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Influence of bond coat thickness on the cyclic rumpling of thermally grown oxides

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Abstract

Recent experimental measurements have revealed that the amplitudes of undulations in the thermally grown oxide (TGO) formed on a bond coat subject to cyclic thermal histories depend on the bond coat thickness, h_{bc}, and exhibit a maximum when $h_{bc} \approx 100$ μm. The existing rumpling model does not predict the maximum. To account for this effect, the model has been extended to include finite substrate thickness. The embellished code predicts the maximum and demonstrates close correspondence between calculated and measured undulation amplitudes (provided that all of the strain misfits between the bond coat and substrate are included: thermal expansion, martensite transformation and swelling). The presence of the maximum is attributed to two opposing effects. When thin, the bond coat is unable to deform to the extent needed to accommodate the undulations in the TGO. Conversely, when it has finite thickness relative to the substrate, the strains induced in the substrate reduce the constraint imposed on the bond coat, again reducing its ability to accommodate the undulations.

Keywords: Thermal barriers; Creep; Multilayers; High-temperature deformation; Simulation

1. Introduction

Modern gas turbines use multilayer coatings for environmental and thermal protection. One layer, referred to as the bond coat, provides oxidation protection when its composition allows the formation of α-Al_2O_3 known as a thermally grown oxide (TGO). Many hot section turbine components incorporate such a layer, roughly 50 μm thick. During service, the TGO grows to about 5 μm. In many cases, an insulating oxide layer is superposed, referred to as a thermal barrier coating (TBC). This layer is typically yttria-stabilized zirconia. One of the preferred commercial bond coats consists of Pt(Ni) aluminide [1–6]. When this bond coat is used, upon thermal cycling, the TGO is susceptible to ratcheting, or rumpling (Fig. 1). Other bond coats are less susceptible [7]. When a TBC is superposed, the TGO displacements cause cracks to form (Fig. 1) [6]. The cracks grow on a cycle-by-cycle basis and eventually coalesce to form spalls.

A model that characterizes rumpling has been developed [8,9]. But, because of the highly non-linear nature of the phenomenon, many different (over 30) constituent properties are needed as input. Most of these properties can be (and have been) independently measured, as elaborated below. The two major consequences of the large number of parameters are as follows:

(i) It is inconceivable that an experimental matrix can be planned that isolates the constituent properties having the greatest influence on rumpling. Instead, reliance must be placed on the model.
(ii) Validation of the model is a challenging prospect because so many parameters must be independently measured.

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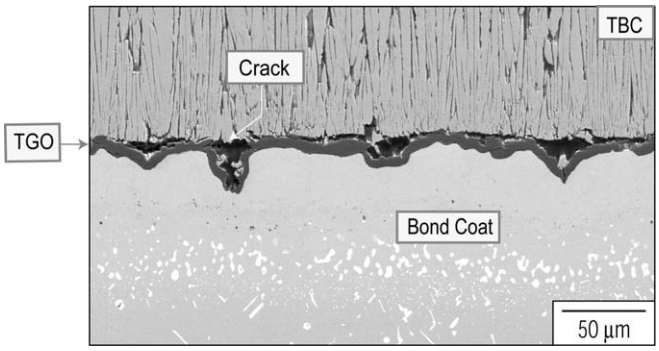

Fig. 1. TGO undulations in a thermally cycled system with a yttria-stabilized zirconia top coat and a Pt aluminide bond coat [3].

Two separate validation studies have been completed, with associated property measurements [10,11], resulting in sufficient confidence in the model that it has been successfully transitioned to the aero-turbine industry. The model is being used to conduct sensitivity studies and to predict rumpling rates over the wide range of thermal scenarios encountered in turbine airfoils. Nevertheless, as with any model, assessment and validation are continuing processes. Specifically, as distinctive new results emerge, the model should be used to assess possible shortcomings. The goal of the present article is to extend the model in a manner that enables it to reproduce recent experimental observations that the rumpling rate of aluminide bond coats depends on their thickness (Fig. 2) [12]. In this study, the thickness of the bond coat, h_{bc}, was systematically varied (by a thinning process), with all other characteristics remaining constant. The measurements were performed using a substrate with thickness $h_s = 3$ mm. The amplitude of the undulations induced upon thermal cycling (absent a thermal barrier oxide) varied with h_{bc} in the manner plotted in Fig. 2(a), exhibiting a maximum at $h_{bc} \approx 120$ μm. Simultaneously, the wavelength corresponding to the maximum amplitude increased slightly with an increase in h_{bc} (Fig. 2(b)).

