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THERMODYNAMIC STUDY OF Cr-Co-Al AND Cr-Co-Mo SYSTEMS

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ABSTRACT

The results of the calculation of the thermodynamic properties for ternary systems Cr-Co-Me (Me = Mo, Al) using general solution model, Kohler and Toop models are presented in this work. For five sections (with molar ratio Co:Me=1:4, 1:1, 4:1) investigated in each ternary system at temperature of 2000K, integral molar excess Gibbs energies were calculated and compared mutually.

Keywords: alloy thermodynamics, thermodynamic predicting, Cr-Co-Mo system, Cr-Co-Al system

1. INTRODUCTION

Alloys based on the Cr-Co-Me (Me = Mo, Al) systems are of great practical interest in the production of Ni-based super alloys, surgical implants, heat-resistant and corrosion-resistant protective coatings.

In spite of this fact, thermodynamic study of such multicomponent systems has not yet been completely reported in the literature, while there are a lot of articles dealing with the thermodynamics of the constituent binary systems [1-8]. Having in mind such problems, it is anticipated that most of the thermodynamic data of ternary and multicomponent systems will come from theoretical calculations rather than from direct experimentation. The main reasons are experimental difficulties, especially the high investigation temperatures required.

Therefore, calculation procedure according to general solution model [9], Kohler [10] and Toop model [11], was applied in this paper in order to contribute to a better knowledge of the Cr-Co-Mo and Cr-Co-Al thermodynamics.

2. THEORETICAL FUNDAMENTALS

Kohler [10] and Toop [11] models belong to a group of traditional geometrical, frequently used calculation models. According to the Hillert's classification [12], Toop model is related to asymmetric systems, while Kohler model is usually applied for symmetric systems.

The main equations describing mentioned models are as follows:

$$\textit{Kohler: } G^E = \Sigma(x_i+x_j)^2 G^E_{ij}[x_i/(x_i+x_j);\ x_j/(x_i+x_j)] \quad (1)$$

$$\textit{Toop: } G^E = x_2/(1-x_1)G^E_{12} + x_3/(1x_1)G^E_{31}+(x_2+x_3)^2\ G^E_{23}[x_2/(x_2+x_3);\ x_3/(x_2+x_3)] \quad (2)$$

where are: G^E and G^E_{ij} - integral molar Gibbs excess energies ternary and binary, respectively, x_i – composition of a component *i*.

According to the Chou's general solution model [9] integral molar excess Gibbs energy is given in terms of the regular solution parameters:

$$\Delta G^{xs} = x_1x_2\,(A^o_{12} + A^1_{12}\,(x_1-x_2) + A^2_{12}\,(x_1-x_2)^2) + x_2x_3\,(A^o_{23} + A^1_{23}\,(x_2-x_3) + A^2_{23}\,(x_2-x_3)^2) + x_3x_1\,(A^o_{31} + A^1_{31}\,(x_3-x_1) + A^2_{31}\,(x_3-x_1)^2) + f x_1x_2x_3 \quad (3)$$

where A^o_{ij}, A^1_{ij}, A^2_{ij} are regular-solution parameters for the binary system "ij" independent of composition, depending only on temperature and the function f is the ternary interaction coefficient, derived on the basis of similarity coefficient concept, given by Chou. Detailed description of determination of mention parameters are presented in Refs. [8,9].

3. RESULTS AND DISCUSSION

The thermodynamic calculations in the ternary systems Cr-Co-Mo and Cr-Co-Al were performed along the lines of a constant Co:Mo and Co:Al molar ratio of 1:4; 1:1; 4:1, respectively.

The starting data for the calculation according to the Kohler and Toop model were taken from the articles by Kaufman and Nesor [2-4]. The binary regular-solution parameters for the constitutional binaries in the investigated ternary Cr-Co-Mo and Cr-Co-Al systems are presented in Table 1.

