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## COATING LIFE PREDICTION FOR COMBUSTION TURBINE BLADES

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### ABSTRACT

A life prediction method for combustion turbine blade coatings has been developed by modeling coating degradation mechanisms including oxidation, spallation, and aluminum loss due to inward diffusion. Using this model, the influence of cycle time on coating life is predicted for GTD-111 coated with an MCrAlY, PtAl, or aluminide coating. The results are used to construct a coating life diagram that depicts failure and safe regions for the coating in a log-log plot of number of startup cycles versus cycle time. The regime where failure by oxidation, spallation, and inward diffusion dominates is identified and delineated from that dominated by oxidation and inward diffusion only. A procedure for predicting the remaining life of a coating is developed. The utility of the coating life diagram for predicting the failure and useful life of MCrAlY, aluminide, or PtAl coatings on the GTD-111 substrate is illustrated and compared against experimental data.

### INTRODUCTION

Land-based combustion turbine blades are generally coated with overlay or diffusion coatings to improve oxidation and corrosion resistance. The effectiveness of these coatings diminishes with time after exposure to high temperatures and repeated heat-up and cool-down cycles. These coatings usually fail when a continuous protective oxide layer, e.g., alumina, cannot be formed on the coating surface due to the depletion of Al. The loss of Al from the coating can take place by three means: (1) oxidation, (2) spallation, and (3) inward diffusion. All three degradation mechanisms, which reduce the amount of Al available for forming a protective oxide layer, are detrimental to the useful life of the coatings; consequently, they must be taken into account in any coating life model.

Several investigators (Nesbitt and Heckel, 1984; Lee et al., 1987; Nesbitt, 1989a, 1989b; Nesbitt and Barrett, 1993) have developed life prediction methods for coatings based on consideration of cyclic oxidation, spallation, and diffusion of oxide forming elements. These earlier life prediction approaches were based on an empirical spallation model that contains temperature-dependent material constants (Probst and Lowell, 1988; Lowell et al., 1991). Applications of these models at

low temperatures can be difficult because of the lack of spallation data for obtaining the model constants. For life estimation, two criteria were proposed for defining the onset of coating failure: (1) a critical Al content (Nesbitt and Barrett, 1993) and (2) the volume fraction of the  $\beta$  phase in the aluminide coatings (Lee et al., 1987).

A new coating life model was recently proposed for predicting the useful life of combustion turbine coatings such as MCrAlY, aluminide, and PtAl (Chan et al., 1997). The model, named COATLIFE, includes treatment of oxidation, spallation, and inward diffusion of Al. The mechanism-based model differs from previous models in the treatment of oxide spallation by adapting a fracture mechanics approach that results in explicit relationships between weight of oxide spalled and relevant physical and mechanical properties of the oxide (Chan, 1997). As a consequence, possible temperature dependence of material parameters is easily defined and any extrapolation of model constants with temperature, if necessary, can be justified and done with confidence. Applications of the model to the oxidation, spallation, and lifetime predictions of aluminide and platinum aluminide coatings have been reported earlier for cases without the effect of inward diffusion of the oxide forming element, Al, into the substrate (Chan et al., 1997). In this paper, the effect of oxidation, spallation, and inward diffusion on the coating lives of MCrAlY, aluminide, and PtAl coatings are considered.

### EXPERIMENTAL PROCEDURE

Material and Coatings: Cyclic oxidation data were generated for GTD-111 test specimens coated with MCrAlY, aluminide, and PtAl coatings. These experimental data were used for obtaining the material constants in the coating life model and for verifying the predictive capability and accuracy of the model. The MCrAlY coating was processed by an EB-PVD process while the aluminide and PtAl coatings were processed via a pack cementation process. The MCrAlY coating is a CoCrAlY with a microstructure of approximately equal volume percent of  $\beta$  (NiAl) phase and  $\gamma$ -Ni solid solution. Both the aluminide and PtAl coatings show a microstructure of equiaxed  $\beta$  (NiAl) grains in the as-processed condition. The nominal coating thicknesses were 33.8, 65, and 253  $\mu\text{m}$  for aluminide, platinum aluminide, and MCrAlY

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coatings, respectively. The GTD-111 material was heat-treated to a microstructure containing a bimodal distribution of primary (cuboidal) and secondary (spherical) gamma prime particles.

