



Thermodynamic modelling of a six component (C-Co-Cr-Ni-Ta-W) system for the simulation of Cobalt based alloys



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ABSTRACT

Co-based alloys are key materials for several high temperature applications where high corrosion and wear resistance are required. Main alloying elements, in addition to Co, are Cr, Ni, Ta, Mo, W, Ti, Al, etc. and C. In order to simulate these materials a new thermodynamic database has been implemented which includes the six most important alloying elements: Co, Cr, Ni, Ta, W and C.

The liquid and 30 solid phases have been modelled by means of the Compound Energy Formalism (CEF) with particular attention to the consistency between thermodynamic and crystallographic sublattices. Interaction parameters for all the binary and ternary sub-systems are included. When possible they have been taken from the literature but, for several systems, partial or complete reassessment was needed, due to inconsistency of the phase models or incompatibility between assessments of different authors. As a result phase equilibria in selected commercial alloys are calculated.

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1. Introduction

Co-based alloys are key materials for several high temperature applications where high corrosion and wear resistance are required. They are especially employed in gas turbine vanes and jet engine blades and vanes.

Main advantages of the Co-based alloys with respect to the Ni- or Fe-based ones, are higher melting points and flatter stress-rupture curves, better hot-corrosion resistance in gas turbine atmospheres, better weldability and thermal fatigue resistance. On the contrary they show lower strength, ductility and fracture toughness.

A few typical Co alloy compositions are reported in Table 1. They are characterised by an austenitic matrix (Co-based *fcc* solid solution) where a considerable amount (20–30 mass%) of Cr is dissolved to improve oxidation and hot corrosion resistance, as well as solid solution strengthening. However, an excess of Cr can cause the precipitation of detrimental TCP phases such as *sigma* or *mu*. Ta, W and Mo also contribute to solid solution strengthening, while Ni additions tend to inhibit the low temperature transformation of Co from *fcc* to *hcp*. Finally, small amounts (0.25–1.0 mass%) of carbon

are added to favour precipitation hardening via carbide formation.

Only recently [1] the existence of a ternary Co-Al-W *gamma prime* phase (at the $\text{Co}_3\text{W}_{0.5}\text{Al}_{0.5}$ composition) has opened the possibility to obtain Co superalloys based on the coherent precipitation of *gamma prime* in *gamma*, similar to the traditional Ni-based superalloys, but with improved high temperature performance. However these new alloys are still far from applications, due to the limited stability of the Co-Al-W *gamma prime* phase.

In view of the development of new alloys or improvement of the traditional ones, a detailed description of thermodynamic properties and phase equilibria of the involved multi-component systems is fundamental. Many binary and ternary systems formed by the main alloying elements, namely Co, Cr, Ni, W, Ta, C, Al, Ti, Mo, etc., have already been modelled in literature or have been included in commercial databases. In both cases however there are difficulties and drawbacks: thermodynamic assessments reported in literature are typically performed by different authors, which often use different thermodynamic models for the same phase in different systems. This makes very difficult or even impossible to merge interaction parameters from different assessments in a single multi-component thermodynamic database. Moreover, owing to well reproduced phase equilibria, thermodynamics is often poorly defined and the adopted interaction parameters fail to give reliable higher order extrapolations.

On the other hand, commercial databases, while self-consistent,

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Table 1
Composition (mass%) of selected Co-based alloys. Elements considered in the SuperCo database are in bold.

Alloy	Co	Cr	Ni	W	Mo	Ta	Zr	C	Ti	Al	B	Other
FSX-414	Bal.	29.5	10.5	7	–	–	–	0.25	–	–	0.012	2 Fe
Stellite 21	Bal.	28	2	–	5.5	–	–	0.3	–	–	–	–
Mar-M302	Bal.	21.5	–	10	–	9	–	0.85	–	–	0.005	0.75 Fe
Mar-M509	Bal.	23.4	10	7	–	3.5	0.45	0.6	0.23	–	–	–
ECY-768	Bal.	23	10	7	–	3.5	–	0.6	0.23	0.18	–	–
Haynes-188	Bal.	22	22	14.5	–	–	–	0.1	–	–	–	<3 Fe, 0.9 La
Stellite 31	Bal.	20	10	15	–	–	–	0.1	–	–	–	–

are usually reliable only in restricted composition ranges. Moreover thermodynamic models introduced several years ago have not been improved because a change would require a complete re-assessment of all the systems included in the database. So the development of a new self-consistent thermodynamic database for Co-based alloys with improved phase models is highly advisable.

A first version of SuperCo, a new Co alloy database, is presented in this work. As a first step appropriate phase models have been selected, with special attention to their physical, chemical and crystallographic soundness. This is discussed in the section entitled *Thermodynamic Phase Models*.