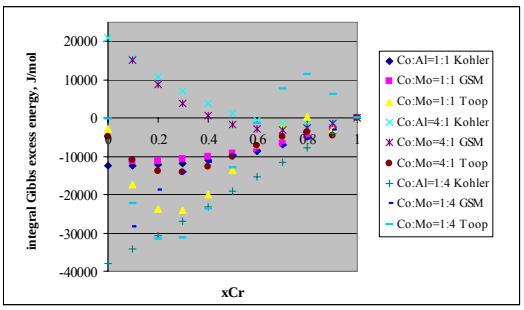
Based on these starting data, similarity coefficients were determined according to the procedure of general solution model [9] and their values are:

* for the *Cr-Co-Al* system: $\xi_{Cr\text{-}Co} = 0.083$, $\xi_{Co\text{-}Al} = 0.910$, $\xi_{Al\text{-}Cr} = 0.522$, and
* for the *Cr-Co-Mo* system: $\xi_{Cr\text{-}Co} = 0.470$, $\xi_{Co\text{-}Mo} = 0.997$ and $\xi_{Mo\text{-}Cr} = 0.004$.

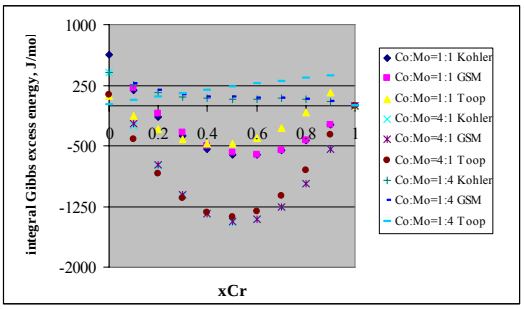
Table 1 - Binary regular-solution parameters for the constitutional binaries (i-j) in the ternary systems Cr-Co-Mo and Cr-Co-Al

System	A^{o}_{ij} (T)	A^{1}_{ij} (T)
Cr-Co	-8368	0
Co-Mo	2510	0
Cr-Mo	19037 - 8.58T	6485 - 2.72T
Co-Al	-281347 + 118.003T	174264 + 0.379T + $0.03612T^2$
Cr-Al	-46442	0

Further calculations were carried out for 27 alloys in all of the selected cross sections in each of the investigated ternary system at the temperature of 2000K, according to the fundamentals of general solution model, Kohler and Toop models, as given by Eqs.(1-3). The results of the thermodynamic predictions for the Cr-Co-Mo and Cr-Co-Al systems are given in Fig.1 as a graphic illustration of the dependence of the integral excess Gibbs energy on composition, for both investigated systems.



a)



b)

Fig. 1. The dependence of the integral excess Gibbs energy on composition for investigated systems at 2000K: (a) Co-Cr-Al and (b) Co-Cr-Mo

As can be seen from Fig.1, system Co-Cr-Mo exhibits more uniform behavior and better agreement between applied calculation models may be

noticed. Slight, but not significant, deviation of Toop results occurs comparing to the other two models. The negative values for G^E is typical for the sections with Co:Mol=4:1 and 1:1, while for the section Co:Mo.=1:4 G^E has positive values.

Concerning the other system, Co-Cr-Al, it is obvious that some discrepancies between three applied models are presented, and Toop results, in this case also, are much different than GSM and Kohler results, especially for sections with Co:Al=4:1 and 1:1. Such trend changes for the third section Co:Al.=1:4, in which all three models show mutual agreement.

All the facts mentioned during the comparison of obtained results may be explained by the nature of the considered systems. Namely, similarity coefficients, presented in the text above, point out to a symmetrical nature of both investigated systems, which explains deviation of Toop results in both ternary systems Cr-Co-Me (Me=Al,Mo). Therefore, results obtained by Kohler and general solution model should be taken as more accurate ones.

4. CONCLUSIONS

The obtained results for the thermodynamic properties in the ternary systems Cr-Co-Mo and Cr-Co-Al are a contribution to the better understanding of the thermodynamic behaviour of these alloys, which is very important in the present day wide field of material designing.

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