A two-step process is used to extend the model:

(i) Establish the mechanics principles underlying an intrinsic bond coat thickness effect, consistent with Figs. 2(a) and (b).
(ii) Determine whether the model predicts undulation amplitudes similar to the measurements.

The experiments [12] were performed using (so-called) overlay bond coats, which differ from commercially used Pt aluminide coatings in their chemistry and microstructure. While the differences are not specified in the published articles [12,13], the results for the undulation amplitudes and the TGO thickness are reported [12] to be in the same range as those for commercial coatings. These similarities suggest that the parameters affecting undulation growth are comparable. Consequently, in the absence of independent property information for the overlay coatings, the numerical assessment is conducted using the material parameters previously determined for commercial coatings [11]. Discrepancies are attributed to this limitation.

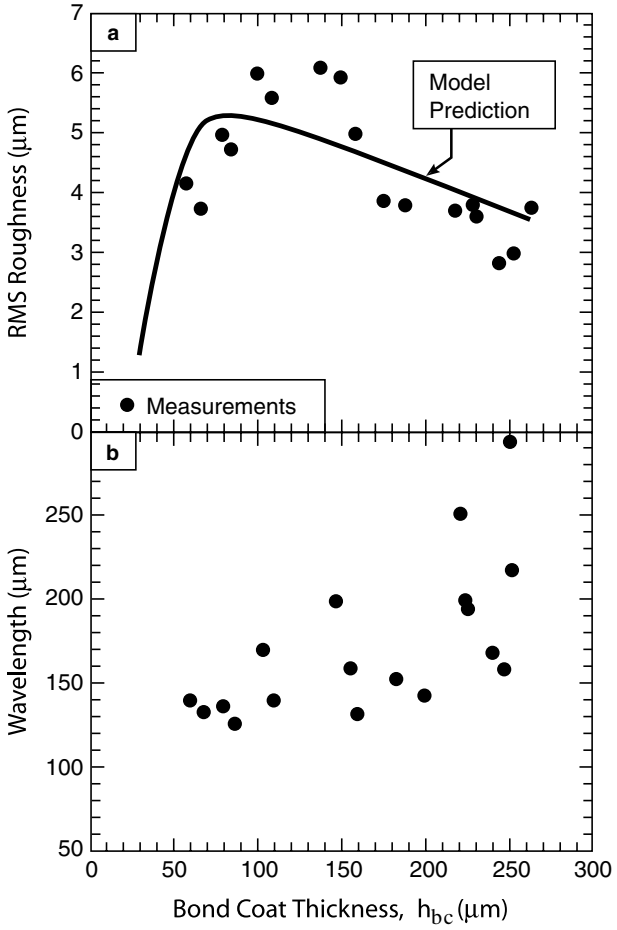

Fig. 2. Experimental observation that the rumpling rate of a Pt aluminide bond coat depends on its thickness [12]. The simulation result is superposed.

2. Synopsis of the model

In the model [8,9], the layers are modelled individually. The result is a set of coupled, ordinary non-linear differential equations that can be readily solved numerically. Changes in the TGO stress due to lateral growth, overall lengthening and thermal mismatch are taken into account. At the beginning, the TGO has an initial sinusoidal undulation with amplitude δ_0 and fixed wavelength $2L$. The undulation gives rise to a sinusoidal normal traction at the interface, which deforms the creeping bond coat, causing the undulation to grow if the film is under compression.

