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

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I. Introduction

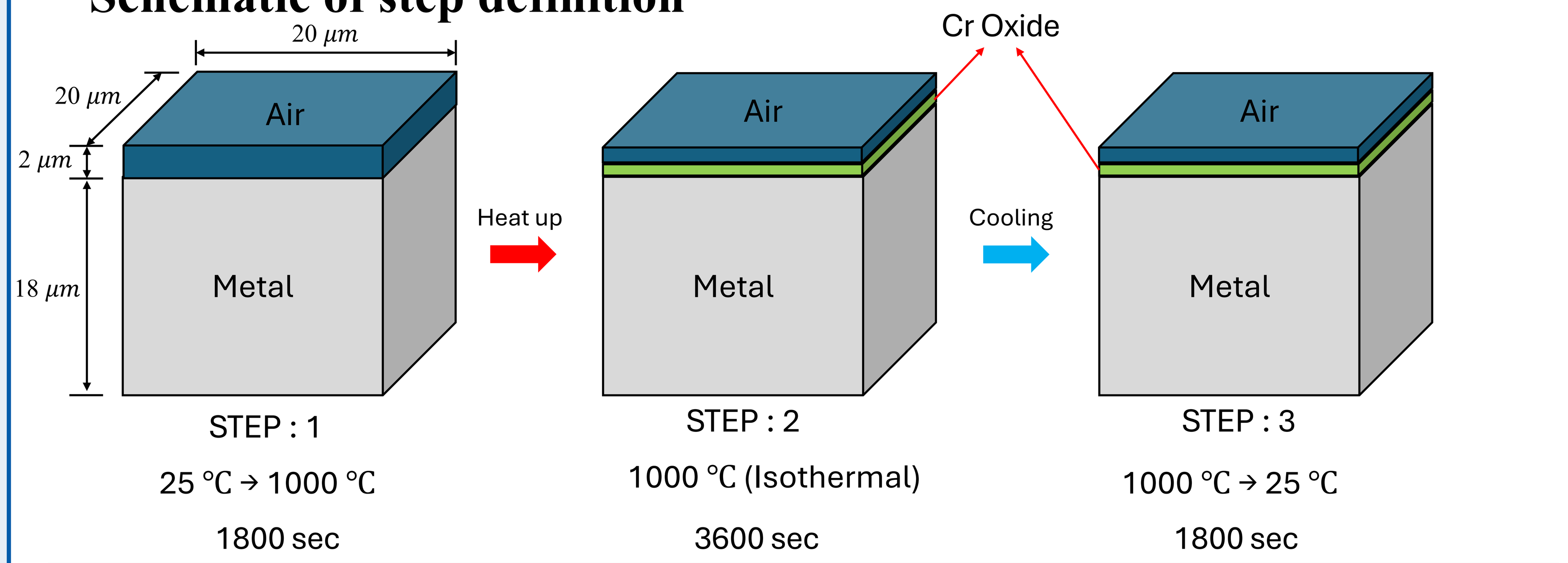
- The longevity of metallic alloys in high temperature environments relies almost entirely on their ability to form and sustain a protective oxide scale.
- However, at elevated temperatures, the kinetics of oxide growth accelerate that leads to mechanical failures such as spallation or cracking. [1]
- Most existing studies relies on ex-situ characterization, where samples are analyzed after cooling to room temperature; this makes it difficult to decouple growth stress at high temperature from thermal stresses induced during cooling.
- In this study, we conducted simulations to analyze stress evolution using UMAT (User Material) subroutine with comprehensive thermomechanical model.

II. Thermomechanical Model V&V

* Strain decomposition in benchmark system [2]

$$\left(\frac{\varepsilon_{elastic}}{dt}+\frac{\varepsilon_{creep}}{dt}+\frac{\varepsilon_{thermal}}{dt}+\frac{\varepsilon_{diffusion}}{dt}\right)_m = \left(\frac{\varepsilon_{elastic}}{dt}+\frac{\varepsilon_{creep}}{dt}+\frac{\varepsilon_{thermal}}{dt}+\frac{\varepsilon_{growth}}{dt}\right)_{ox}$$

