Thermo-Calc and DICTRA modelling of the β-phase depletion behaviour in CoNiCrAlY coating alloys at different Al contents

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ABSTRACT

The β-phase depletion kinetics in MCrAlY coating alloys at different Al contents has been investigated by diffusion simulations and comparing with available experimental data. The thermodynamic software, Thermo-Calc, and the finite difference software, DICTRA, were employed to calculate phase equilibriums and to perform diffusion calculations using the thermodynamic database, TTNi7, and the mobility database, MOB2. The phase fractions and compositions in MCrAlY alloys with different Al contents were calculated by Thermo-Calc. At high temperature exposures, the β-NiAl phase in MCrAlY coating alloys depletes progressively due to the consumption of Al during oxidation and interdiffusion. The Al flux due to oxidation was approached from the oxide growth kinetics at the oxide/coating interface in the DICTRA diffusion model. Initial oxides and the associated initial β-phase depletion zones were assumed as the initial conditions. It is found that the MCrAlY with highest Al content exhibits the least β-phase depletion due to its large β-phase fraction and high Al content. In addition, it is shown that the loss of β phase to the substrate due to interdiffusion is more significant than the β-phase depletion from oxidation.

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1. Introduction

MCrAlY (M = Co and/or Ni) coatings are widely used for surface protection of high temperature components in gas turbines due to their outstanding oxidation resistance by forming the continuous and protective oxides, predominantly alumina, at the surface [1–8]. MCrAlYs are typically multi-component and multi-phase alloys and can have customised compositions to achieve particular performance requirements [9–14]. Depending on the compositions, MCrAlYs can consist of γ-Ni, γ′ and β-NiAl phases [15,16]. Among the various phases that present in the MCrAlY alloys, one of the vital phases is the Al-rich β-NiAl phase, which acts as the Al reservoir to allow sufficient Al to form the protective alumina scale [17–19]. Since Al is mainly from the β-NiAl phase, the growth of the alumina scale causes the continuous loss of Al and subsequently the β-phase depletion zone is formed in contact with the alumina scale [20,21]. As the Al_2O_3 continues to grow, the β phases progressively deplete. The loss of the β phase also occurs from interdiffusion between MCrAlY and substrate [22,23]. Eventually the protective effects of the MCrAlY coating alloy diminish when the β phases are completely consumed [24–29].

The evolution of the β-phase depletion in MCrAlY alloys is mainly governed by the oxidation kinetics, the β-phase fraction and the interdiffusion with substrates [30,31]. The oxide growth kinetics of the MCrAlY coatings have been extensively reported, which generally exhibit a parabolic behaviour though some divergent arguments still exist [32–34]. The β-phase fraction and composition vary with the MCrAlY composition, especially the Al content. It was reported that the β-phase fraction increased with Al and the changes of the Al content in MCrAlY compositions could significantly influence the evolution of the β-phase depletion [35]. It was further found that the loss of the β phase due to the interdiffusion with substrate was also significant [36]. To achieve a theoretical evaluation in the lifetime prediction of MCrAlY alloys, modelling of the β-phase depletion in different MCrAlY compositions is of particular interest for the alloy design and application. Early work by Nebsitt [36–40] and Lee et al. [41] have demonstrated the capability of using finite difference modelling methods to evaluate the microstructure evolution of MCrAlY coatings during oxidation and interdiffusion. With the recent development of computational software and thermodynamic databases, many diffusion modelling work of MCrAlYs have been reported [42–48]. Among the reported studies, the MCrAlY coatings used are limited to some commercial compositions and specific concerns on the β-phase depletion kinetics in MCrAlY coatings with different Al contents

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and β-phase fractions have not been detailed yet. Due to MCrAlYs with various Al contents are not commercially available, thus modelling of the β-phase depletion in such compositions becomes important to reveal the effects of Al content on β-phase depletion. However, studies on this aspect do not appear to have been previously reported.

Therefore, given the importance of the β-phase depletion in influencing the durability of MCrAlY coating alloys and considering the significance of Al content on the β-phase depletion, the aims of this paper are to investigate β-phase depletion in MCrAlYs during oxidation and interdiffusion, specifically at different Al content. The commercially available thermodynamic software, Thermo-Calc [49], and the multi-component diffusion software, DICTRA [50], along with the TTNi7 thermodynamic database [51] and MOB2 mobility database are used. Phase equilibrium calculations are performed by Thermo-Calc and the β-phase depletion at different Al content is simulated by DICTRA at 1100 °C using a previously developed β-phase depletion model [31]. This paper is aiming at reporting the β-phase depletion behaviour at different Al content in MCrAlY coating systems during oxidation and interdiffusion.