The treatment of the TGO in the model merits comment. During growth, the TGO not only thickens, but also elongates at a strain rate that produces a compressive stress [14]. This growth stress is a measure of the creep strength of the TGO at the elongation strain rate. In practice, it is measured in situ at the growth temperature [15]. The stress is $\sigma_g \approx -300 \pm 100$ MPa for the TGO that forms on Pt alu-

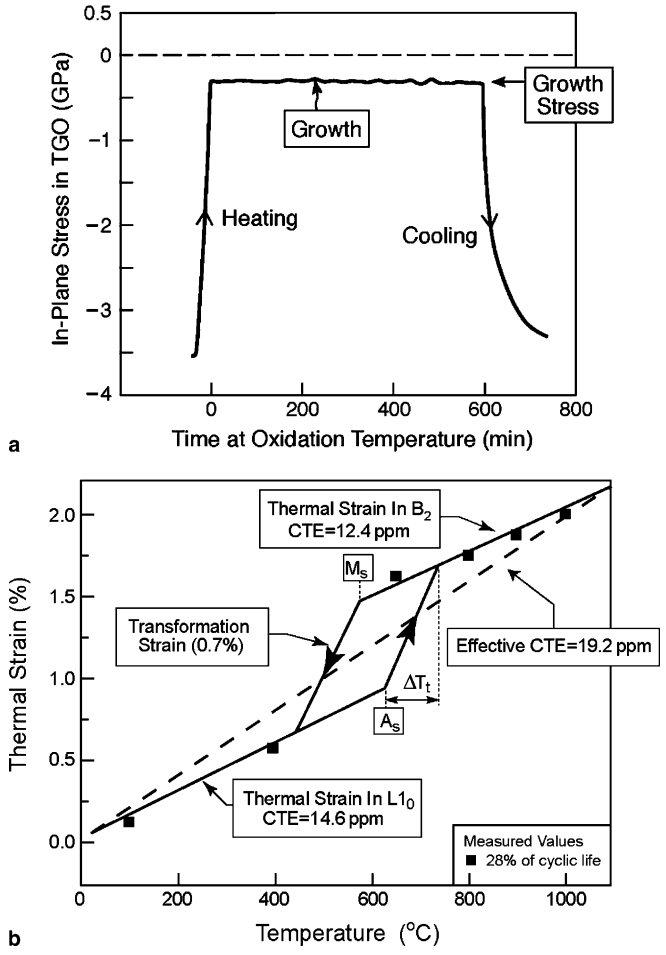

Fig. 3. (a) Growth stress in a TGO on a Pt aluminide bond coat [15]. (b) Martensite transformation in a Pt aluminide bond coat [19].

minide (Fig. 3(a)) [15,16]. This behaviour can be faithfully incorporated in the model by assigning the TGO a strength $\sigma_Y^{\mathrm{tgo}} = \sigma_g$ at the growth temperature, and elastic at all other temperatures [8,9,12]. Its thermoelastic properties are $E = 375$ GPa, $\nu = 0.2$ and $\alpha = 8.5 \times 10^{-6}\ ^{\circ}\mathrm{C}^{-1}$. Based on prior assessments, the lateral growth strain rate is taken to be proportional to the rate of thickening [17,18], with average 0.5×10^{-3} per cycle.

The Pt aluminide bond coats experience various strain misfits with the substrate that radically affect rumpling by enhancing creep. It is essential to incorporate these strains into the simulations. Three misfits are important. (a) Thermal expansion misfit with the substrate. (b) A martensite transformation having the strain characteristics depicted in Fig. 3(b) [19]. In general, the martensite start temperature, M_s, is a parameter. (c) This bond coat is susceptible to swelling due to a flux of Ni from the substrate [13] (Fig. 4). The swelling strain rate is a parameter in the model. The volume change accompanying the martensite transformation is incorporated by using an effective thermal expansion coefficient of $86 \times 10^{-6}\ ^{\circ}\mathrm{C}^{-1}$ between 600 and 700 °C on heat-up, and between 550 and 450 °C on cool-down, giving a 0.7% linear strain change relative to the substrate over

