Thermal-Structural Modeling of Additively Manufactured Ni-YSZ Layers for SOFC Electrodes

Sachin Poudel[1], Anna Timofiejczuk[1], Dhruba Panthi[2], Nele Moelans[3], Anil Kunwar[1]

[1]Faculty of Mechanical Engineering, Silesian University of Technology, Poland
[2]Kent State University at Tuscarawas, USA
[3]Department of Materials Engineering, KU Leuven, Belgium

Motivation

- **Why Ni-YSZ for SOFC-Electrodes?**
  - Ni: electronic conduction, catalytic sites.
  - YSZ: high ionic conductivity, mechanical stability.
  - Controlled porosity (20-30%) maximizes gas transport and triple-phase-boundary (TPB) density.
- **Additive Manufacturing Advantage**
  - Solid state Selective laser sintering (SLS) below melting retains tailored porosity [1].
  - Insitu densification and microstructure control via laser parameters.
  - Need for predictive, coupled thermal-sintering-mechanical models to optimize process.
- **Gap and Objective**
  - Existing studies focus on separate thermal or mechanical aspects.
  - We simulate SLS of Ni-YSZ composites **(dissimilar joints)** by capturing simultaneous thermal gradients, densification kinetics, and stress evolution.

Computational Framework

- **1. HeatTransfer Model**

  Solve transient conduction with a volumetric Gaussian laser source:

$$\rho_{\mathrm{eff}}(T)\, c_{p,\mathrm{eff}}(T)\, \frac{\partial T}{\partial t} = \nabla\big[k_{\mathrm{eff}}(T)\, \nabla T\big] + q_{\mathrm{laser}}.$$

  Laser power distribution:

$$q_{\mathrm{laser}}(r) = \alpha\, \frac{2P}{\pi r_0^2}\, \exp\big[-2(r/r_0)^2\big].$$

  Effective properties account for local porosity [2]:

$$\rho_{\mathrm{eff}}(T) = (1-\psi)\, \rho_{\mathrm{bulk}}(T) + \psi\, \rho_{\mathrm{air}}(T), \quad k_{\mathrm{eff}}(T) \approx (1-\psi)\, k_{\mathrm{bulk}}(T) + \psi\, k_{\mathrm{air}}.$$

- **2. Porosity Evolution**

  Densification kinetics follows a thermally activated law:

$$\dot{\rho}_r = A\, (1-\rho_r)^m \exp\Big(-\frac{Q}{RT}\Big),$$

  where $\rho_r = 1 - \psi$ is the local relative packing density.
  Activation energies: $Q_{\mathrm{Ni}} \approx 200$ kJ/mol, $Q_{\mathrm{YSZ}} \approx 400$ kJ/mol.
  User-defined parameters (A, m) set in preprocessor (Elmer) based on material data.
- **3. Thermo-Mechanical Response**
  - Enforce static equilibrium with thermal strains:

$$\nabla \cdot \boldsymbol{\sigma} = \mathbf{0},$$

$$\sigma_{ij} = 2\mu(T)\, \epsilon_{ij} + \lambda(T)\, \mathrm{tr}(\epsilon)\, \delta_{ij} - \alpha(T)\, E(T)\, [T - T_{\mathrm{ref}}]\, \delta_{ij}.$$

  - Ni plasticity: via von Mises criterion and **Hollomon powerlaw** (strain-hardening) when $\sigma_{\mathrm{eq}} > \sigma_{Y,\mathrm{Ni}}(T)$.
  - YSZ treated as brittle elastic ceramics with no plastic deformation.
- **All bulk thermal & mechanical properties are temperature dependent.**

