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MCrAlY coating design based on oxidation–diffusion modelling. Part II: Lifing aspects

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ABSTRACT

Coatings from MCrAlY-type alloys are commonly used for oxidation and corrosion protection in gas turbines. As coated components are exposed to high temperature, the coating provides oxidation protection by the formation of an alumina scale, thus depleting the coating of Al which, eventually, will cause the coating to fail. The present study deals with MCrAlY alloy design from a lifing perspective. A previously developed coupled oxidation–diffusion model was used to study the influence of coating composition, substrate composition and oxidation temperature on the expected life of MCrAlY coatings. Eight model coatings, covering the wide range of MCrAlY compositions used industrially, and two model substrates, corresponding to a blade material and a combustor material, were evaluated by the oxidation–diffusion model. Three life criteria were tried: 1) β-phase-depletion, 2) critical Al content at the coating surface, and 3) a critical TGO thickness. It was shown that the critical TGO thickness was the most conservative life criterion for high-Al coatings on high-Al substrates. For low-Cr and low-Co coatings, the β-depletion criterion was usually the most conservative. For cases where β-stability was high (such as at low temperatures and for coatings high in Cr, Co and Al) the critical-Al criterion was often the most conservative.

1. Introduction

Overlay coatings made of MCrAlY-type alloys are commonly used for oxidation/corrosion protection both on their own, and as bond coats in thermal barrier coating systems [1–3]. The base element, M, may be Ni and/or Co, and Cr and Al are added in varying amounts to promote oxidation and corrosion resistance. Minor amounts of reactive elements, most commonly Y, are also added, mostly to improve the coating's performance during oxidation [4]. Common manufacturing methods include atmospheric plasma spraying (APS), vacuum plasma spraying (VPS) and high velocity oxy-fuel spraying (HVOF) [1,4,5]. They all use powders as feedstock and give a characteristic "splat-on-splat" structure.

During high-temperature exposure, the coating will oxidise and form an outer layer of thermally grown oxides (TGO) [6]; in the case of APS, "intersplat" TGOs may also form internally in the coating [7]. The coatings provide oxidation protection of the underlying substrate through the formation of a continuous layer of alumina [8]; MCrAlY coatings are consequently rich in Al which partitions to the Al-rich phases γ'-Ni_3Al and/or β-NiAl. At prolonged exposure to high temperature, the coatings will eventually reach a point where they can no longer maintain a protective layer of alumina and they will fail. The failure may be induced by depletion of Al, so that alumina is no longer the preferred oxide, or by the TGO reaching a critical thickness where it cracks and spalls [9,10]. Both cases will cause non-protective oxides to form and the oxidation protection of the substrate becomes compromised.

The expected high-temperature life of the coating is an important property that should be considered during MCrAlY alloy design. Several papers exist on Al-depletion-based life modelling of MCrAlY coatings [10–18], but none which studies the life as function of different alloy compositions. This is the second part of a two-part paper investigating various aspects of MCrAlY alloy design: part I of this study deals with the microstructural aspects of MCrAlY alloy design [19] and the current paper deals with lifing issues. The current paper presents a study on the composition dependence of the expected coating life for a wide range of alloy compositions. The computational thermodynamics software Thermo-Calc, and its diffusion module DICTRA, were used together with an oxidation model to simulate Al depletion for coatings with varying Co, Cr and Al contents deposited on two different substrates. The expected lives of the coatings were evaluated at 850–1050 °C from β-depletion, Al-depletion

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and a critical TGO thickness. The paper concludes with a discussion on the composition and temperature dependence of coating life and the suitability of the three life criteria.

2. Modelling work

2.1. Model description

A coupled oxidation–diffusion model has previously been developed and was used as basis for the current work; see, for example, Refs. [7,19,20] for a more thorough description of the model. The substrate–coating couple was represented in 1D by a set of 98 nodes reaching from the coating surface through the coating and into the substrate. At locations where large concentration gradients were expected (close to the coating surface and the substrate–coating interface) the node spacing was 1 μm; at other locations the node spacing was 2–50 μm. Each node represented a location in the substrate–coating system and contained the composition of the material at that point. The substrate had a thickness of 1 mm and the coating was 150 μm thick. The coupled oxidation–diffusion was implemented as an iterative process as outlined below.

1. A suitable time step is chosen; shorter at the beginning, when oxidation occurs rapidly, and longer towards the end of the simulation.
2. The composition of the outermost coating nodes is adjusted to account for the oxidation that occurs during the chosen time step (i.e. Al is removed from these nodes to simulate oxidation); experimentally established oxidation kinetics is used as input. A Matlab script was written to perform this. As Al is consumed, the metal–oxide interface is allowed to regress.
3. Optionally (and especially for APS coatings), intersplat oxidation can be simulated by adjusting all nodes in the coating according to an experimentally established oxidation law.
4. The adjusted composition profile is passed on to DICTRA which performs the diffusion calculations and thus adjust the composition profiles for substrate–coating interdiffusion during the chosen time step.
5. Start again from point 1.

