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On the elastic and creep stress analysis modeling in the oxide scale/metal substrate system due to oxidation growth strain

J.L. Ruan [a], Yongmao Pei [b], Daining Fang [a,b,*]

[a] AML, Department of Engineering Mechanics, Tsinghua University, Beijing 100084, China
[b] LTCS, College of Engineering, Peking University, Beijing 100871, China

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ABSTRACT

Considering the case of asymmetric oxidation, new elastic and creep analysis models are developed to elucidate the stress evolutions in an oxide scale/metal substrate system during isothermal oxidation, due to the oxidation growth strain in oxide scale. The theoretical works allow for the experimental inference of growth strain and stresses from the curvature measurements during oxidation. Moreover, they provide ways to explore and identify the main mechanisms for oxidation. Two sets of published experimental data are employed and analyzed by the elastic and creep analytical approaches. A novel simple determination method of the growth parameter is proposed and validated.

1. Introduction

High-temperature metals and alloys that operate in demanding high-temperature oxidizing environments are widely used as structural components in many applications, such as aircraft propulsion, power generation, and marine propulsion. They rely on thermal grown oxide (TGO), commonly alumina, for corrosion protection. Strains that develop in TGO during operating can reduce the protectiveness of the TGO [1]. However, despite decades of effect, the occurrence and evolution of growth strains in TGO, and mechanisms that cause them, are poorly understood [2]. Hence, knowledge of the growth strain in TGO and the accompanying stress generation and relaxation in oxide/metal systems during high-temperature oxidation is essential in order to evaluate their integrity.

Nowadays, there have been a number of attempts made to measure the growth strains and stresses, including X-ray diffraction [3–5], deflection test in monofacial oxidation (DTMO) [6–10], Raman spectroscopy [11,12], photoluminescence piezospectroscopy [13,14], and synchrotron X-ray diffraction [2,15–17]. In spite of the advantages and limitations of those methods, the measurement results are with little success [2], the reported values of stress range from 1.7 GPa compressive [18] to 0.5 GPa, or more, tensile [19]. Because of its simplistic nature, curvature-based technique for the measurement of stress in thin film/substrate systems is traditionally the most widely acknowledged method [20–23]. Many measurement schemes have been made to improve and enhance this technique. For example, Rosakis et al. [24] introduced coherent gradient sensing (CGS) as an optical, full-field, real-time, in situ, non-intrusive and non-contact technique for the instantaneous measurement of curvature and curvature changes in thin film structures.

Although the existence of a stress accompanying the growth of the oxide has been known for many years and is manifest in many ways as described above, the origin of oxidation growth strain and stress has intrigued investigators for many years [25]. Huntz and Pieraggi [26] summarized several main possible origins for the growth strain during isothermal oxidation. Among them, the Pilling and Bedworth approach (incompatibility of the molar volumes) [27] and the formation of new oxide in the preexisting oxide grain boundaries [25,28,29] are the well-known models to describe the growth mechanism during oxidation. Furthermore, Rhines and Wolf [28] indicated that it was necessary to take explicitly into account elements of the microstructure. Now many models with a microstructural origin exist [29–34], with their own advantages and disadvantages. Recently, Clarke [25] and Panicaud et al. [35] successively developed models based on a microstructural approach and on a general thermodynamical explanation, respectively. They both demonstrated that the lateral growth strain rate increased linearly with the oxide thickening rate during isothermal oxidation, namely Clarke model. This model is acknowledged and used by many authors [36–40].

At the same time, much work has been undertaken to investigate the accompanying stress generation and relaxation process

* Corresponding author at: LTCS, College of Engineering, Peking University, Beijing 100871, China. Tel.: +86 10 62772923; fax: +86 10 62781824.
E-mail addresses: fangdn@pku.edu.cn, fangdn@mail.tsinghua.edu.cn (D. Fang).

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during oxidation. Although there have been a number of techniques made to measure the growth stresses as mentioned above, credible methods of stress analysis are still scarce. Among them, most analyses are about deflection test and have assumed either elastic [6,7,41–43] or athermal plastic [7,44] deformation. Under most oxidation temperature conditions, it is much more likely that deformation will occur by thermally activated creep processes. This was firstly accomplished by Evans [45], who provided a stress analysis of deflection test assuming nonlinear creep deformation of both oxide and metal phases. He adopted two neutral axes of the metal and oxide to express strains in them. Recently, in accordance with Evans' approach and in conjunction with the growth strain based on the Clarke model, Maharjan et al. [39] proposed an analytical modeling of residual stress for the metal/oxide composite of the deflection test. However, in order to simplify and solve the problem, elastic strain rate is not considered in both their works [39,45], which may play an important role in the stress evolutions as performed by Veal et al. [2], so their analyses may lead to inexact results. Furthermore, in their approach, people need to solve simultaneously a set of two nonlinear and complex equations by a rather sophisticated numerical method to determine the positions of the two neutral axes and then to obtain the stress solutions, which makes the use of their approach relatively difficult [10]. There are several other creep analysis models of the modified deflection test [46,47], yet have assumed uniform oxide stress distribution and also not considered elastic strain rate.

