using the CALPHAD (CALculation of PHAse Diagram) approach. There are no ternary and quaternary compounds in this quaternary system. The solution phases, i.e. liquid, bcc ((βTi), (Mo), (Cr) and (V)) and hcp (αTi), are described by the substitutional solution model. The Laves phase αCr_2Ti is modeled using the two sublattice model $(Cr, Mo, Ti,V)_2(Cr, Mo, Ti,V)_1$ with Mo and V entering both sublattices. A set of self-consistent thermodynamic parameters for the Ti–Mo–Cr–V systems is obtained. The present thermodynamic description can satisfactorily account for most of the reliable experimental data. The complete liquidus and solidus projection of the Ti–Mo–Cr, Ti–Mo–V and Mo–Cr–V systems are also presented.

1. Introduction

Titanium alloys have been widely used in aviation, aerospace, biomedical applications etc. due to their attractive combination of mechanical properties, such as high specific strengths, good corrosion resistance, excellent toughness and good biocompatibility [1–3]. Additions of transition metal elements such as Mo, V and Cr to titanium can stabilize the high temperature β phase to room temperature following rapid cooling. Mo and V are the most frequently used β isomorphous elements in titanium alloys, and Cr is the β eutectoid forming element [4]. The design of compositions of Ti–Mo–Cr–V based novel titanium alloys requires information about the phase equilibria of the Ti–Mo–Cr–V quaternary system. In the present work, thermodynamic description of the this quaternary system is developed.

The Ti–Mo–Cr–V quaternary system has been extrapolated by Lee et al. [5] based on thermodynamic parameters of the Ti–Mo–Cr and Ti–Mo–V systems reported by themselves and thermodynamic description of the Ti–Cr–V system in their previous work [6]. However, the thermodynamic parameters of these constitutive binary systems adopted in the work of Lee et al. [5] were ambiguous. For the Ti–Mo system, they used the set of parameters from Kaufman and Nesor [7]. The unary data used by Kaufman and Nesor [7] disagreed with those used in the other binary datasets. For the Ti–V system, Lee et al. [5] adopted the set of parameters from their previous work [6]. However, the solubility of V in (αTi) was low in their modeling and should be improved based on the experimental data [8]. Lee et al. [5] adopted the thermodynamic parameters of the Ti–Cr and Mo–V systems from Lee et al. [5] and Rudy [9], respectively, which have been updated by Ghosh [10] and Zheng et al. [11]. Lee et al. [5] used three ternary interaction parameters for the bcc phase in both Ti–Mo–Cr and Ti–Mo–V systems and calculated some isothermal and vertical sections along with the extrapolated ones based on the constitutive binary systems. The calculated phase boundaries nearly overlaps with the extrapolated ones (see Figs. 1 and 2 in [5]). It demonstrated that these ternary interaction parameters had little effect on the phase equilibria. In addition, the Ti–Cr–V system has been reassessed by Ghosh [10] based on the available experimental thermodynamic and phase diagram data.

Therefore, a thorough thermodynamic assessment of the Ti–Mo–Cr–V quaternary system is necessary for providing a set of reliable thermodynamic parameters for thermodynamic extrapolations to related higher order systems. The purposes of the present work are to critically evaluate the measured phase diagram data available in the literature and to obtain a set of self-