The DICTRA run was performed using the TCNI5 and MONI2 databases; the γ, γ', α and β phases were included and their relative contribution to the overall diffusivity of the material was modelled using "homogenisation model 5" which assumes a rule-of-mixtures distribution of the phases. Further information about the Thermo-Calc and Dictra software can be found in, for example, Refs. [21–23]. The development and calibration of the oxidation–diffusion model have been made based on experimental data from several coatings and temperatures and the agreement with experimental results has generally been good [20]; comparisons between model results and experimental observations are available in part I of this paper [19].

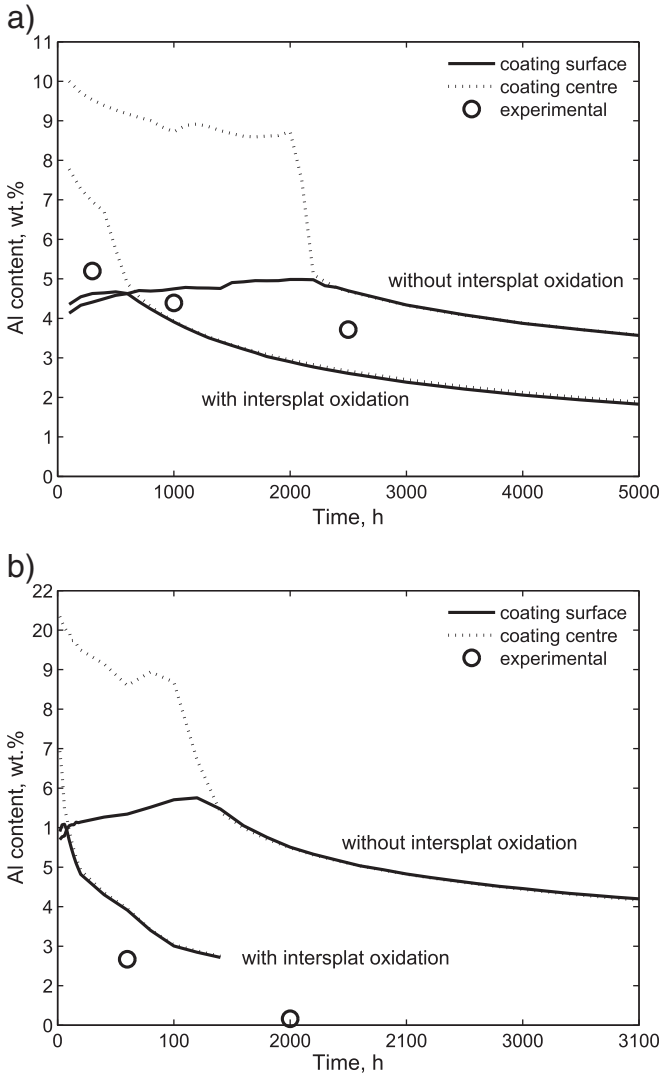

Fig. 1. Comparison of EDS results and simulation results with and without intersplat oxidation: a) 980 °C and b) 1050 °C.

2.2. The oxidation model

The current oxidation–diffusion model requires oxidation kinetics to be established experimentally and used for input during simulation. The model oxidation assumption must be adjusted depending on the manufacturing method: for APS coatings, where intersplat oxidation may be prevalent, in-coating Al removal must be incorporated into the oxidation simulation, whereas, for VPS and HVOF coatings, it is sufficient to perform just the surface oxidation. This is illustrated in Fig. 1 which shows the variation in Al content with time in the coating centre and at the coating surface for an APS coating oxidised at 980 °C and 1050 °C. Fig. 1 includes experimental EDS results and simulation results using two different oxidation models: 1) surface oxidation only and 2) surface and intersplat oxidation. Using intersplat oxidation improved the agreement with experimental results for APS coatings.

In the current study, the modelling work was limited to only consider external oxidation and, therefore, mainly concerns VPS and HVOF coatings. The TGO thickness, h, was assumed to follow a parabolic oxidation law

$$h = (kt)^{1/2} \tag{1}$$

where

$$k = k_0 e^{-\frac{Q}{RT}} \tag{2}$$

Table 1
Substrate and coating compositions used for modelling.

Material	Symbol	Ni, wt.%	Cr, wt.%	Co, wt.%	Al, wt.%	Ti, wt.%
Substr. 1	s1	79.5	15	5	0.5	–
Substr. 2	s2	61	15	15	5	4
Coat. 1	c1	59	15	20	6	–
Coat. 2	c2	52	15	20	13	–
Coat. 3	c3	49	25	20	6	–
Coat. 4	c4	42	25	20	13	–
Coat. 5	c5	39	15	40	6	–
Coat. 6	c6	32	15	40	13	–
Coat. 7	c7	29	25	40	6	–
Coat. 8	c8	22	25	40	13	–