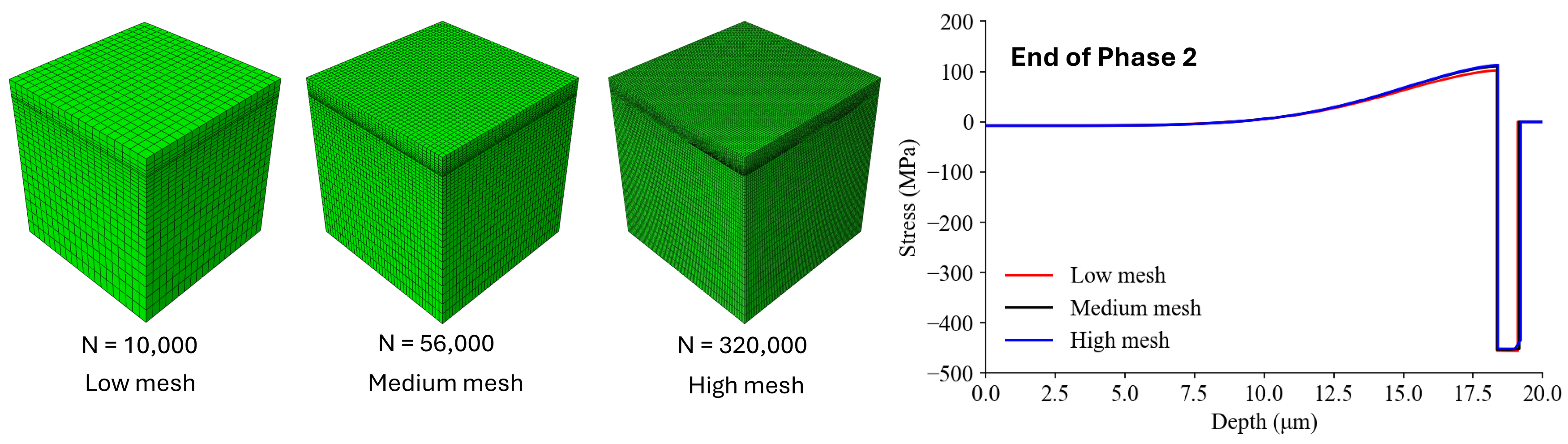
* Schematic of step definition



* Input parameters used in NiCr V&V [2]

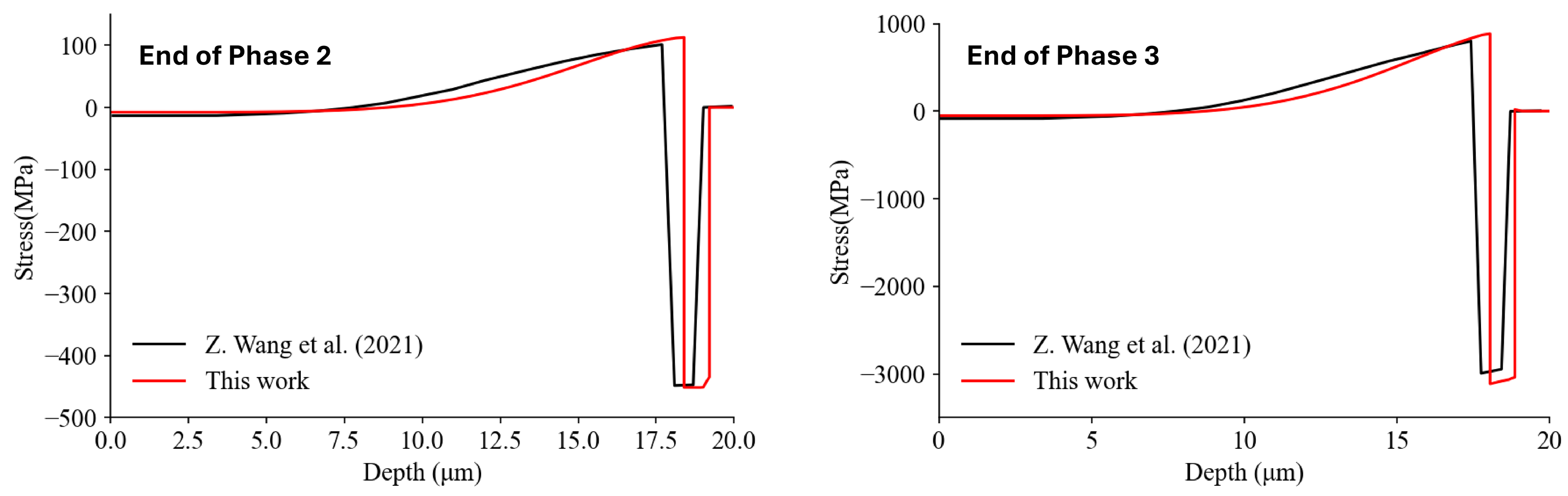
Parameter	Metal(Ni30Cr)	Oxide	Air
E(MPa)	160,000	205,000	1E-6
υ	0.3	0.29	0.0
N	1	1	-
K $(MPa^{1/N})$	1.88E15	3.5E7	-
$\alpha(K^{-1})$	2.02E-5	7.24E-6	-
η	-8.98E-03	-	-