The purpose of this paper is to develop an integrated theoretical framework, including an elastic analysis model and a creep analysis model, for the more precise and efficient description of stress evolutions in the oxide scale/metal substrate system during isothermal oxidation process and for some explorations of the main mechanisms for oxidation. The relations between the growth strain and system curvature, and between the system stresses and system curvature are derived, which will allow for the accurate experimental inference of such growth strain and stresses from the real-time and in situ curvature measurements during oxidation by curvature-based technique. First, an elastic analysis model of the stress evolutions is proposed, and some explicit and simple expressions are acquired to calculate the growth strain and stresses for preliminary analysis and evaluation. Second, a creep analysis model of the stress evolutions that particularly considers the elastic strain rate in both oxide and metal phases is developed, and the forward Euler method is adopted. It realizes our goal of providing a precise and efficient means for the description of realistic stress evolutions in the oxide scale/metal substrate system. Finally, two sets of published experimental data are employed and analyzed by the elastic and creep analytical approaches, and some curves and conclusions are obtained.

2. Modeling approach

For the case of asymmetric oxidation, attention will be focused on a system with a circular metal or alloy substrate of diameter $2R$, and isothermal oxidation is only happening on the top surface of this substrate. Meanwhile, the other surfaces are perfectly protected by oxidation-resistant coatings, which can be ignored in the model analysis. A polar section of the system is shown in Fig. 1, with the oxide scale and substrate thicknesses labeled as $h_o(t)$ and $h_s(t)$, respectively, here and below the subscripts "o" and "s", respectively, denote the oxide scale and substrate, t is the time. Cylindrical coordinates (r, θ, z) are adopted with the origin on the center of the bottom surface of substrate, and z axis is perpendicular to the bottom surface and points to the oxide scale as shown. The total thickness of system is $h(t) = h_s(t) + h_o(t)$. Both the oxide scale and metal substrate are assumed to be homogeneous isotropic materials, and the deformation is assumed axisymmetric.

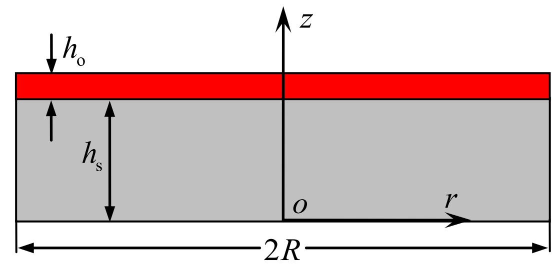

Fig. 1. Schematic diagram of the oxide scale/metal substrate system.

2.1. Elastic analysis of stress evolution

For the time being, it will be assumed that only linear and elastic deformations are occurring in both oxide and metal phases. A schematic illustration of the oxide scale/metal substrate system at different stages of oxidation is given in Fig. 2 (a) (based on the symmetry, only one-half of the polar section is shown).

When a metal is exposed to a high-temperature oxidizing atmosphere, an oxide scale generally appears at its surface. The growing process is accompanied by the growth strain. According to Clarke model [25,35], the growth strain rate is proportional to the oxide growth rate, that is,

$$\dot{\varepsilon}_g(t) = D_o \dot{h}_o(t) \tag{1}$$

where a superposed dot denotes differentiation with respect to time t, ε_g represents the lateral growth strain in the oxide scale, that would occur if no constraints were imposed [25]. Growth parameter D_o may depend on microscopic, microstructural, and kinetic parameters. It should be noted that, since the growth parameter D_o is unknown and the oxidation growth strain mechanism is sophisticated, Eq. (1) is not directly used in this paper; on the contrary, it should be inferred from experiments and the Clarke model needs to be confirmed.

As a matter of fact, the oxide scale is adherent to the metal substrate, so the oxide scale cannot be free to expand laterally. The substrate constraint will produce in-plane elastic strain ε^e and corresponding elastic stress in the oxide scale/metal substrate system as shown in Fig. 2 (a). Finally, together with the thermal expansion strain, the actual total strains in system due to high-temperature oxidation are

$$\begin{aligned} &\varepsilon_s(z,t) = \varepsilon_s^e(z,t) + \alpha_s \Delta T \quad 0 < z < h_s \\ &\varepsilon_o(z,t) = \varepsilon_o^e(z,t) + \alpha_o \Delta T + \varepsilon_g(t) \quad h_s < z < h \end{aligned} \tag{2}$$

where α is the linear thermal expansion coefficient and ΔT is the temperature change.

Under such above strain field, the oxide scale/metal substrate system will deform, leading to stress redistribution within the system and releasing part of the oxidation stresses. It is assumed that the system releases stresses only by the system curvature changes, and any nonlinear stress relaxation mechanisms, such as recrystallization, phase transition, misfit dislocations and creep deformation, are not considered here. From the classical plate theory analysis [48], the total strains in oxide scale and metal substrate can be expressed as

$$\begin{aligned} &\varepsilon_s(z,t) = \varepsilon_0(t) + \kappa(t) z \quad 0 < z < h_s \\ &\varepsilon_o(z,t) = \varepsilon_0(t) + \kappa(t) z \quad h_s < z < h \end{aligned} \tag{3}$$

where ε_0 is taken to be the reference strain at the bottom surface of substrate and κ represents the curvature of system.