**Cyclic Oxidation Testing:** The cyclic oxidation tests were performed in the cyclic oxidation testing facility at SwRI. During cyclic oxidation tests, the specimens were inserted in a furnace maintained at a constant peak temperature, which was 1066°C (1950°F) or 954°C (1750°F). They were held in the furnace for 30 or 55 minutes and then moved to the cooling system and cooled by forced air for five minutes. The specimens took approximately four minutes to reach the peak temperature and one minute to cool from the peak temperature to room temperature. They were then returned to the furnace and the thermal cycle repeated. The cyclic oxidation test was interrupted at specified intervals to weigh the specimens. After a selected number of thermal cycles, microsections were prepared from some coated specimens for metallographic evaluation. The microstructure and coating composition were determined using optical and scanning electron microscopy and energy dispersive spectroscopy (EDS). Details of the experimental procedure are described elsewhere (Chan et al., 1997; Cheruvu et al., 1998).

### COATING LIFE MODEL

The coating life model used in this investigation is COATLIFE, which is a computer program that simulates cyclic oxidation on a cycle-by-cycle basis and predicts the useful life of a coating based on a critical Al criterion. The development of the cyclic oxidation model is described in a paper by Chan (1997), while an extension of the model for predicting the usable life of coatings under cyclic oxidation without the effect of inward diffusion is presented in Chan et al. (1997). In this paper, the influence of inward diffusion on coating life is modeled. The result is then used to develop a coating life diagram for predicting the remaining life of combustion turbine coatings.

Figure 1 shows a schematic of the cyclic oxidation model and the proposed methodology for predicting the usable life of a coating. The important features in the coating life model are: (1) oxidation kinetics, (2) oxide fracture and spallation, (3) inward diffusion, (4) overall kinetics of cyclic oxidation and depletion of the oxide-forming element, Al, due to oxidation, spallation, and inward diffusion, and (5) a life predicting scheme based on a critical concentration of Al for the formation of a protective oxide layer. A brief description of these essential features of the coating life model is presented in the next five sections.

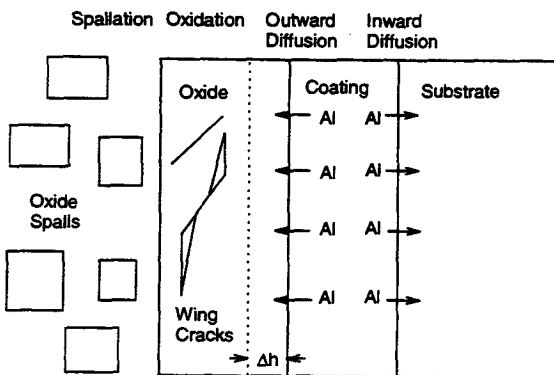


Figure 1. Schematics of degradation mechanisms treated in the COATLIFE model.

### 1. Oxidation Kinetics

The weight of oxide,  $W_{ox}$ , formed during a thermal cycle is modeled using a parabolic growth law that relates the weight of oxide formed to the weight of oxygen gained by the coating, as given by

$$W_{ox} = Z\sqrt{k_p t} \quad (1)$$

where  $k_p$  is the oxidation kinetic constant,  $t$  is time of oxidation, and  $Z$  is the ratio of the molecular weight of the oxide to the atomic weight of oxygen in the oxide. After spallation occurs at the end of a thermal cycle, the thickness of the oxide is reduced, leading to an increase in the oxidation rate. This increase in the oxidation rate after spallation is modeled by using the concept of an equivalent time introduced by Probst and Lowell (1988). The equivalent time,  $t_e$ , for cyclic oxidation corresponds to the time required to form an oxide layer of identical thickness under isothermal conditions. The equivalent time,  $t_e$ , is calculated at each cycle based on the cycle time and the current thickness of oxide layer on the coating surface.