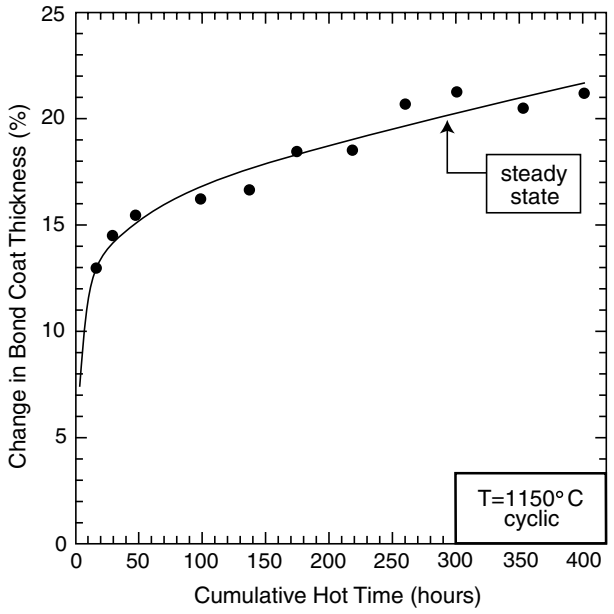

Fig. 4. Bond coat swelling observed as a change in bond coat thickness with high-temperature exposure [13].

a span of 100 °C (Fig. 3(b)) [19]. To deduce the creep strains that accommodate the TGO undulations, power law creep data for the bond coat [20] are incorporated, characterized by a reference strain rate $\dot{\varepsilon}_R = 0.2\ \mathrm{s}^{-1}$, reference temperature $T_R = 1.5 \times 10^4$ K, reference stress $\sigma_R = 25$ MPa and power law exponent $n = 4$. Its elastic properties are: $E = 115$ MPa, $\nu = 0.27$ and $\alpha = 16 \times 10^{-6}\ ^{\circ}\mathrm{C}^{-1}$. The underlying superalloy is modelled as elastically isotropic with $E = 200$ GPa, $\nu = 0.3$ and $\alpha = 16 \times 10^{-6}\ ^{\circ}\mathrm{C}^{-1}$.

The initial state includes a thin TGO (0.5 μm) subject to in-plane stress, $\sigma_g \approx -300$ MPa, while the bond coat and substrate are stress-free. The system is subject to a cyclic thermal history that begins at 1150 °C, is then cooled to room temperature in 1 min, reheated to 1150 °C, also in 1 min, and subsequently held for 1 h. The cycle is repeated 100 times causing the TGO to thicken from 0.5 to 3 μm. The model [9] is enhanced in two ways for this study:

(i) The perturbation solution for the undulation growth rate is adapted to a bond coat of finite thickness. The lower boundary with the substrate is constrained to remain straight such that the interface undulation is zero, consistent with the significantly higher creep strength of the substrate (relative to the bond coat).
(ii) The effect of substrate thickness was added to the formulation by incorporating expressions for the in-plane thermal mismatch stresses in each of the three layers, derived assuming a finite-thickness substrate.

3. General assessment

Initially, the model is used to probe a range of parameter space. Such an assessment is necessary since the initial

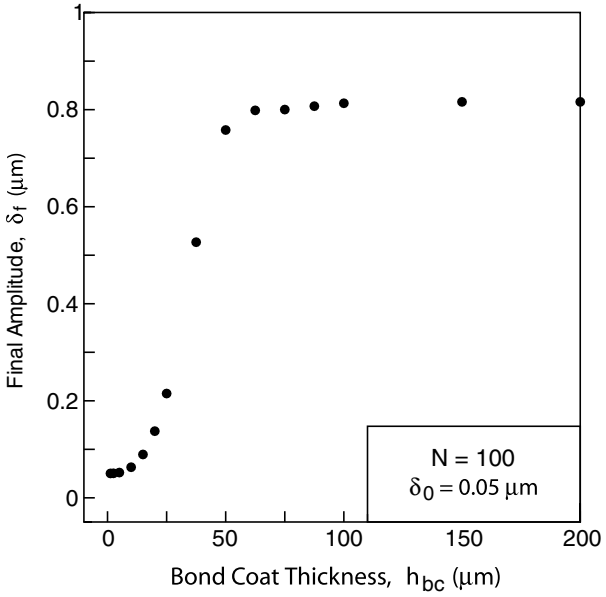

Fig. 5. Variation of the final undulation amplitude with bond coat thickness as predicted by the model with an infinitely deep substrate.