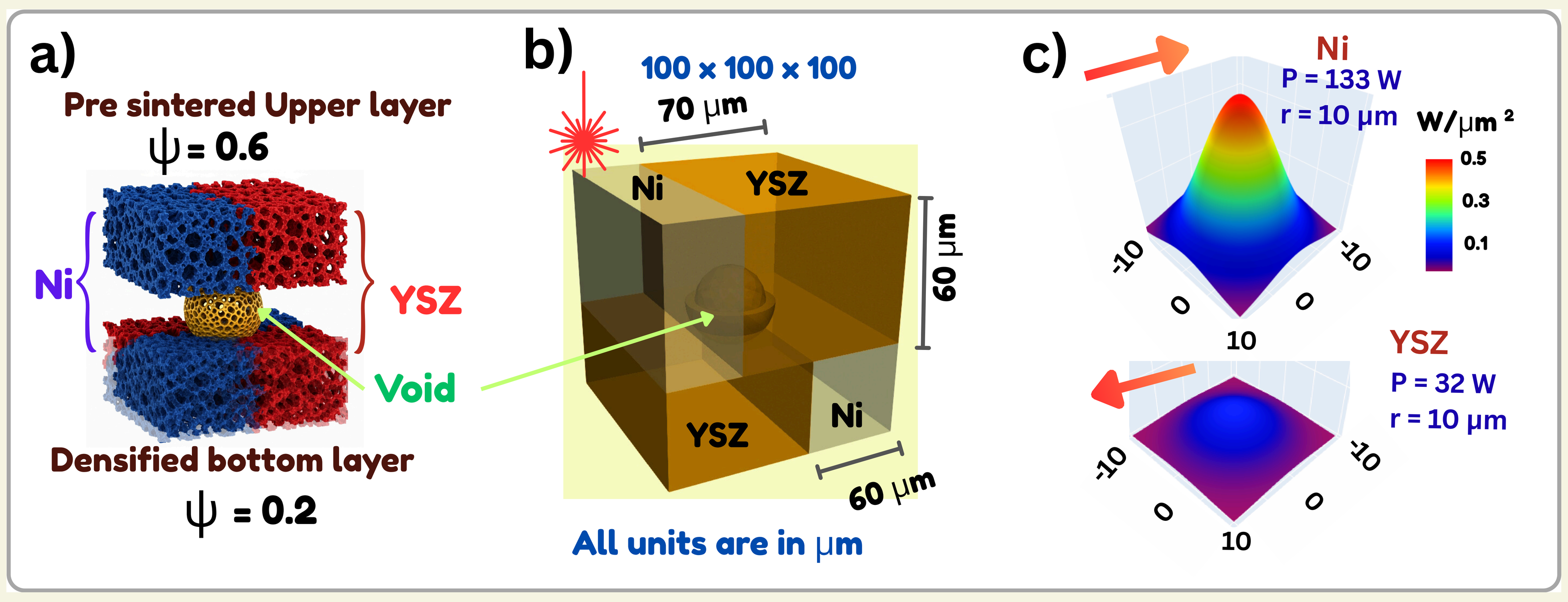

Figure 1: (a) Porous top layer ($\psi = 0.6$) over dense substrate ($\psi = 0.2$) with central void. (b) Computational geometry showing Ni-rich and YSZ-rich zones. (c) Gaussian laser intensity overlaid on Ni and YSZ-rich region under different intensities ($W/\mu m^2$).

Results (Thermal & Stress Distribution)

Thermal Behaviour:

- **Ni-Rich Region:** High thermal conductivity of Ni ($k_{\mathrm{Ni}}(T)$) spreads heat rapidly, resulting in a low temperature gradient (∇T).
- **YSZ-Rich Region:** Low thermal conductivity of YSZ ($k_{\mathrm{YSZ}}(T)$) localizes heat, requiring a bidirectional scanning to avoid overheating and thermal runaway.

