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Finite Element Analysis of Stress Evolution at Metal-Oxide Interface during High Temperature Oxidation

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1. Introduction

Maintaining the structural integrity of materials in high-temperature environments is a critical challenge for ensuring the long-term reliability of materials. Many structural alloys are designed to maintain corrosion resistance by forming a stable, protective oxide film which acts as a diffusion barrier against further degradation. However, at elevated temperatures, the stability of this protective scale is frequently compromised. The primary driver of this instability is the mismatch in thermomechanical properties such as the coefficient of thermal expansion between the oxide layer and the underlying metal substrate. As the oxide film thickens, these incompatibilities generate significant residual stresses that can lead to mechanical failures, including cracking or spallation [1].

Understanding and analyzing the spatial distribution of these stresses is essential for predicting material service lifetimes. Despite its importance, obtaining in-situ data during high-temperature oxidation is remarkably difficult because the extreme conditions often exceed the operational limits of standard analytical equipment. Consequently, many existing studies are forced to rely on ex-situ experimental data gathered after the material has cooled, which requires complex back-calculations to estimate the stress states present during the actual oxidation process.

To overcome these experimental limitations, this study utilizes Finite Element Analysis (FEA) to simulate stress and strain evolution at the metal-oxide interface. Using Abaqus/Standard [2], we implemented a comprehensive thermomechanical model via a UMAT (User Material) subroutine. This computational approach allows for the precise calculation of localized stress concentrations that are otherwise inaccessible.

The present work focuses on the Verification and Validation (V&V) of this model using a NiCr alloy system as a benchmark. By replicating established theoretical frameworks, we aim to establish a robust numerical foundation. This validated framework will serve as the basis for future work extending the analysis to FeCr based systems which are widely used in nuclear industry.

2. Thermomechanical Model V&V

To establish a reliable computational framework, it is imperative to conduct a rigorous verification and validation procedure. Verification serves to ensure that the mathematical model is implemented correctly and that the numerical solution is stable and independent of the discretization parameters, such as mesh density. Validation, on the other hand, assesses the degree to which the computational model provides an accurate representation of the real-world physical phenomena by comparing the simulation results with established experimental or high-fidelity benchmark data. In this study, we utilize the NiCr system as a primary benchmark to confirm the robustness of our thermomechanical model.

2.1 Abaqus implementation

The computational domain for this analysis is a 20 * 20 * 20 μm cubic representative volume element. To effectively capture the phenomena at the critical region, the top 2 μm of the domain is specifically partitioned to accommodate the evolving oxide layer and an initial air layer. A key strategy in our modeling approach is the inclusion of this air layer, which serves as a placeholder for future oxide growth. As the simulation progresses during the isothermal phase, these elements are dynamically converted from air properties to oxide properties according to the prescribed growth kinetics. To ensure that the air layer does not influence the mechanical state of the substrate before conversion, it is assigned a near-zero Young's modulus and Poisson's ratio.

The mechanical behavior is governed by a UMAT subroutine implemented within Abaqus/Standard, which allows for the simultaneous consideration of various strain components. The total strain increment is decomposed into elastic, thermal, creep, diffusion, and growth components. For the metal substrate, elastic, thermal, diffusion, and creep strains are considered, while the oxide layer incorporates growth strain instead of diffusion strain. The material properties utilized for the NiCr validation cases are summarized in Table 1, where A_p is the kinetics coefficient of the global chemical oxidation reaction, E and v represent the Young's modulus and Poisson's ratio, K and N are the viscoplastic (creep) parameters, α is the thermal expansion coefficient, D_{ox} is the growth strain parameter, η is the constant coefficient coupling chromium concentration to diffusion strain, and D is the diffusion coefficient of chromium in the NiCr alloy.