imperfections are unknown and because, for the specific bond coat composition used by Tolpygo and Clarke [12], the martensite start temperature, as well as the swelling rate, are uncertain. As previously mentioned, the transformation strains depicted in Fig. 3 are used in the calculations and swelling is incorporated in accordance with Fig. 4. Preliminary results are presented for a semi-infinite substrate with sinusoidal imperfections having wavelength $2L = 100$ μm and small initial amplitude ($\delta_0 = 0.05$ μm). The trends (Fig. 5) indicate that, when the bond coat thickness h_{bc} is large, the undulation amplitude at the conclusion of thermal cycling, δ_f, is invariant with bond coat thickness. But, when $h_{bc} < 100$ μm, δ_f decreases, such that $\Delta\delta \to 0$ as $h_{bc} \to 0$. The thinness effect is attributed to the constraint imposed by the substrate on the creep strains in the bond coat occurring in the vicinity of the TGO undulations. That is, thinness reduces the capacity of the bond coat to accommodate permanent changes in the amplitude of the undulations through creep. The predicted rumpling characteristics are thus consistent with the measurements at small h_{bc} (Fig. 2(a)), but differ for large h_{bc}.

The deviation between measurements and these calculations is attributed to an influence of the substrate thickness. Namely, the bond coat induces a net in-plane strain in the substrate when sufficiently thin. In turn, this strain reduces the constraint that the substrate imposes on the creep deformation of the bond coat. To examine this feature, results are obtained with a 3 mm thick substrate (that used in the experiments [12]). The trends obtained using the same input parameters are presented in Fig. 6. The results reveal that the undulation growth rate now decreases as the bond coat becomes thicker, reproducing the trends found experimentally. However, the actual amplitude changes are sensitive to (among other parameters) the wavelength of the undulations, as well as their initial amplitude. Detailed comparisons between predictions and simulations thus await the additional sensitivity assessments described next.