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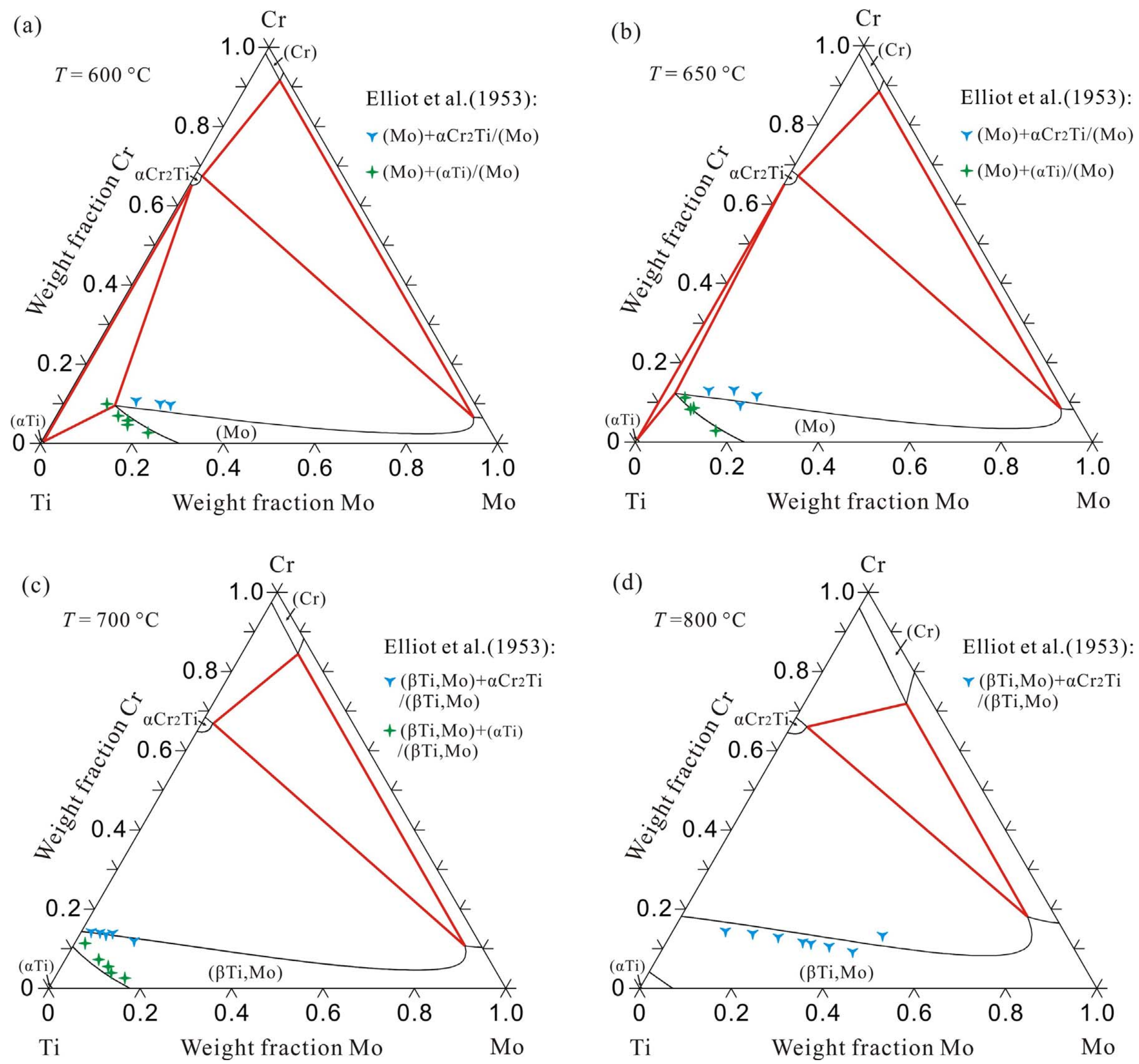

Fig. 1. Calculated isothermal sections of the Ti–Mo–Cr system along with the experimental data from Elliott et al. [12]: (a) 600 °C, (b) 650 °C, (c) 700 °C, and (d) 800 °C.

consistent thermodynamic parameters for the Ti–Mo–Cr–V systems by means of the CALPHAD approach.

2. Evaluation of the literature data

To facilitate reading, the symbols used to denote the solid phases in the Ti–Mo–Cr–V quaternary system and their crystal structure are listed in Table 1.

2.1. The Ti–Mo–Cr system

No experimental thermodynamic data for the Ti–Mo–Cr system were found in the literature. The phase equilibria data were mainly experimentally determined by three groups of authors [12–15]. In 1953, more than 60 ternary alloys were prepared and phase equilibria in the Ti–Mo–Cr system with the composition range from 40 to 100 wt% Ti and the temperature range from 550 to 1300 °C were firstly investigated by Elliott et al. [12] by means of X-ray diffraction (XRD), micrography and contactless thermal analysis. In the work of Elliott et al. [12], the isothermal sections were determined at 50 °C intervals between 550 °C and 900 °C, and at 100 °C intervals between 900 °C and 1300 °C. The vertical sections at 4 and 8 wt% Mo, 4 and 8 wt% Cr, and 70, 80 and 90 wt% Ti were constructed. No ternary compound was detected in the Ti–Mo–Cr system. Contrary to the (βTi, Mo, Cr) phase, the solubilities of Mo and Cr in the low temperature (αTi) phase were neglected. The liquidus surface projection in the Ti-rich corner of the Ti–Mo–Cr system was also constructed by Elliott et al. [12]. The experimental data from Elliott et al. [12] are utilized in the present modeling.

The solidus surface of the Ti–Mo–Cr system was investigated by Grum-Grizhimailo and Gromova [13] by preparing 39 ternary alloys. At the solidus temperature, Ti, Mo and Cr form continuous solid solutions over the entire composition. Subsequently, the same authors [14] investigated the full isothermal sections at 600, 900 and 1200 °C. In the Ti-rich corner, the measured results agree well with the results reported by Elliott et al. [12]. The Laves phases Cr_2Ti formed in the Ti–Cr system extend to about 8 wt% Mo into the ternary system and form two-phase fields of Cr_2Ti and (βTi, Mo, Cr) solid solution. However, the high- and low-temperature Laves phases have not been distinguished at 900 and 1200 °C in the work of Grum-Grizhimailo and Gromova [14]. In addition, the miscibility gap of (Cr) and (Mo) in the Mo–Cr binary system, which should extend into the ternary Ti–Mo–Cr system, was overlooked in the isothermal section at 600 °C by Grum-Grizhimailo and Gromova [14]. Hence, the experimental data reported by Grum-Grizhimailo and Gromova [14] are employed in