### 2. Spallation

The spallation law proposed by Chan (1997) was used in COATLIFE. As described earlier, the spallation model treats both bulk and interface spallation. In the current model, the weight of oxide spalled,  $W_s$ , during an arbitrary thermal cycle is given by

$$W_s = q_c (\Delta T - \Delta T_c)^2 H(\Delta T - \Delta T_c) \left[ 1 + p \left( \frac{W_o}{W_{ox}} \right)^m \right] \left[ \frac{W_{ox}}{W_o} \right]^{1+m} \quad (2)$$

where  $p$  and  $q_c$  are the interface and bulk spallation constants, respectively;  $m$  is the spallation exponent;  $H(\ )$  is the Heaviside function;  $\Delta T$  is the temperature drop,  $\Delta T_c$  is the critical temperature drop below which spallation does not occur. The parameter  $q_c$  incorporates material parameters concerning the length ( $l_o$ ), angle ( $\psi$ ), and density ( $\zeta_o$ ) of microcracks, the Young's modulus ( $E_{ox}$ ), fracture toughness ( $K_{ox}$ ), and the difference in the CTE,  $\Delta\alpha$ , between the oxide and the coating. The parameter  $p$  relates interface defect length and fracture toughness to their counterparts for the bulk. The referenced weight,  $W_o$ , is arbitrary and can be taken as 1 mg/cm<sup>2</sup> or any other convenient value. In general, only the constants  $p$ ,  $q_c$ ,  $\Delta T_c$ , and  $m$  need to be evaluated from experimental data if one adopts a phenomenological approach. In the present paper, the values for these model constants were evaluated from the experimental weight change data.

### 3. Inward Diffusion

The current version of COATLIFE includes a treatment of inward diffusion of Al from the coating to the substrate. The diffusion of aluminum into the substrate requires a multicomponent analysis since most engineering alloys and coatings contain several elements in their compositions. In an  $n$ -component system the diffusivity  $[D]$  is an  $(n-1) \times (n-1)$  property matrix, and the corresponding Fick's second law is given by (Kirkaldy, 1970)

$$\frac{\partial[C]}{\partial t} = \frac{\partial}{\partial x} [D] \frac{\partial[C]}{\partial x} \quad (3)$$

where [C] is concentration, x is distance, and t is time. A simple but approximate solution to Eq. (3) was developed and used in COATLIFE. The validity of this simplified diffusion was verified using the a finite-difference diffusion code, COSIM, developed at NASA-Lewis (Nesbitt, 1984). The input to the simplified diffusion model is coefficients of diffusion of Al and Cr in the diffusion matrix. In many cases, the coefficients of diffusion are not known for the coating of interests and must be evaluated by calibrating the coating life model to pertinent experimental data.

#### 4. Overall Kinetics of Cyclic Oxidation

The overall kinetics of cyclic oxidation has been modeled as a process that involves the formation and spallation of oxides during thermal cycling. The weight of oxide remained,  $W_r$ , on the coating surface after a thermal cycle can be expressed as (Probst and Lowell, 1988; Lowell et al., 1991)

$$W_r = W_{ox} - W_s \quad (4)$$

where  $W_{ox}$  and  $W_s$  are given by Eqs. (1) and (2), respectively. Expressions for the cumulative weight change, total weight of oxide spalled, and the weight of aluminum loss have been formulated as a function of number of thermal cycles. The expression for the cumulative weight change per unit area,  $W_c$ , after n thermal cycles is (Probst and Lowell, 1988; Lowell et al., 1991)

$$W_c(n) = (1/Z)W_r(n) - (1 - 1/Z) \left( \sum_1^n W_r(n) \right) \quad (5)$$

while the cumulative metal loss,  $W_m$ , of the oxide-forming element from the coating due to oxidation and spallation is given by (Probst and Lowell, 1988; Lowell et al., 1991)

$$W_m(n) = (1 - 1/Z) \left[ W_r(n) + \sum_1^n W_r(n) \right] \quad (6)$$

for the  $n^{\text{th}}$  cycle. The parameters of  $W_{ox}$ ,  $W_r$ ,  $W_s$ ,  $W_c$ ,  $W_m$ ,  $t_e$ , and weight gain,  $W_g$ , are calculated for each of the thermal cycles. The loss of Al due to inward diffusion is then subtracted from Eq. (6).