Table 1: Input material properties [3-6]

Parameter	Metal	Oxide	Air
$A_p(mm/s^{0.5})$	-	1.43E-5	-
E (MPa)	160,000	205,000	1E-6
ν	0.3	0.29	0.0
N	1	1	-
K $(MPa^{1/N_{ox}})$	1.88E15	3.5E7	-
$\alpha(K^{-1})$	2.02E-5	7.24E-6	-
η	-	-8.98E-3	-
$D_{ox}(mm^{-1})$	-	51.9	-
D$(mm^2$/s)	-	4.19E-10	

The simulation is conducted over three distinct operational phases to mimic a full high-temperature oxidation cycle, as shown in Fig. 1. The first phase is a heating step where the temperature is increased from 25℃ to 1000℃ over 1800 seconds, primarily inducing thermal expansion stresses. This is followed by an isothermal phase where the model is held at 1000℃ for 3600 seconds, during which the oxide film grows and the metal-oxide interface undergoes stress redistribution due to creep and diffusion. The final phase is a cooling step back to 25℃ over 1800 seconds. While this phase is dominated by significant residual stresses generated by the thermal expansion mismatch, the model continues to account for creep strain relaxation to ensure a comprehensive representation of the stress evolution during the rapid temperature drop.

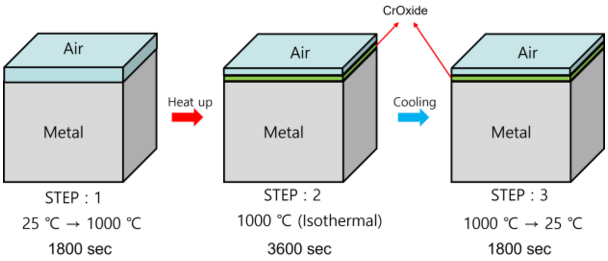


Fig. 1. Schematic of step definition

2.2 Verification: Mesh Sensitivity Analysis

Verification was centered on evaluating the mesh dependency of the stress results to confirm that the spatial discretization was sufficient. We analyzed three distinct mesh cases categorized as low, medium, and high densities. The low-density case utilized 20 * 20 seeds on the horizontal plane with 20 vertical seeds for the metal and 5 seeds for the oxide-air zone. The medium-density case utilized 40 * 40 seeds on the horizontal plane, with 25 vertical seeds for the metal and 10 seeds for the oxide-air zone. The high-density case, which replicates the benchmark literature standards [3], employed 80 * 80 horizontal seeds with 30 vertical seeds for the metal and 20 for the oxide-air zone.

To precisely capture the steep stress gradients typically found at the interface, a seeding bias of 5 was applied toward the metal-oxide boundary in all cases.

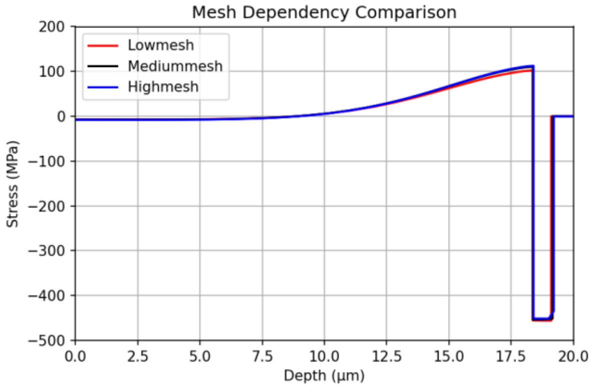
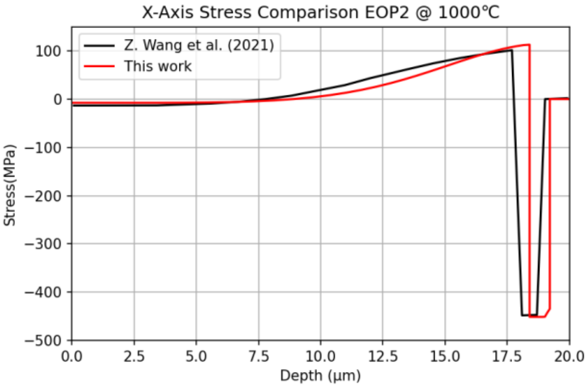


