STRESS DISTRIBUTION AT METAL-OXIDE INTERFACE DURING HIGH-TEMPERATURE OXIDATION

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ABSTRACT

Fe-Cr based alloys such as stainless steels are widely used thanks to its superior corrosion resistance by forming stable passive chromium oxide film. However, in high temperature environment, incompatibility between substrate and oxide layer induces residual stresses as oxide layer grows. These stresses may result in spallation or cracking of oxide layer ultimately compromising loss of corrosion resistance. This study estimates stress distributions using commercial finite element software Abaqus/Standard enhanced with a custom UMAT subroutine.

KEY WORDS

High temperature oxidation, Thermomechanical model, Fe-Cr alloy, finite element analysis

1. INTRODUCTION

Fe-Cr based alloys are among the most commonly used materials due to their superior corrosion resistance by forming stable Cr_2O_3 film in general. However, in high-temperature environments, maintaining this protective film becomes challenging. Elevated temperatures accelerate oxidation, leading to thickening of the oxide scale. As Cr_2O_3 film grows from the surface, incompatibility between substrate and oxide film forms residual stresses. These stresses can lead to failure such as spallation or cracking of the oxide layer, which ultimately reduce corrosion resistance[1]. This failure can affect the lifetime of metal or even structure. Therefore, the presence of residual stress during high temperatures has been studied for a long time. However, many of the studies relies on experimental data that taken after cooling. This approach requires calculations to estimate stresses during experiments.

In this study, it is tried to conduct simulation of stress and strain evolution at the oxide-substrate interface during high temperature oxidation using finite element analysis (FEA). The finite element software that we used is Abaqus, which is superior for simulating high temperature oxidation phenomena by applying full thermomechanical model. Moreover, UMAT subroutine, which stands for User Material, invokes during calculations so we can consider stress differences for each spatial location.

2. THEORETICAL BACKGROUND FOR THERMOMECHANICAL MODELLING

In this section, we present the theoretical foundation for simulating high-temperature oxidation that has been studied in previous works[2-3]. To clearly implement the equations, strain decomposition by phase is shown in Fig. 1.

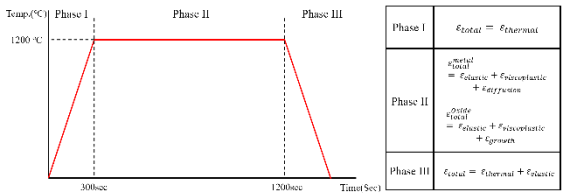

Fig. 1: Strain decomposition by phase.

The following subsections detail each equation used in this study:

2.1 Elastic strain

The elasticity for isotropic isothermal can be described by Hooke's model as in Eq. (1) with Lame's constants:

$$\sigma_{ij} = \lambda\delta_{ij}\varepsilon_{kk} + 2\mu\varepsilon_{ij} \tag{1}$$

This can be implemented as Jaumann rate equation by integrating in a corotational framework:

$$\Delta\sigma^{J}_{ij} = \lambda\delta_{ij}\Delta\varepsilon_{kk} + 2\mu\Delta\varepsilon_{ij} \tag{2}$$

2.2 Creep strain

A Norton-Hoff power law is used for creep strain:

$$\varepsilon_{creep} = sign(\sigma)J|\sigma|^{N} \tag{3}$$

Where J stands for creep parameter and N is the Norton exponents.

2.3 Thermal strain

Difference between temperature generates thermal stress during simulation. For thermal strain, classical thermal equation is being used:

$$\varepsilon_{thermal} = \alpha(\Delta T) \tag{4}$$

Thermal expansion coefficient α should vary with temperature. However, we assume that it is constant in this study.

2.4 Diffusion strain

As oxidation continues, chrome diffuses from metal to form chrome oxide. Nevertheless, the diffusion leads to changing lattice spacing that can generate strain especially near the metal surface:

$$\varepsilon_{diffusion}(z) = \eta([Cr](z,t) - [Cr]_i)\bar{\bar{I}} \quad (5)$$

Where η is constant coefficient coupling the chromium concentration profiles to the diffusion strain. $[Cr](z,t)$ is chromium concentration profiles as function of z. $[Cr]_i$ is initial chromium concentration which is 16.0 in this study. $\bar{\bar{I}}$ is second-rank identity tensor of dimension 3.

2.5 Growth strain

During the oxidation process, we assume that thickness of oxide grows as follows:

$$h_{ox} = A_p\sqrt{t} \quad (6)$$

For oxide growth strain, we consider Clarke relation that has been studied in previous work:

$$\varepsilon_{growth} = D_{ox} * h_{ox} \quad (7)$$

Where D_{ox} is the parameter for growth strain. D_{ox} is varies with temperature following Arrhenius relation. For simplified calculations, the parameter is assumed to be constant.

2.6 Thermomechanical modeling

We assume there are no non-linear mechanical phenomena such as buckling, spallation, etc. Furthermore, two-dimensional behavior is also neglected. With these assumptions, we can possibly prove the continuity of strain. With the proposed strain decomposition, we can propose the relation between metal and oxide that leads to:

$$(\varepsilon_{elastic} + \varepsilon_{creep} + \varepsilon_{thermal} + \varepsilon_{diffusion})_m = (\varepsilon_{elastic} + \varepsilon_{creep} + \varepsilon_{thermal} + \varepsilon_{growth})_{ox} \quad (8)$$

3. ABAQUS IMPLEMENTATION

The simulated geometry is a single 1 x 1 x 1μm cubic part, partitioning top of 0.1μm for oxide layer. The input parameters used in simulation are shown in Table. 1

Table 1: Input material properties[2,4-6]

Parameter	Metal	Oxide
E (MPa)	200,000	231,000
ν	0.285	0.29
N	1	1
J ($MPa^{-1}s^{-1}$)	1.2e-10	1.2e-10
$\alpha(K^{-1})$	11e-6	3e-5
η	-0.01	-

As shown in Fig 1, the simulation process consists of three steps. The detailed schematic for model implementation is illustrated in Fig. 2

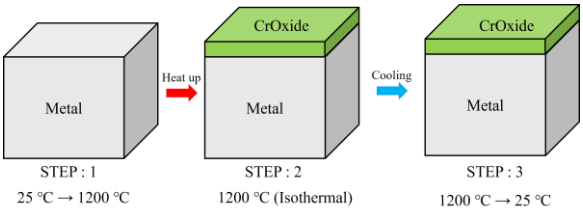

Fig 2: Schematic of step definition

4. CONCLUSION

This study addresses the use of finite element method to predict stress distribution during high temperature oxidation. The current modeling work has some limitations on, for example, material properties. Resolving these limitations in future work is essential to improve model accuracy. Additionally, validating the model through comparisons with experimental data is necessary. Despite these limitations, this work is beneficial to propose spatial stress distribution during high temperature oxidation, particularly at the interface between oxide and metal. Since damage often initiates at this interface, analyzing localized stress may contribute to predicting material lifetime.

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