Then, selected binary and ternary sub-systems formed by the main alloying elements have been assessed or adapted from previous assessments reported in literature. This is reported and discussed in the section *Assessed Systems*.

2. Thermodynamic phase models

The Gibbs energy of a generic phase ϕ is given by the sum of several contributions:

$$G^\phi = {}^{ref}G^\phi + {}^{id}G^\phi + {}^{ex}G^\phi + {}^{mag}G^\phi \quad (1)$$

where ${}^{ref}G^\phi$ is the reference Gibbs energy, ${}^{id}G^\phi$ and ${}^{ex}G^\phi$ are the ideal and excess mixing contributions, respectively, and ${}^{mag}G^\phi$ is the magnetic contribution, which is only relevant when magnetic ordering occurs. Each term in the summation may assume different expressions, depending on the nature of the phase.

The different phases included in the database are modelled according to the interaction and mixing mechanism between the component elements within the Compound Energy Formalism (CEF) which is briefly introduced in the following.

2.1. Elements

For a pure element in the phase Φ , the Gibbs energy is defined, as a function of temperature, by the expression:

$$G^\phi(T) = A^\phi + B^\phi T + C^\phi T \ln T + D^\phi T^2 + \dots \quad (2)$$

where A , B , C , D , ... are empirical parameters evaluated on the basis of the experimental information. They can be retrieved from the SGTE Pure Element Database [2]. Several temperature ranges with different sets of parameters can actually be needed to accurately describe $G^\phi(T)$ in a wide temperature range.

For magnetic elements eq. (2) refers to the paramagnetic state and the ${}^{mag}G^\phi$ term is added to account for magnetic ordering. It is expressed according to the model introduced by Inden [3] and subsequently adapted by Hillert and Jarl [4]:

$${}^{mag}G^\phi = RT \cdot f(\tau) \cdot \ln(\beta(x) + 1)$$

where β is the average magnetic moment per mole of atoms in Bohr

magneton, τ is the ratio T/T_C (T_C = critical temperature for magnetic ordering), and $f(\tau)$ is a polynomial expression obtained by expanding Inden's description of the magnetic heat capacity into a power series of τ . Magnetic parameters for pure elements are available in the SGTE Pure Element Database [2].

2.2. Disordered solutions

The liquid phase and the disordered solid solutions are modelled as substitutional random solution of the component elements. All atomic species mix in a single sublattice and in this case the first three addenda of eq. (1) can be written as:

$$\begin{aligned} {}^{ref}G^\phi &= \sum_i x_i G_i^\phi(T) \\ {}^{id}G^\phi &= RT \sum_i x_i \ln x_i \\ {}^{ex}G^\phi &= {}^{ex2}G^\phi + {}^{ex3}G^\phi + \dots \end{aligned} \quad (3)$$

where: x_i is the mole fraction of component i , $G_i^\phi(T)$ is the Gibbs energy of the pure component i in the Φ phase, ${}^{ex2}G^\phi$ and ${}^{ex3}G^\phi$ are the binary and ternary interaction terms, respectively, contributing to the excess Gibbs energy. They are expressed as:

$${}^{ex2}G^\phi = \sum_{i=1}^{n-1} \sum_{j=i+1}^n x_i x_j \sum_{\nu} {}^{\nu}L_{ij}^\phi(T) (x_i - x_j)^{\nu} \quad (4)$$

and

$${}^{ex3}G^\phi = \sum_{i=1}^{n-2} \sum_{j=i+1}^{n-1} \sum_{k=j+1}^n x_i x_j x_k (u_i L_i^\phi(T) + u_j L_j^\phi(T) + u_k L_k^\phi(T)) \quad (5)$$

respectively, with:

$$\begin{aligned} u_i &= x_i + \frac{1 - x_i - x_j - x_k}{3}, \quad u_j = x_j + \frac{1 - x_i - x_j - x_k}{3}, \quad u_k \\ &= x_k + \frac{1 - x_i - x_j - x_k}{3} \end{aligned} \quad (6)$$

$L^\phi(T)$ in equations (4) and (5) are empirical parameters whose temperature dependence is similar to that of $G^\phi(T)$ given in equation (2).

For a binary solution with magnetic ordering the composition dependence of ${}^{mag}G^\phi$ results from the composition dependence of T_C and β , which are expressed by a Redlich–Kister series expansion:

$$\begin{aligned} T_C^\phi(x) &= x_A T_C^\phi(A) + x_B T_C^\phi(B) + x_A x_B \sum_{\nu=0}^n {}^{\nu}T_C^\phi(x_A - x_B)^{\nu} \\ \beta_C^\phi(x) &= x_A \beta_C^\phi(A) + x_B \beta_C^\phi(B) + x_A x_B \sum_{\nu=0}^n {}^{\nu}\beta_C^\phi(x_A - x_B)^{\nu} \end{aligned}$$

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