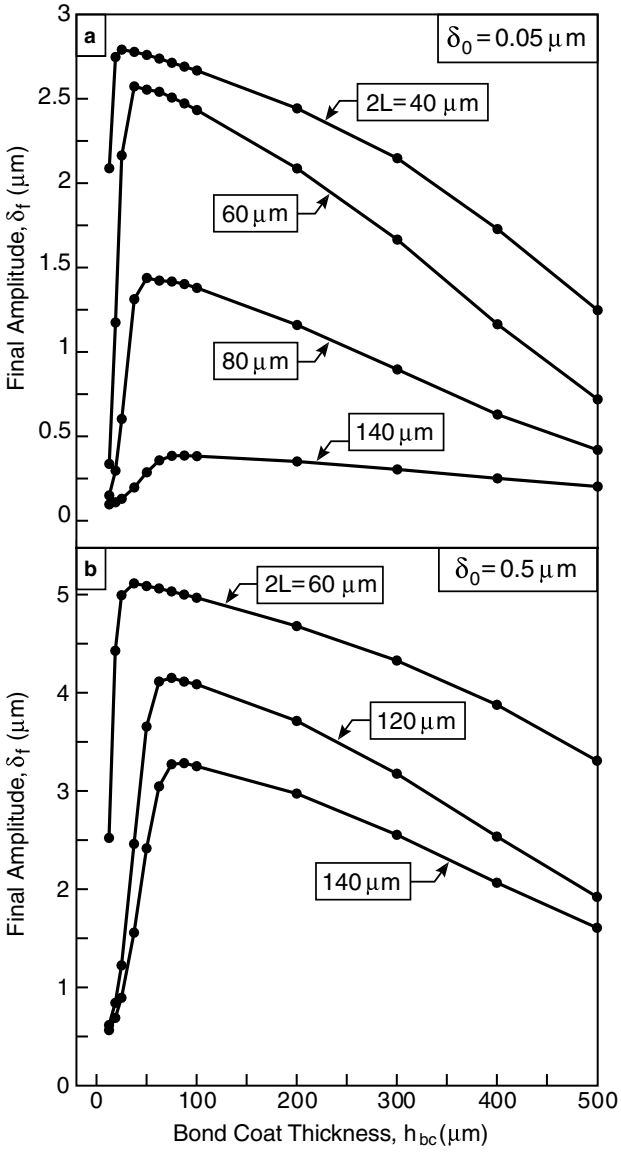

Fig. 6. Variation of the final undulation amplitude with bond coat thickness, for various initial undulation shapes, as predicted by the model with a finite thickness substrate. Swelling is not included.

The trend with initial amplitude (Fig. 7), for $2L = 100$ μm, indicates that the final amplitudes only become comparable to the measurements (Fig. 2) when $\delta_0 > 0.3$ μm. Consequently, $\delta_0 = 0.5$ μm is used in the ensuing detailed assessment. The relative roles of the martensite transformation and of swelling are summarized in Fig. 8 for two different wavelengths. In the absence of the strain misfits from both the martensite transformation and swelling, the undulation growth is negligible. The influence of swelling without martensite has been ascertained by cycling between 950 °C (above the transformation temperature) and 1150 °C. Undulations develop, but they are much smaller than those found experimentally (Fig. 2). The incorporation of the transformation and swelling strains

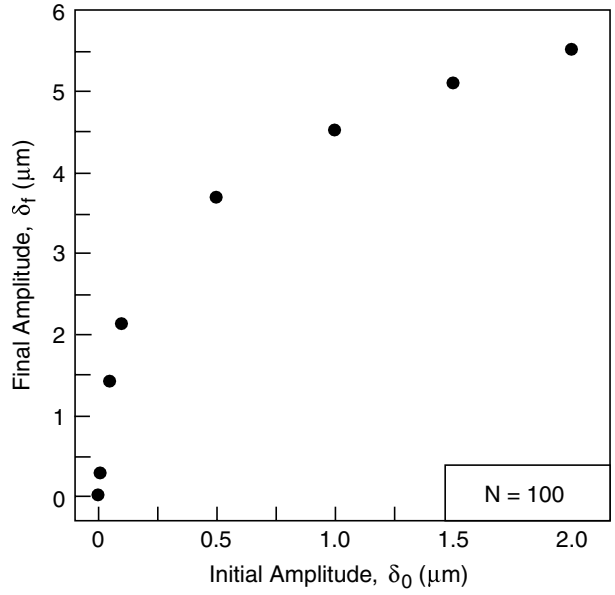

Fig. 7. Variation of the final undulation amplitude with initial amplitude.

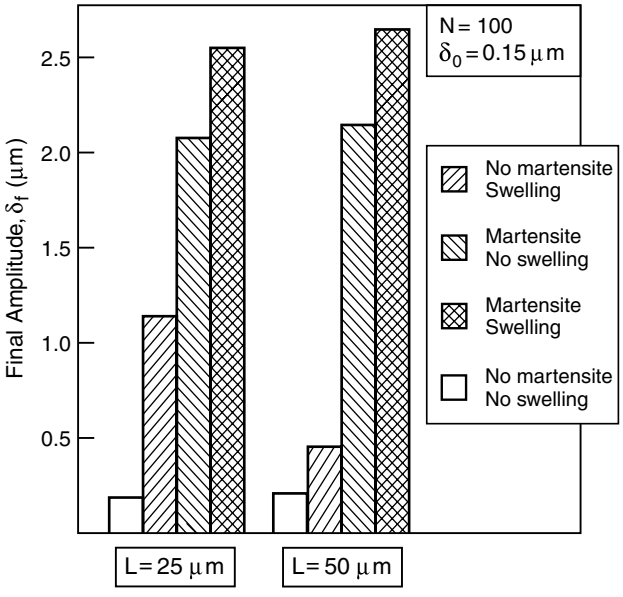

Fig. 8. Comparison of final undulation amplitude with and without swelling and martensite. Results are shown for two wavelengths.