Fig. 2. Mesh dependency comparison

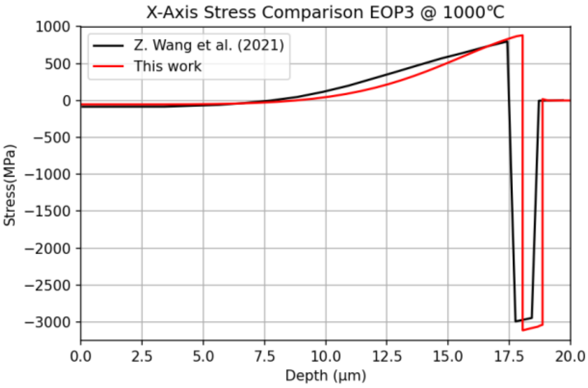
Upon comparing the stress distributions along a central path for all three mesh densities, the results appeared virtually identical, as shown in Fig. 2. Only minor deviations were observed in the low-mesh case, indicating that the solution has successfully converged. This confirms that the numerical results are stable and the chosen mesh density is sufficient for further analysis.

2.3 Validation: Comparative Stress Analysis

Validation was performed by comparing the calculated stress distribution along the depth of the central path with high-fidelity benchmarks data provided by Wang et al. [3]. The validation focused on the stress states at the end of the isothermal holding period and the final cooling phase.



(a)



(b)

Fig. 3. X-Axis stress comparison along the center path; (a) End of phase 2 (b) End of Phase 3.

At the end of Phase 2 (see Fig. 3a), the model predicts a tensile stress of approximately 100 MPa in the metal substrate near the interface, while the oxide layer exhibits a compressive stress of nearly 450 MPa. These values align closely with the benchmark data, reflecting the stress generation from oxide growth and the subsequent relaxation provided by creep at 1000℃.

Following the cooling phase, the stresses intensify dramatically due to the thermomechanical mismatch. As shown in Fig. 3b, the tensile stress in the metal side increases to nearly 800 MPa, while the oxide layer experiences a high compressive stress of approximately 3100 MPa. The general tendency and magnitudes observed in our simulation are highly consistent with the benchmark results. While minor discrepancies exist largely due to unknown exact solver configurations not detailed in the reference study, the strong correlation in the trend and peak stress values validates the model's ability to accurately simulate the stress evolution in these complex high-temperature systems.

3. Conclusions & Future Work

In this study, a comprehensive thermomechanical finite element model was successfully developed using Abaqus/Standard coupled with a user-defined UMAT subroutine to simulate the complex stress evolution at the metal-oxide interface during high-temperature oxidation. The model's reliability was rigorously established through a multi-step verification and validation procedure using a NiCr alloy system as a benchmark.

The verification phase confirmed numerical stability and mesh independence, while the validation phase demonstrated a strong correlation with established literature. Specifically, the model accurately captured the transition from the isothermal oxidation phase, characterized by moderate tensile stresses in the substrate and compressive stresses in the oxide, to the critical cooling phase, where thermal mismatch induced significant stress intensification, reaching nearly 800MPa in the metal and -3100MPa in the oxide layer. These results underscore the model's ability to resolve localized stress concentrations at the interface, which are known to be the primary drivers for mechanical degradation mechanisms such as cracking and spallation.

While the current work provides a robust numerical foundation, it serves as a precursor to more specialized applications within the nuclear industry. Future work will expand this computational framework to FeCr-based systems, specifically targeting stainless steel 316H, a material of high relevance for high-temperature reactor components. Building upon the validated NiCr model, we will conduct a detailed parametric study focusing on two dominant variables: diffusion coefficients and creep parameters.

These specific parameters were selected because they are hypothesized to be the most critical factors influencing the generation and relaxation of stresses, respectively. By systematically varying these inputs, we aim to quantify their individual and synergistic effects on interface integrity. This research will provide crucial insights in to long-term structural reliability of SS316, contributing to more accurate life prediction models and enhanced safety for nuclear power plant systems.

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