#### 5. Life Prediction Methodology

The volume fraction of the  $\beta$  phase (NiAl),  $V_\beta(n)$ , in the coating at the  $n^{\text{th}}$  cycle is calculated using the lever rule and is given by

$$V_\beta = 1 \text{ for } X_{Al} \geq X_{Al}^\beta \quad (7)$$

and

$$V_\beta(n) = \frac{X_{Al}(n) - X_{Al}^*}{X_{Al}^\beta - X_{Al}^*} \text{ for } X_{Al}^\beta \geq X_{Al}(n) \geq X_{Al}^* \quad (8)$$

where  $X_{Al}^\beta$  is the aluminum content in the  $\beta$  phase and  $X_{Al}^*$  is the aluminum content in the  $\gamma'$  or  $\gamma$  phase at the appropriate phase boundary in equilibrium with the  $\beta$  phase.

The remaining life, RL, is defined based on the assumption that the useful life of the coating is zero when the volume fraction of the  $\beta$  phase is zero, leading to

$$RL = \frac{X_{Al}(n) - X_{Al}^*}{X_{Al}(0) - X_{Al}^*} \text{ for } X_{Al}^\beta \geq X_{Al}(n) \geq X_{Al}^* \quad (9)$$

which gives a remaining life of unity when  $X_{Al}(n) = X_{Al}(0)$  but a zero remaining life when  $X_{Al}(n) < X_{Al}^*$ .

### COMPARISON OF MODEL PREDICTION AND EXPERIMENTAL DATA

The COATLIFE model was applied to predict the useful life of coatings on laboratory specimens subjected to cyclic oxidation. The experimental data were those generated on GTD-111 specimens coated with an aluminide, PtAl, or MCrAlY coating. They were thermally cycled between room temperature and a peak temperature of either 954°C (1750°F) or 1066°C (1950°F). Experimental weight change curves were obtained and used to determine the material constants in the coating life model. Once the model constants have been determined, COATLIFE was used to compute the aluminum content, volume fraction of  $\beta$ , and the remaining life of the coating as a function of thermal cycles.

Figure 2 shows a comparison of the calculated and measured weight change curves for thermal cycling between 25°C and a peak temperature of 1066°C in one-hour and half-hour cycles. The calculated and measured Al content in the coating as a function of thermal cycling between 25°C and 1066°C is shown in Fig. 3. The experimental values of Al content were calculated based on experimental values of the volume fraction and aluminum content of  $\beta$  and  $\gamma'$  in the coating. Model calculations with and without diffusion are presented in Fig. 3. The dash-dotted line shows that the model prediction without diffusion slightly overpredicts the Al content in the coating during thermal cycling. The COATLIFE model calculation with diffusion is shown as the solid curve in Fig. 3. This result was obtained by matching the calculation with diffusion to the experimental values of the Al content in order to establish the effective diffusion coefficient. Once the effective diffusion is calibrated at one temperature, the model can be used to predict the coating life at any other temperatures.

Comparison of the calculated and measured weight change curves for PtAl coating at two temperatures is shown in Fig. 4. The volume fraction of  $\beta$  in the platinum aluminide coating is compared against model calculations as a function of thermal cycle in Fig. 5 for the case of a maximum cycling temperature of 1066°C. Model calculations with and without inward diffusion are presented in Fig. 5, which shows the

model overpredicted the volume fraction of the  $\beta$  phase when inward diffusion was ignored. Agreement between model calculations and experimental data was improved when inward diffusion was included in the model, Fig. 5. This result indicates that inward diffusion was important and affected the life of the PtAl coating significantly.

