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Computational Modelling of Full Interaction between Crystal Plasticity and Oxygen Diffusion at a Crack Tip

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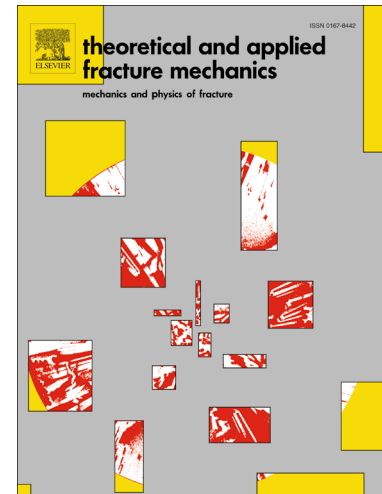
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**Computational Modelling of Full Interaction between Crystal Plasticity and Oxygen  
Diffusion at a Crack Tip**

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**Abstract**

Oxidation-promoted crack growth, one of the major concerns for nickel-based superalloys, is closely linked to the diffusion of oxygen into the crack tip. The phenomenon is still not well understood yet, especially the full interaction between oxygen diffusion and severe near-tip mechanical deformation. This work aimed at the development of a robust numerical strategy to model the full coupling of crystal plasticity and oxygen diffusion in a single crystal nickel-based superalloy. In order to accomplish this, finite element package ABAQUS is used as a platform to develop a series of user-defined subroutines to model the fully coupled process of deformation and diffusion. The formulation allowed easy incorporation of nonlinear material behaviour, various loading conditions and arbitrary model geometries. Using this method, finite element analyses of oxygen diffusion, coupled with crystal plastic deformation, were carried out to simulate oxygen penetration at a crack tip and associated change of near-tip stress field, which has significance in understanding crack growth acceleration in oxidation environment. Based on fully coupled diffusion-deformation analyses, a case study was carried out to predict crack growth rate in oxidation environment and under dwell-fatigue loading

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