* Verification: Mesh sensitivity



- No significant difference was shown between mesh quality

* Validation: σ_{xx}(X-Axis stress) comparison with benchmark

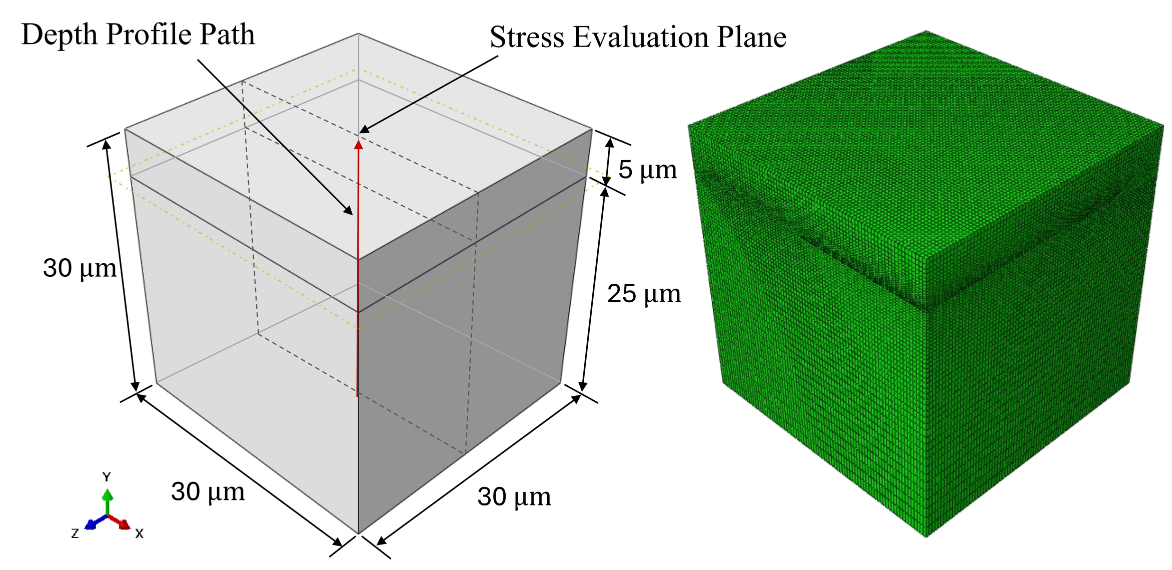


~ 100 MPa at metal / 450 MPa at oxide

~ 700 MPa at metal / -3100 MPa at oxide

III. Application Case Study

- The validated framework was applied to 316 SS to demonstrate the model's generalizability beyond the NiCr benchmark
- Geometric configuration: 30 × 30 × 30 μm RVE (expanded to accommodate higher oxidation kinetics)

