Simulating Fracture in SOFC Anode Materials

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Background

The anode of a solid oxide fuel cell (SOFC) is a porous composite consisting of a metallic conducting phase (typically nickel) and a brittle electrolyte phase (yttria-stabilized zirconia). Oxidation of the metallic phase due to the presence of excess oxygen results in an expansion to its corresponding oxide phase. This structural transformation exerts stress on the brittle phase and has been observed to result in brittle fracture throughout the cell, as shown in the experimental image to the left [1]. These microfractures can jeopardize the mechanical integrity and electrochemical performance of the cell.

Objective

We are studying the detrimental effects that oxidation-reduction cycles have on the microstructural properties of solid-oxide fuel cell (SOFC) anodes. How much oxidation is allowable without incurring severe crack formation and propagation? Which microstructural characteristics affect this degradation mechanism? Can the materials and/or microstructure be engineered to mitigate fracture?

Phase Field Model

A crack can be represented with a continuous field, often called the order parameter [2,3]. This fracture field evolves to minimize the global free energy of the system (F). With this method, the crack forms a diffuse interface and can feature complex fracture topologies. The free energy accounts for the release of strain energy during fracture propagation, as well as the increase in the crack interface energy. The strain energy features a tension/compression split and allows for the transmission of compressive stress across the crack faces [4].

SOFC Fracture

The SOFC anode features a porous microstructure that consists of a metallic phase (orange) and a brittle electrolyte (grey). Due to the elevated operating temperatures, the brittle particles have sintered together, and the metallic phase coarsens. This forms the initial configuration for the fracture simulations.

Oxidation of the metallic phase and its structural expansion induces large stresses in the anode system. The results of the fracture simulation show many microcracks throughout the brittle phase. The right face of the system box exhibits a large, transgranular crack that has propagated through multiple particles.

2D Fracture Tests

The images show snapshots of the spatio-temporal evolution of an initial defect in an elastically homogeneous, two dimensional system. Black lines are drawn for contours of the fracture parameter and indicate the crack interface. Stress contours are colored by the component of stress perpendicular to the initial crack direction. The system is rapidly loaded by increasing the displacement, and the stress concentrates around the crack tip. The crack quickly begins propagating to relieve the system of excess strain energy and forms branching paths.

Discussion

Initial tests indicate that the phase field fracture model is capable of reproducing essential features of brittle fracture including stress concentration at the crack tip, propagation, and splitting events. Results from the multiphase, three dimensional anode structures reveal a sudden and dramatic onset of fracture at only 2-3% phase transformation. This is followed by continued propagation that shows some dependence on microstructure and phase interactivity (as measured by the contact angle).

References