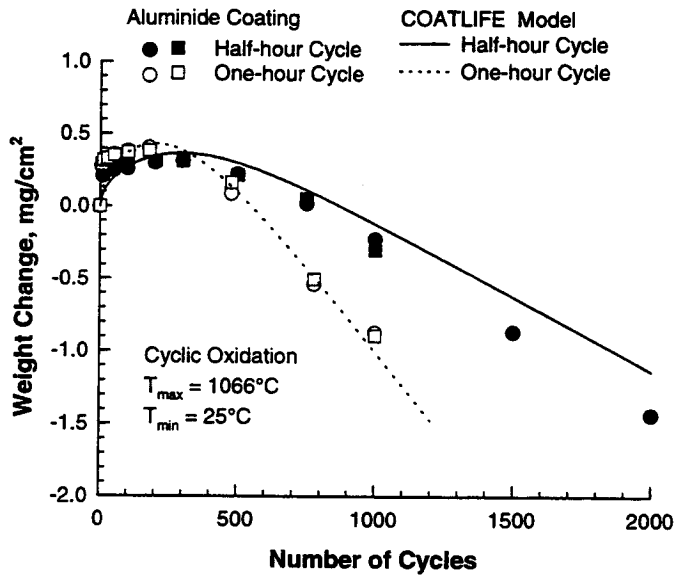


Figure 2. Experimental weight change data compared against model calculation for aluminide coated GTD-111.

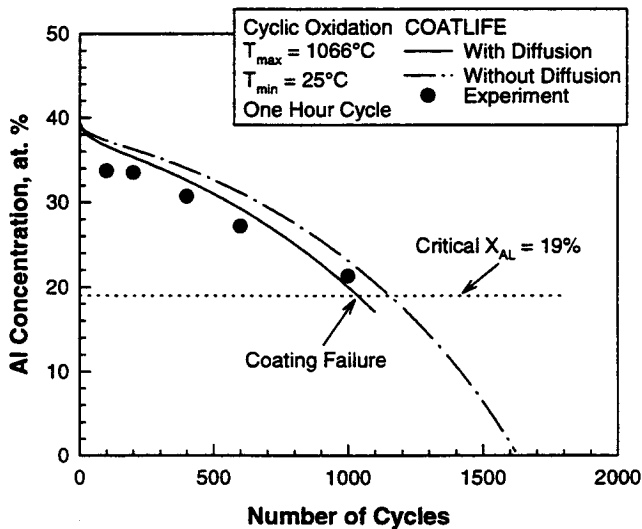


Figure 3. Comparison of calculated and observed Al content as a function of thermal cycles for aluminide-coated GTD-111.

A comparison of the calculated and measured weight change curves for MCrAlY coatings at 954° and 1066°C is presented in Fig. 6. Both experimental data were used to obtain the material constants in the oxidation kinetics and spallation equations. The Al content and volume

fraction of the  $\beta$  phase have been calculated; the result for the Al content is compared against experimental data in Fig. 7, which shows good agreement between model and experiment.

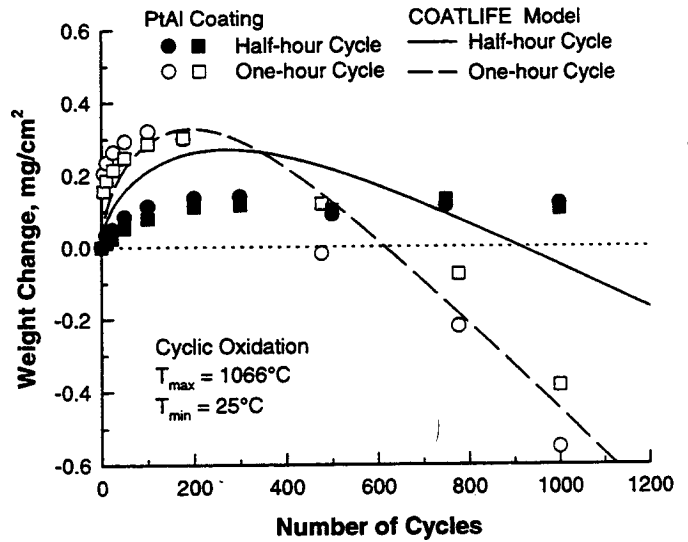


Figure 4. Experimental weight change data compared against model calculation for platinum aluminide-coated GTD-111.

