Oxygen Diffusion and Its Coupling with Crystal Plasticity in a Nickel-Based Superalloy

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Abstract

Nickel-based superalloys, consisting of γ-matrix phase and superior γ′-precipitate phase, are strategically important class of high temperature and corrosion-resistant materials, which are widely used in power generation, nuclear and aerospace industries. The usage of nickel superalloys is irreplaceable and critical in gas turbine systems (e.g. aero-engines). As a structural material that is usually exposed to high static or cyclic loads in aggressive environments (up to 1000°C), it is important to understand the resistance to crack initiation and propagation to improve service-lifing accuracy of components and provide guidance to future alloy development. At high temperature, fatigue crack growth in such alloys exposed to air can be drastically accelerated by two or three orders (10^2~10^3) of magnitude due to oxidation damage, which is one of the major concerns for structural integrity of gas turbines. Oxidation-accelerated failure process is closely linked with the diffusion of oxygen along rapid diffusion paths, such as slip planes or grain boundaries, into a local area with increasing tensile stress, such as crack tips. The oxygen, through chemical reactions with alloy elements, embrittles the surrounding metal and prompts accelerated crack propagation.

In literature, diffusion of oxygen into a crack tip was generally modelled using a simplified approach, which considered only the influence of hydrostatic stress (i.e., trace of the Cauchy stress) and neglected the full interaction between mechanical deformation and oxygen diffusion. In this paper, efforts were made to model the full coupling of mechanical deformation and oxygen diffusion in a single crystal nickel base superalloy. Both Cauchy stress and Elsheby stress were considered in the chemical potential to model the fully coupled deformation-diffusion process. The approach has been numerically incorporated into a crystal plasticity model, which has not been previously reported yet. Using this method, finite element analyses of oxygen diffusion, coupled with crystal plastic deformation, have been carried out to predict oxygen penetration at a crack tip and associated change of near-tip stress field. A direct comparison was made to understand the difference between Cauchy stress and Eshelby stress that are used in modelling stress-assisted oxygen diffusion at a crack tip.

Keywords: Crystal plasticity; Oxygen diffusion; Full coupling; Finite element; Crack tip; Nickel-based superalloy.

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