Development of a Mechanistic-Based Healing Model for Self-Healing Glass Seals

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OVERVIEW

The usage of self-healing glass as hermetic seals is a recent advancement in sealing technology development for the planar solid oxide fuel cells (SOFCs). Because of its capability of restoring the mechanical properties at elevated temperatures, the self-healing glass seal is expected to provide high reliability in maintaining the long-term structural integrity and functionality of SOFCs. In order to accommodate the design and to evaluate the effectiveness of such engineering seals under various thermo-mechanical operating conditions, a mechanistic-based, two-stage computational model was developed to accurately capture and predict the stress and temperature-dependent crack-healing behavior of the self-healing glass materials. The model was first calibrated by experimental measurements combined with the kinetic Monte Carlo (kMC) simulation results and then implemented into finite element (FE) analysis. The effects of various factors, i.e. stress, temperature, crack morphology, on the healing behavior of the glass were investigated and discussed.

OBJECTIVES

- Develop a mechanistic based model to quantify the healing behavior of the self-healing glass seal materials.
- Investigate the effects of various thermo-mechanical operating conditions on the healing performance.
- Assist the development of the reliable stack-level SOFC design integrated with the self-healing glass sealing system.

DISCRETE MECHANISTIC BASED HEALING MODEL

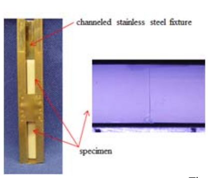
- Conceptually divided the entire healing process into two sequential stages:
  1) Creep-driven crack closure;
  2) Interdiffusion-driven crack healing.
- Developed a temperature-dependent dwelling time to characterize the interdiffusion-driven crack healing process and calibrated it by controlled experimental measurements and kMC predictions.
- Implemented the healing mechanism into FE analyses to predict the healing behavior under different operating conditions.

Viscous flow	$\dot{\varepsilon} = \frac{1}{\eta}\sigma$
Temperature-dependent viscosity	$\eta = \eta_0 \exp(\frac{Q_v}{RT})$
Characteristic dwelling time	$\tau_0 = \alpha \exp(\frac{\beta}{T})$

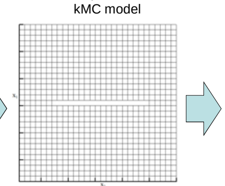
MODEL CALIBRATION

- In controlled experiments, two bars were placed vertically and exposed to elevated temperatures to mimic the healing process of one glass bar of double length but with a closed cross-sectional crack. The measured flexural strength recovery was used to calibrate the healing probability function of the kMC model, whose predictions then extrapolated the experimental data to a wider temperature range and formulated the functional form of the characteristic dwelling time.

Controlled experimental setup



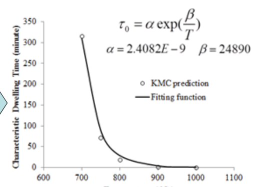
Geometrically non-dimensional kMC model



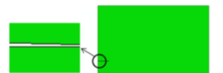
The lattice spacing denotes the covalent bond, the central crack then represents a closed but not healed crack.

$$P = w_h \times \exp(-\frac{E_h}{kT}) \quad w_h = 6.02E9Hz \quad E_h = 2.555eV$$

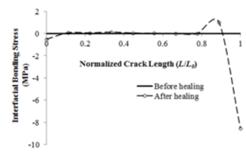
Characteristic dwelling time



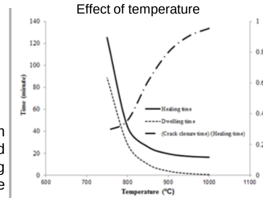
PARAMETRIC STUDY USING FE MODEL



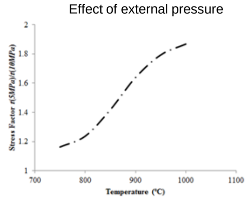
2D plane-strain model (100×100mm square) with a 0.1mm wide and 10mm long V-type edge crack having its bottom fixed and uniform pressure applied onto its top is exposed to elevated temperatures.



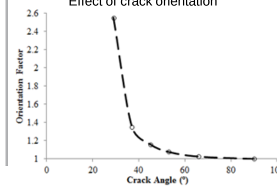
Effect of temperature



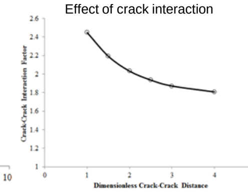
Effect of external pressure



Effect of crack orientation



Effect of crack interaction



CONCLUSIONS

A mechanistic-based healing model, which can quantify the healing behavior of the self-healing glass seal materials, was developed. The following conclusions were derived in this research:

- High temperature leads to faster healing. The total healing time is mostly determined by the crack closure at extremely high temperatures when the cracks instantly heal as the crack surfaces come into contact, while it is primarily dominated by the crack healing at low temperatures when diffusion is considerably slow.
- External confining stresses help accelerate crack healing. However, such influence becomes less effective as the temperature drops because the crack closure primarily affected by stresses is less influential on the total healing at low temperatures.
- Both stress magnitude and directions of local stresses affect the healing behavior. The healing time drastically increases as the crack orientation (θ) deviates from the direction normal to the applied pressure (θ=90º) while asymptotically reaching a plateau as it approaches 90º.
- The presence of multiple cracks increases the healing time. As cracks get closer, the adverse effects on the healing behavior induced by the crack–crack interaction appear to be more significant.

The findings of the discrete crack healing model can be utilized to provide the missing links between the behavior of the individual cracks and the overall structural response for the upscale continuum damage-healing modeling and SOFC stack-level simulation.

FUTURE WORK

- Develop a continuum damage-healing model to accommodate stack-level simulations
- Comparative prediction and optimization of seal designs: compliant seal vs. rigid seal

PUBLICATIONS

- W Xu, X Sun, E Stephens, I Mastorakos, MA Khaleel, HM Zbib, 2012. "A Mechanistic-based Healing Model for Self-healing Glass Seals Used in Solid Oxide Fuel Cells", Journal of Power Sources (accepted).

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