2. Thermodynamic calculation of phase equilibrium

2.1. Procedure for phase equilibrium calculation

Phase equilibrium calculations using Thermo-Calc can provide useful information on the fractions and compositions of various phases at given alloy compositions under specified conditions. The CALPHAD approach employed in Thermo-Calc is based on minimising the total Gibbs free energy of the alloy system to determine the optimal fractions and compositions of its constituting phases as a function of temperature. In this study, three Co-based CoNiCrAlY alloys at different Al content are examined, of which the compositions are summarised in Table 1. The composition of CoNiCrAlY-8 with 8 wt%Al has been widely used for oxidation protection (i.e. AMDRY-995 and Praxair CO-210-24 powders) [52,53], while the other two compositions at 10 wt%Al and 12 wt%Al are not yet commercially available. The compositions from Table 1 are entered in Thermo-Calc excluding Y due to its small amount and unavailability in the TTNi7 database. The suitability of this thermodynamic database to the CoNiCrAlY alloys has been demonstrated in previous studies [23,53]. To perform phase equilibrium calculations, the phases considered in this alloy system are liquid, γ, β-NiAl, γ′ and σ. Interesting data for these three alloy compositions are the fraction and composition of β-NiAl phase at high temperatures since this will directly influence the subsequent β-phase depletion calculations.

2.2. Results

The computed phase diagram as a function of Al content is presented in Fig. 1. It can be seen the melting points of the MCrAlY alloys are generally between 1330 and 1400 °C, depending on the Al content. The phase transformation occurs from γ to γ + β when Al content increases at high temperatures. It can be seen at high Al content, i.e. above 6 wt%, only γ and β-NiAl phases present at high
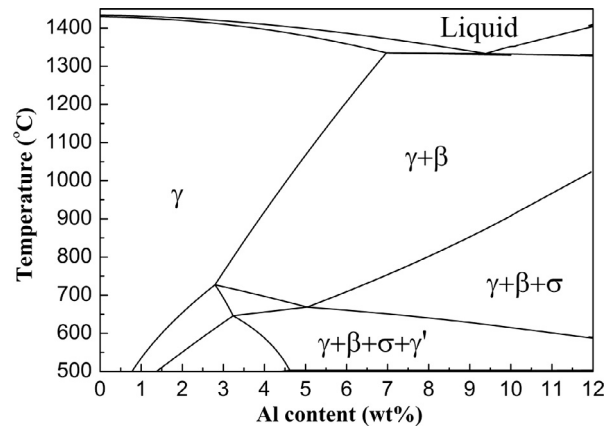

Fig. 1. The calculated phase diagram of CoNiCrAlY alloys as a function of Al content using the TTNi7 database.

temperatures and the minor phases, σ and γ′, start to precipitate at low temperatures. It is noticed that the temperature for the σ phase precipitation increases with Al content. The calculated phase changes are γ → γ + β upon increasing the Al content at 1100 °C. The computed phase fraction maps as a function of temperature at Al content of 8 wt%, 10 wt% and 12 wt% are shown in Fig. 2, suggesting the primary phases are γ and β-NiAl phase at high temperatures. It is seen that the fraction of the phases that present at different temperatures varies with Al content. For the minor σ and γ′ phases, it is found that the fraction of σ increases with Al content but γ′ fraction remains largely unchanged. The β-phase fraction increases as Al content increases, showing good agreement with reported studies on Al stabilising the β phase [35]. The fraction of the γ matrix decreases due to the increase of σ and β phases. To elucidate the effect of Al content on the calculated phase equilibria, the evolution of γ and β phase fractions as a function of Al content at 1100 °C is summarised in Fig. 3. An approximately linear relationship is seen between the phase mass fractions and the Al content. Since Al is the major element in the β phase, the β-NiAl phase forms quite strongly with the Al content. Indeed, the fraction of the β-NiAl increases with Al content whilst the γ-phase fraction decreases with Al content, as seen from Fig. 3. Eventually, the fraction of the β-NiAl phase becomes larger than the γ phase at 12 wt% Al. Although the fractions of various phases change with Al content in the three MCrAlY alloys, they still exhibit the γ + β dual phase structure at 1100 °C. The equilibrium compositions of the γ and β phase versus Al content at 1100 °C are illustrated in Fig. 4. It is seen the Ni concentration decreases and the Cr concentration increases with Al content in the γ phase. Since the changes of the Al content is only from 8% to 12%, no significant changes occur on the β-phase compositions, indicating the increase of Al content mainly contributes to the increase of the β-phase fractions.

The fraction and composition of γ and β phases at 8%Al have shown good agreement with previous experimental measurements [31,53], of which the microstructure after 2-h heat treatment at 1100 °C is shown in Fig. 5. A two phase structure is clearly seen

Table 1
Three compositions of CoNiCrAlY alloys at 8 wt%, 10 wt% and 12 wt%Al.

	Elements (in wt%)				
	Co	Ni	Cr	Al	Y
CoNiCrAlY-8	Bal.	31.7	20.8	8	0.5
CoNiCrAlY-10	Bal.	31.7	20.8	10	0.5
CoNiCrAlY-12	Bal.	31.7	20.8	12	0.5