rectifies the discrepancy. While the larger contribution is that attributed to martensite (especially at the larger wavelength), nevertheless, to attain amplitudes that match the measurements, both the martensite and swelling contributions are required. The assessment described in the next section is thus conducted with both misfits incorporated.

4. Detailed comparisons between measurements and simulations

Based on the insights gained from the general assessment, the detailed comparison is conducted in the following manner. The initial undulation amplitude ($\delta_0 =$

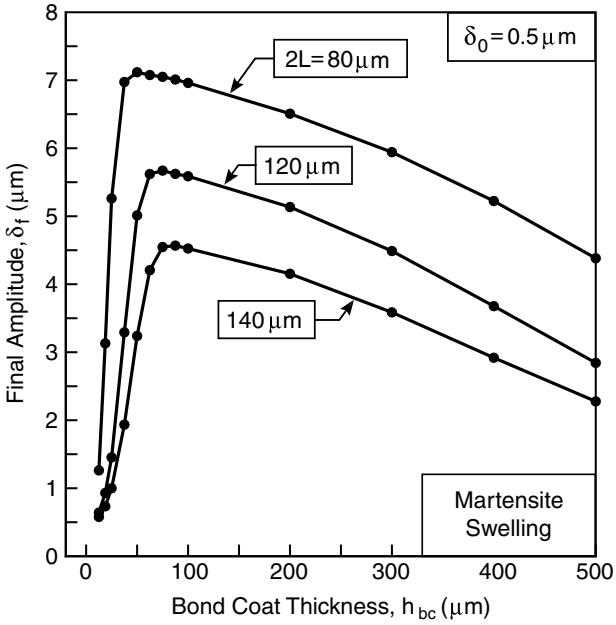

Fig. 9. Variation of the final undulation amplitude with bond coat thickness, for various initial undulation shapes, as predicted by the model with a finite thickness substrate. Swelling is included.

0.5 μm) and wavelengths ($2L = 60$–140 μm) are chosen to give final amplitudes in the requisite range. The trends are ascertained as a function of bond coat thickness for cases that include both the martensite transformation and the swelling (Fig. 9). Overlaying the predictions with the measurements (Fig. 2(a)) indicates that the model captures the general features quite well within the measurement uncertainty, given the lack of independent information about M_s and the initial imperfections. There is a small discrepancy in the wavelength. To achieve amplitudes comparable to the measurements, the model requires that $2L \approx 120$ μm, whereas the measurements indicate a wavelength $2L \approx 150$ μm. This difference is undoubtedly related to the choice of material parameters used in the simulations, which has been based on those for the commercial Pt aluminide coatings, not the overlay coatings used in the experimental investigation [12].

5. Concluding remarks

Recent observations have revealed that the bond coat and substrate thickness affect TGO rumpling [12]. Most notably, the undulations exhibit maximum amplitude at a bond coat thickness $h_{bc} \approx 100$ μm. To provide a basic understanding of this effect, a rumpling model [8,9] has been extended by incorporating finite substrate thickness. The presence of the maximum is attributed to two opposing effects. When the bond coat is thin, it is unable to deform to the extent needed to accommodate the undulations in the TGO. Conversely, at a finite fraction of the substrate thickness, the strains induced in the substrate reduce the constraint imposed on the bond coat, again reducing its ability to accommodate the undulations.

Close correspondence between the calculated and measured undulation amplitudes has been demonstrated, provided that all of the strain misfits between the bond coat and substrate are included: thermal expansion, martensite transformation and swelling. Small differences are attributed to the choice of material parameters used in the simulations, based on those for the commercial Pt aluminide coatings, not the overlay coatings used in the experimental investigation.

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