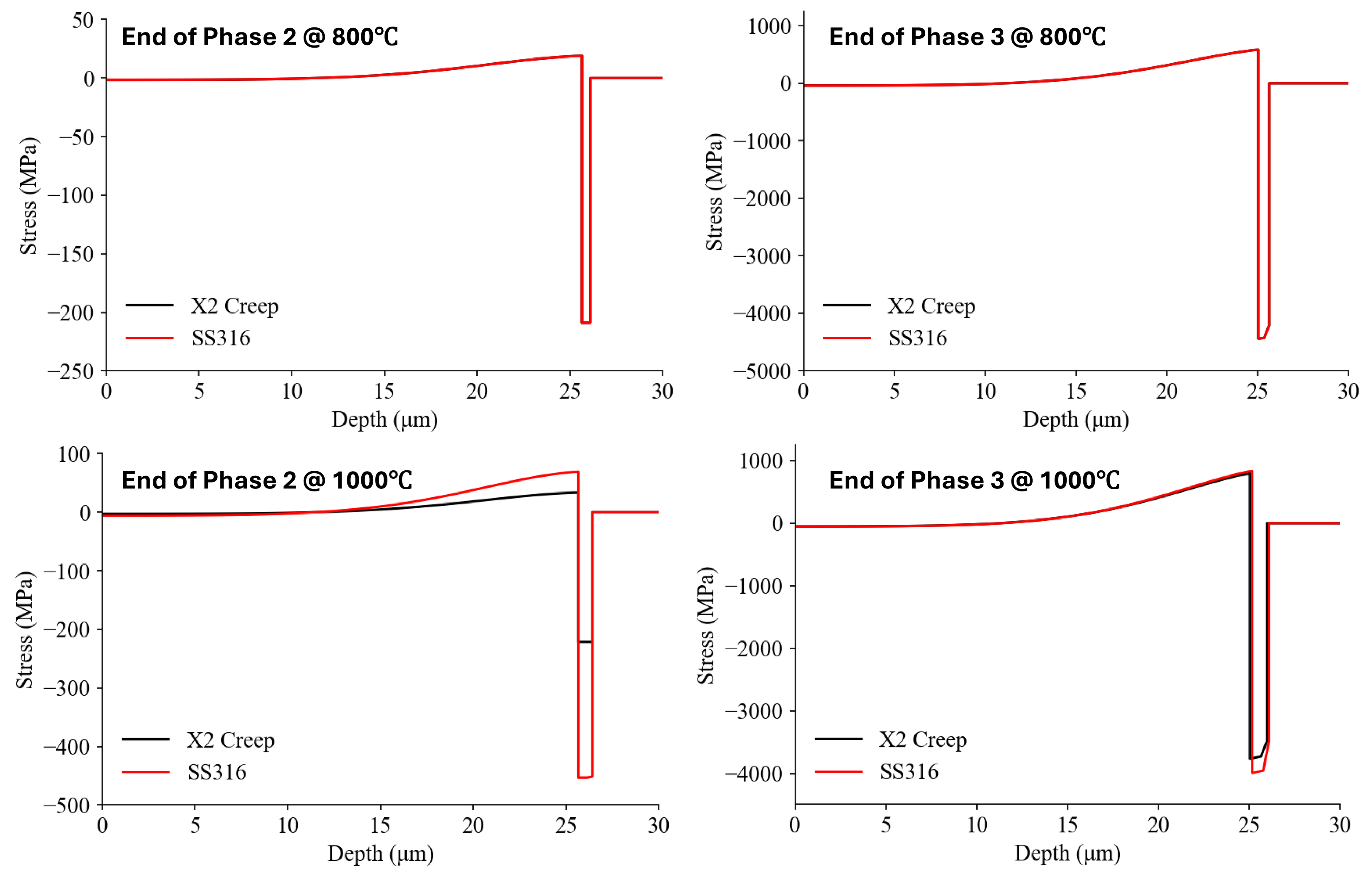


- Isothermal(phase II) conditions: 800℃ (10 hr) and 1000℃ (1 hr)
- Independently varied Dorn creep constant and diffusion coefficient

* Input parameters used in application case study [2-6]

Temperature(℃)	$A_p(mm/s^{0.5})$	$E_{ox}(MPa)$	v_{ox}	$A_{ox}(MPa^{1/N_{ox}})$	N_{ox}	$\alpha_{ox}(K^{-1})$
800	2.83E-6	225,000	0.29	1.887E-9	1	6.99E-6
1000	1.43E-5	205,000	0.29	1.428E-8	1	7.24E-6
	$D_{ox}(mm^{-1})$	$E_m(MPa)$	v_m	$A_m(MPa^{1/m})$	N_m	$\alpha_m(K^{-1})$
800	51.4	138,000	0.3	4.58E-25	7.9	2.08E-5
1000	51.9	120,000	0.3	1.61E-22	7.9	2.15E-5
	$[Cr]_0$	η	$D\ (mm^2/s)$			
800	0.18	-6.57E-3	2.59E-12			
1000	0.18	-5.7798E-4	1.20E-10			

* σ_{xx} comparison in 316 SS case with creep parametric study



- Creep acts as a critical stress buffer during isothermal holds at 1000℃.
  - ➢ Doubled A effectively halves growth stress
- Diffusion coefficient variation shows negligible mechanical effect in both 800℃ and 1000℃.
- Stress difference intensified mostly by CTE mismatch regardless of creep capacity, indicating failures in oxide layer tends to occur in cooling phase.

IV. Conclusion and Future work

- In this study, we validated the thermomechanical FEA framework against NiCr system benchmark showing strong correlation in stress magnitude and interfacial behavior.
- Case study on 316 SS identified viscoplastic relaxation as the dominant stress-relief mechanism during isothermal oxidation, while CTE mismatch governs the final stress state.
- As future work, we plan to develop an advanced model considering plastic deformation and fracture to overcome the limitations of purely elastic analysis.
- We also plan to assess the model's consistency through comparison with experimental results.

Reference

[1] Birks, Neil, Gerald H. Meier, and Frederick S. Pettit. *Introduction to the high temperature oxidation of metals*. Cambridge university press, 2006.

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