A COMBINED MICROMECHANICS/MATERIALS SCIENCE APPROACH TO UNDERSTANDING HIGH TEMPERATURE HYDROGEN ATTACK

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High temperature hydrogen attack (HTHA) is degradation of carbon steels whereby internal hydrogen reacting with carbides forms methane gas bubbles typically on grain boundaries which grow and coalesce, leading to loss of strength and toughness. Current design practice against HTHA is based on Nelson curves which are constructed based on the data from previous HTHA failures and define the conditions for safe operation in a temperature/hydrogen-partial-pressure diagram. Nelson curves are empirical and do not account for the underlying failure mechanism(s), microstructure, carbide stability, and applied stresses. To this end, we present a constraint-based model for failure of carbon steels by HTHA. The model is based on constrained growth and coalescence of grain boundary voids under the influence of internal cavity methane gas pressure and applied macroscopic loads. Void growth is constrained because voids nucleate only on some of the grain boundaries and therefore uncavitated grains geometrically constrain the growth of voids on cavitated boundaries. Void growth is simulated by coupling grain boundary diffusion and bulk deformation of the grains under applied stresses and gas pressure. The methane gas pressure is calculated by employing a combined atomistic-kinetics approach that involves 1) hydrogen uptake and carbide dissolution, 2) migration of carbon and hydrogen atoms to the void surface, 3) surface reaction of carbon and hydrogen atoms to form methane and hydrogen gas molecules, and 4) desorption of the gas molecules into the void. The essential kinetic parameters involved in the model are computed using density-functional theory (DFT). An important ingredient of the model is the incorporation of the effect of hydrogen on the constitutive response of the steel at temperatures relevant to HTHA. Experimental work for this effect in carbon steel is almost non-existent in the open literature. We quantified the hydrogen effect by measuring the activation parameters that govern the deformation during HTHA. The synthesized results provide a chemomechanical model for the prediction of growth and coalescence of voids during HTHA. The model is used to construct physically-based Nelson-type curves indicating lifetime under given applied stresses. The proposed methodology can be considered a step toward improving the current design practice against HTHA while maintaining the simplicity of the original Nelson curve approach.