

Thermodynamic re-assessment of the Al-Co-W system



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ABSTRACT

The Al-Co-W system and its binary sub-systems Al-Co, Al-W and Co-W were critically reviewed. The thermodynamic description of the Al-Co-W system including all three binaries was developed considering thermodynamic and constitutional data of the systems. Results from density functional theory calculations were employed to improve reliability of the descriptions. The Gibbs energy for the thermal vacancy (G_{v_a}) in the BCC_A2 phase is discussed. The revised descriptions obtained for the Al-W and Co-W systems describe the thermodynamic and phase equilibrium data well and are free of undesired artefacts for temperatures below 6000 K. The ordered γ' phase of the Al-Co-W system is described as a metastable phase in the entire temperature range. The calculated Gibbs energy of the γ' is only slightly above that of the equilibrium state, which indicates that there is good possibility of stabilizing the γ' phase with the addition of γ' -stabilizing elements, such as Ti, Ta, Hf, Nb and Ni.

1. Introduction

Superalloys are used in aircraft engines, turbo superchargers and chemical plants that require high performance at elevated temperatures [1–3]. The most widely used superalloys are Ni-based alloys which are strengthened by γ' phase ($L1_2$, $AlNi_3$) while traditional Co-based alloys, lacking this phase, have limited applications due to their lower high-temperature strength. The efficiency of gas turbine cycles increases with increasing turbine inlet temperature, thus continuous efforts are made to increase the γ' solvus temperature of Ni-based alloys, such as the addition of γ' stabilizing elements. Although these Ni-based superalloys have a very high ratio of absolute working temperature to melting temperature, the higher melting point of Co compared to Ni makes Co-based alloys attractive candidates for high temperature applications. In addition, Co-based alloys are receiving more attention because of the potential for superior hot corrosion resistance, better weldability and thermal fatigue resistance compared to Ni-based superalloys [4]. The key for the application of Co-based alloys as superalloys is improving their high-temperature strength. Already in 1971, Lee [5] found that a Co-0.04 Al-0.25 W alloy (mass fraction) with ordered γ' phase ($L1_2$) precipitates in a γ phase matrix (FCC_A1) exhibited precipitation-hardened characteristics. More recent work by Sato et al. [6] found that Al-Co-W alloys showed increased high-temperature

strength compared to conventional Ni-base superalloys as result of γ' precipitates in a γ matrix. This suggested a promising future for the application of Co-based γ/γ' superalloys. However, subsequent experiments showed that the ternary γ' phase $Co_3(Al,W)$ is a thermodynamically metastable phase [7–9], unless additional elements are added to stabilize this phase [10]. The use of CALPHAD (CALCulation of PHase Diagrams) type simulations is essential for efficient development of new alloys. Indeed it is now widely accepted that the most effective strategy for accelerated development of such alloys is the CALPHAD-based design technology now known as the Materials Genome [11]. Using preliminary databases, this approach has already delivered a novel γ' -strengthened Co alloy optimized for wear resistance applications [12]. For realistic predictions, more accurate thermodynamic and diffusion mobility databases are needed. Therefore, a multicomponent database for the development of new Co-based γ/γ' superalloys must have a sound thermodynamic description of phase stability of the γ' phase of the Al-Co-W system.

The thermodynamic descriptions of the ternary Al-Co-W system have been assessed by Cui et al. [13], Yang et al. [14] and Zhu et al. [15]. However, in all three assessments the metastable γ' phase was described as a stable phase. It should be noted that Yang et al. [14] did not report the parameters of their thermodynamic description. Zhu et al. [15] used assessments from the literature for the thermodynamic

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Table 1

Summary of the crystallographic information and the enthalpies of formation at 0 K from DFT calculations from AFLOW [22], OQMD [21] and Materials Project [23] databases for the phases of the Al-Co-W system.

Phase name	Crystallographic information					ΔH_f (kJ/mole-atoms)		
	Strukturbericht	Prototype	Pearson symbol	Space group	Ref.	OQMD	Materials Project	AFLOW
(Al), (α Co)	A1	Cu	cF4	$Fm\bar{3}m$	[25]	–	–	–
(W)	A2	W	cI2	$Im\bar{3}m$	[25]	–	–	–
(ϵ Co)	A3	Mg	hP2	$P6_3/mmc$	[25]	–	–	–
BCC_B2, AlCo	B2	CsCl	cP2	$Pm\bar{3}m$	[26]	–58.37	–58.18	–58.46
Al ₅ Co ₂	D8 ₁₁	Al ₅ Mn ₂	hP28	$P6_3/mmc$	[27]	–44.38	–44.28	–44.57
Al ₃ Co	–	–	–	$P2_1/m$	[28]	–	–	–
o-Al ₁₃ Co ₄	–	–	–	$Pmn2_1$	[29]	–	–	–
m-Al ₁₃ Co ₄	–	–	–	$C2/m$	[30]	–	–	–
y-Al ₁₃ Co ₄	–	–	–	$C2/m$	[31]	–	–	–
o'-Al ₁₃ Co ₄	–	–	–	$Pnma$	[32]	–	–	–39.46
Al ₉ Co ₂	–	–	mP22	$P2_1/c$	[33]	–31.64	–31.45	–
Al ₁₂ W	–	Al ₁₂ W	cI26	$Im\bar{3}$	[34]	–7.53	–7.24	–7.57
Al ₅ W	–	Al ₅ Mo	hP12	$P6_3$	[35]	–15.73	–15.44	–15.82
Al ₄ W	–	Al ₄ W	mC30	Cm	[36]	–	–14.86	–
Al ₇₇ W ₂₃	–	–	–	–	–	–	–	–
Al ₇ W ₃	–	–	–	–	–	–	–	–
Al ₂ W	–	Cr ₂ Si	–	$P6_422$	[37]	–	–3.09	–
Co ₃ W	D0 ₁₉	Ni ₃ Sn	hP8	$P6_3/mmc$	[38]	–7.72	–7.81	–7.94
μ	D8 ₅	Fe ₇ W ₆	hR13	$R\bar{3}m$	[38]	–	–	–3.66
γ' (Co ₃ (Al,W) ₁)	L1 ₂	Cu ₃ Au	cP4	$Pm\bar{3}m$	[6]	–	–	–