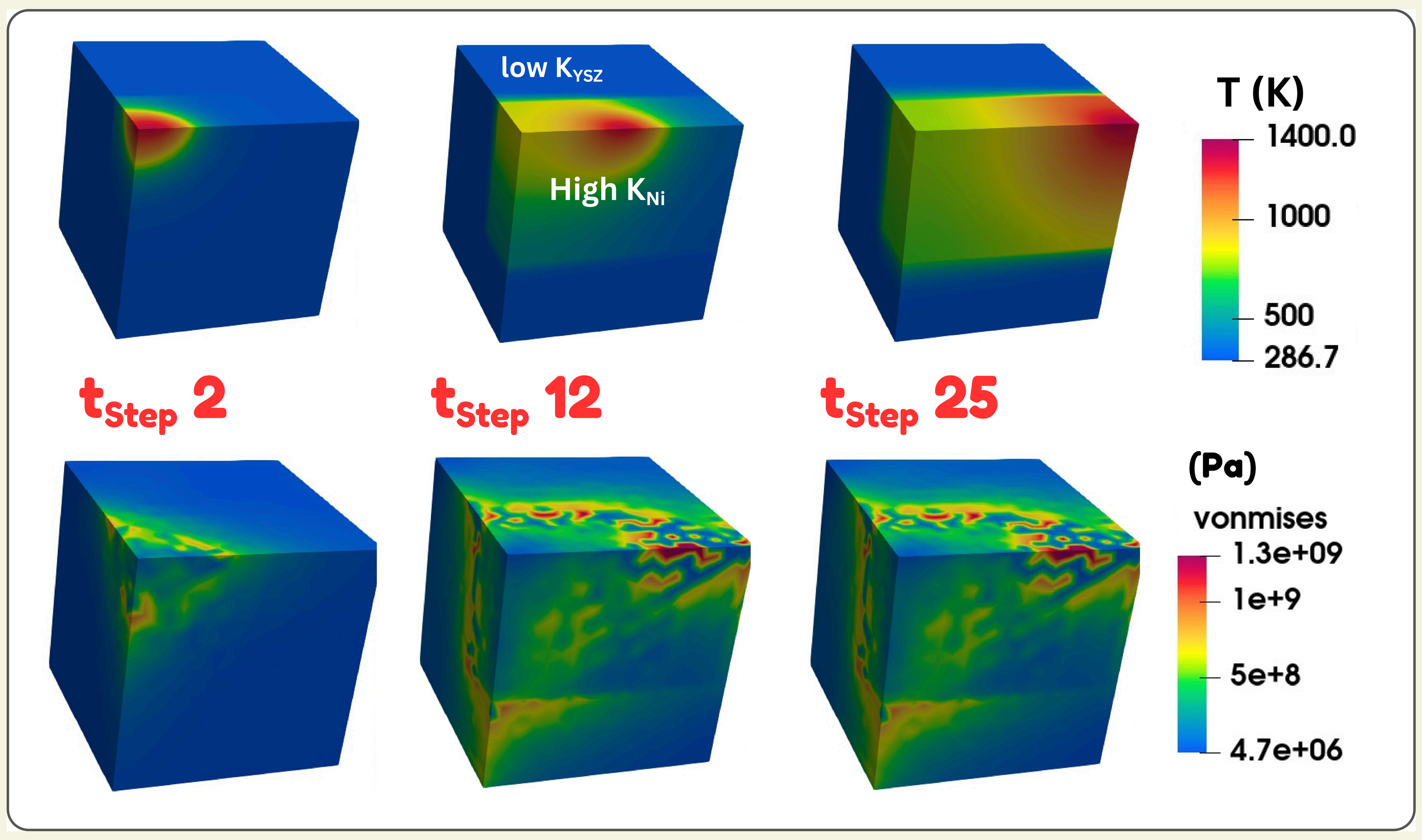

Figure 2: (a) Temperature field when laser scans Nirich layer (peak ~ 1300 K). (b) Ni plastic flow results a peak von Mises stresses (max $\sigma_{\mathrm{VM}} \approx 1300$ MPa) in a localized region. The time steps used in the simulation is $\Delta t = 3\mu s$. The laser is operated in forward directions.

Mechanical Consequences:

- Ni region's plastic flow reduces peak von Mises stresses.
- YSZ remains elasticbrittle; localized tensile stresses exceed fracture strength, leading to microcrack initiation.