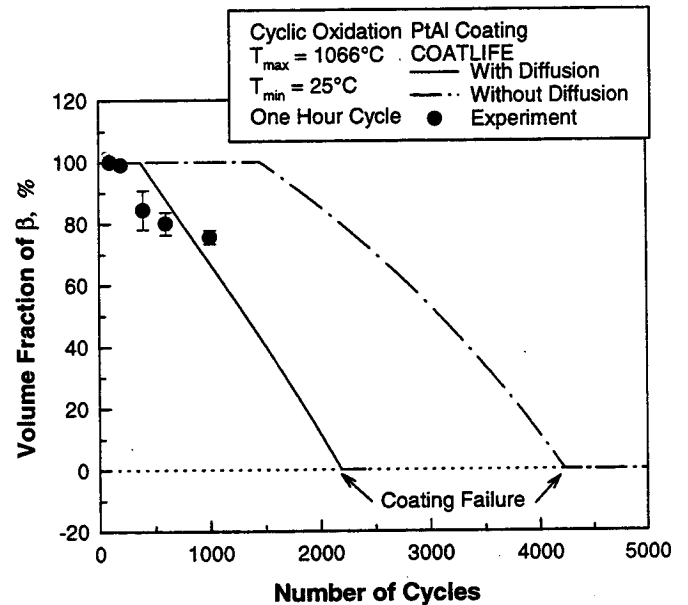


Figure 5. Calculated and measured values of the volume fraction of  $\beta$  as a function of thermal cycles for PtAl-coated GTD-111.

### COATING LIFE DIAGRAM

Once a set of model constants has been obtained for a coating, COATLIFE can be used to calculate the time to failure of the coating by varying the cycle time. The calculated values of the times-to-failure are

then divided by the cycle time to obtain the number of startup cycles to coating failure. A coating life diagram is then obtained by plotting the number of startups as a function of cycle time in a log-log plot. As an illustration, a coating life diagram calculated for MCrAlY coatings subjected to cycling between 25° and 1066°C is presented in Fig. 8. The solid line, calculated via COATLIFE, represents the failure boundary for the coating under the imposed temperature. The coating is protective when the number of startup cycles at a given cycle time, e.g., point P, is less than that of the failure boundary. Conversely, the coating has failed if the number of startup cycles exceeds the coating failure boundary, as illustrated by point F in Fig. 8. The coating life diagram thus provides a simple and rigorous means for forecasting the remaining life of a coating after it has been in service. The controlling failure mechanism along the coating failure boundary varies with cycle time and temperature. In general, oxidation and spallation dominate at short cycle times while oxidation and inward diffusion dominate at long cycle times. At intermediate cycle times, coating failure involves oxidation, spallation, and inward diffusion, as shown in Fig. 8.

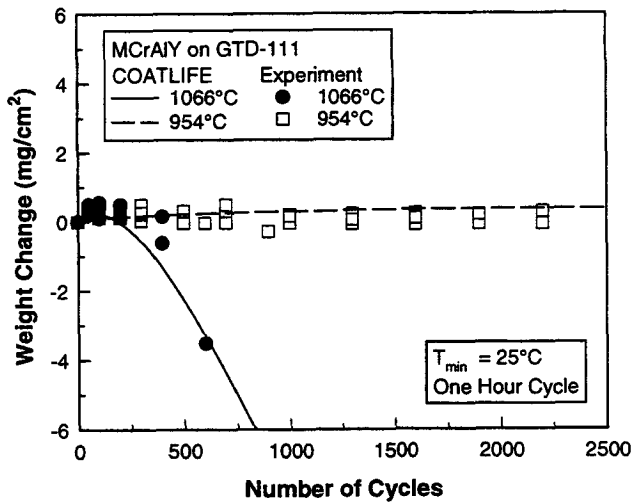


Figure 6. Experimental weight change data compared against model calculation for MCrAlY-coated GTD-111.

For illustration, Fig. 9 shows the coating life diagram calculated for PtAl coating on IN738 and compared against field data. The actual operating temperatures of the blades were not known but were estimated to be in the range of 870°C to 927°C. The coating life boundaries were computed for 870°C and 927°C and the results are shown as the solid and dotted lines, respectively. COATLIFE predicted that the coatings in these five blade are still functional and protective. EDS measurements indicated the Al content in the coatings ranged from 24% to 39%, which are in accord with model calculations. The remaining life of these coatings are represented by the difference in the number of startup cycles from their current positions to the failure boundary at a given cycle time.