description of the binary sub-systems, Al-Co [16], Al-W [17] and Co-W [18]. However, the calculated phase diagrams of the two binary Co sub-systems show noticeable deviations from recent experimental data [19,20].

As part of the development of a thermodynamic database for multicomponent Co-based alloys, the present work provides a comprehensive CALPHAD assessment of the Al-Co-W system including the description of the metastable γ' phase and incorporating data from density functional theory (DFT) calculations from open databases, such as the Open Quantum Materials Database OQMD [21], Automatic-Flow for Materials Discovery AFLOW [22], Materials Project [23] and Alloy Database [24]. The data for the binary sub-systems Al-Co, Al-W and Co-W are critically reviewed and the thermodynamic descriptions are reassessed or modified to ensure the quality of the thermodynamic description of the ternary system. The solid phases occurring in this ternary system are summarized in Table 1 [6,25–38].

2. Literature review

2.1. Al-Co system

Several thermodynamic descriptions are available for the Al-Co system [16,20,39]. Of these descriptions, the description by Stein et al. [20] reproduces the available experimental data best. For the re-optimization of the description, Stein et al. used all available experimental data from the literature and their own data. Although their calculations agree well with the experimental data sets, an inverse miscibility gap, as shown in Fig. 1, occurs above 4800 K. Due to the relatively high melting point of the refractory element W (3695 K), the presence of an inverse miscibility gap at a temperature of 4800 K could interfere with obtaining a reliable description for the Al-Co-W system [40]. Although Al evaporates at 2791 K it is imperative for systems containing refractory elements to have an artifact-free description of the liquid phase even for temperatures that are significantly higher than their melting points. Thus, it was considered necessary to eliminate the occurrence of this inverse miscibility gap in the Al-Co system and to re-assess the thermodynamic description of this system.

McAlister [41] performed a comprehensive review of the experimental data for the Al-Co system that were available in 1985. Dupin and Ansara [16] also reviewed the data that were available in 1997.

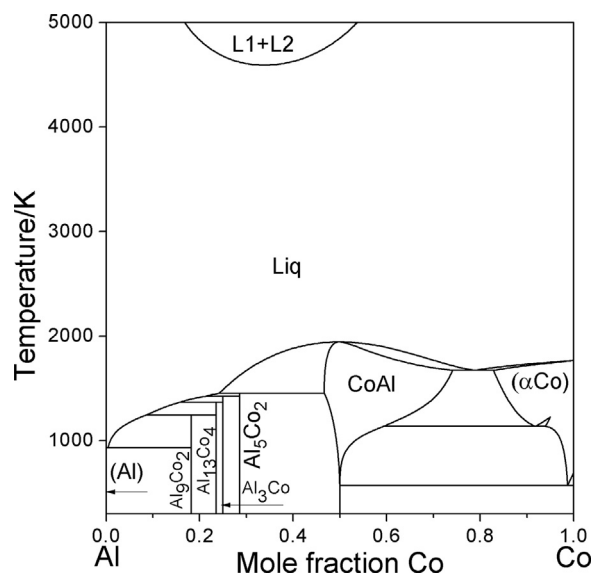


Fig. 1. Calculated Al-Co phase diagram from Stein et al. [20].

Some of these data will be discussed here together with newer experimental and supplemental data and put into context with the older data.

Hishimoto [42] used thermal analysis (TA) during cooling to determine liquidus and solidus in the composition range with 0.4761 Co to 1.0 Co (compositions are in mole fraction, unless otherwise noted). However, the observation of strong supercooling effects [43] casted doubts on the reliability of the data. Therefore, the data from Hishimoto [42] were not used for the parameter optimization.

Kimura et al. [44] prepared alloys with 0.4 Co to 0.98 Co using arc melting. The alloys were annealed at 1273 K for seven days or at 1423 K for two days. The phase equilibria of the AlCo (BCC_B2) and (α Co) (FCC_A1; also named γ in superalloys) phases were measured for annealed alloys using a scanning electron microscope (SEM) equipped with an energy dispersive X-ray spectrometer (EDS). Kimura et al. [44] also measured the solidus and liquidus for alloys with 0.63 Co to 0.98 Co using differential thermal analysis (DTA) with a heating rate of 10 K/min.

Dmitrieva et al. [45] used DTA with a heating rate of 60 K/min to

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