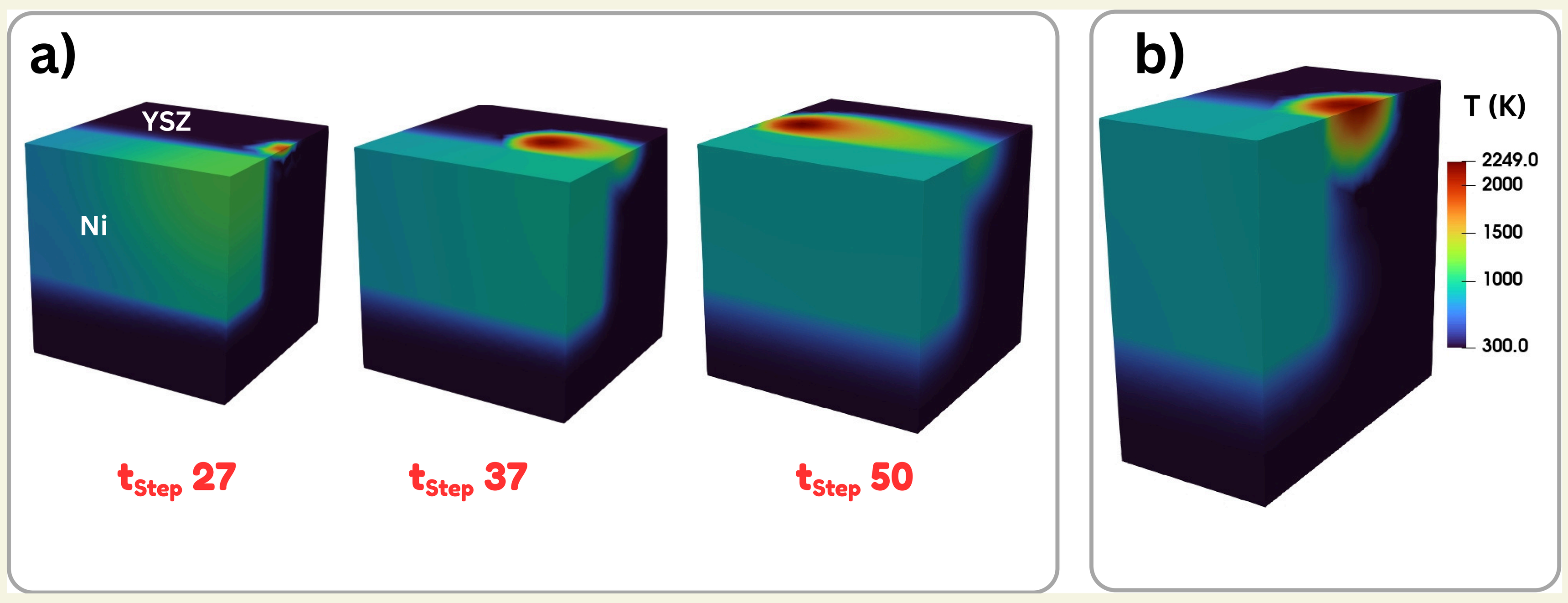

Figure 3: (a) Temperature distribution when laser is applied at the YSZ-rich region in reverse heating. The maximum temperature in YSZ region is 2249 T. (b) Thermal distribution in the internal cross-section in the cube in $t_{step} = 37$.

Analysis & Outlooks

Thermo-Mechanical Insights:

- Ni-rich regions exhibit moderate ∇T, enabling gradual densification with low residual stress accumulation.
- YSZ-rich areas experience steep thermal gradients, promoting rapid sintering but increasing micro-crack risk due to thermal stress.

Role of Voids:

- Voids at Ni-YSZ interfaces act as barriers to heat and stress propagation.
- The stress is concentrated around the void surface.

Outlook:

- Engineering interface porosity enables control of sintering behavior and mechanical resilience.

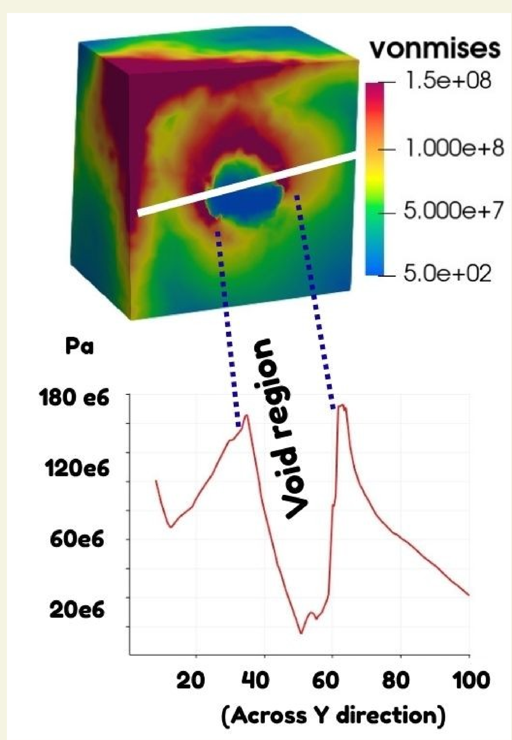

Figure 4: Stress distribution across Ni-YSZ with voids.

Key References

[1] Arantes, V. L., Coutinho, R. B., Martins, S. S., Huang, S., and Vleugels, J., "Solid State Sintering Behavior of ZirconiaNickel Composites," *Ceram. Int.*, vol. 45, no. 17, pp. 22120–22130, 2019. Available: `https://doi.org/10.1016/j.ceramint.2019.07.229`

[2] Geng, Y., Wang, X., Chen, Y., Shan, Z., Zhang, Z., and Kunwar, A., "Stress-Relief Annealing Friendly Fe-Based Metallic Glass-Reinforced Al-Si-Mg-Zr Alloy Fabricated by Laser Powder Bed Fusion," *Virtual Phys. Prototyp.*, vol. 19, no. 1, article e2416518, 2024.

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Corresponding Author Profile:
Sachin Poudel
sachin.poudel@polsl.pl
`https://github.com/Sachinscnpdl/ni-ysz_amm_2025`