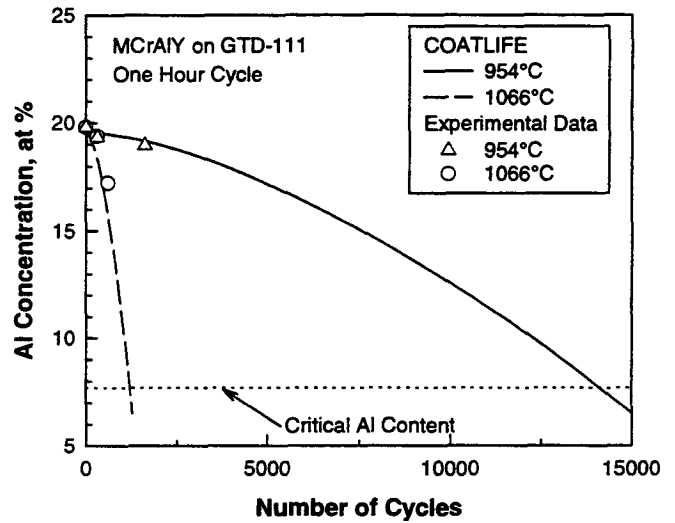


Figure 7. Computed and measured values of the Al content in MCrAlY-coated GTD-111.

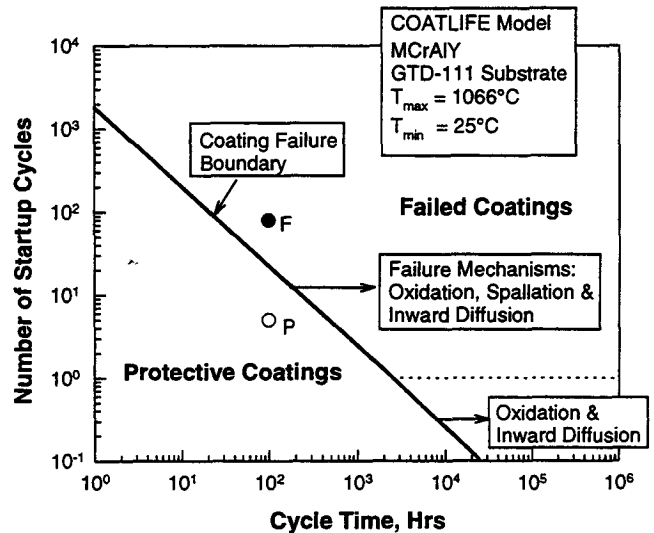


Figure 8. Coating life diagram calculated via COATLIFE shows the protective and failed regimes of MCrAlY-coated GTD-111.

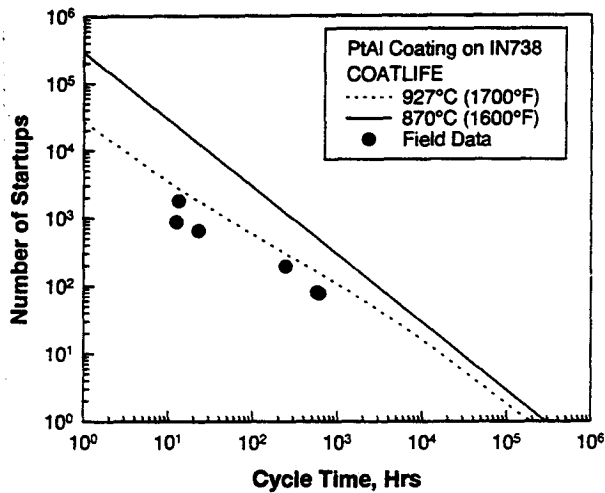


Figure 9. Calculated coating life diagram for PtAl-coated IN738 compared against field data.

### CONCLUSIONS

A recent coating life model, COATLIFE, has been extended to treat the effect of inward diffusion on coating life. Applications of the model for GTD-111 with MCrAlY, PtAl, and aluminide coatings are demonstrated using laboratory specimens. A life prediction methodology based on COATLIFE and a coating life diagram is introduced. The utility of the coating life diagram is explained and evaluated with a comparison of model calculations against field data for PtAl-coated IN738 blades. The result indicates that COATLIFE shows promise as a predictive tool for forecasting the useful life of combustion turbine coatings in service.

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