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Continuum level simulation of the grain size and misorientation effects on hydrogen embrittlement in nickel

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Abstract

This paper addresses the size and misorientation effects on hydrogen embrittlement of a four grain nickel aggregate. The grain interior is modelled with orthotropic elasticity and the grain boundary with cohesive zone technique. The grain misorientation angle is parameterized by fixing the lower grains and rotating the upper grains about the out-of-plane axis. The hydrogen effect is accounted for via the three-step hydrogen informed cohesive zone simulation. The grain misorientation exerts an obvious weakening effect on the ultimate strength of the nickel aggregate which reaches its peak at misorientation angles around $20°$, but such effect becomes less pronounced in the case with a pre-crack. The misorientation could induce size effect in the otherwise size independent case without a pre-crack. The contribution of misorientation to the size effect is negligible compare to that caused by the existence of a pre-crack. These findings indicate that the misorientation effect in cases with a deep pre-crack is weaker than expected in shallow-pre-crack situations. Most of these conclusions hold for the hydrogen charging situation except that the ultimate strength is lowered in all the sub-cases due to hydrogen embrittlement. Interestingly, it is observed that the size effect becomes less pronounced with hydrogen taken into account, which is caused by the fact that hydrogen takes more time to reach the failure initiation site in larger grains.

Nomenclature

θ grain misorientation angle
L grain length
a half pre-crack length
σ_C cohesive strength
δ_C critical cohesive separation
Γ_C cohesive separation energy

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σ_N nominal stress applied at the remote boundary
σ_{22} opening stress developed in the grain aggregate
σ_f failure initiation stress or ultimate strength of the grain aggregate in the cohesive zone simulation
C_B hydrogen concentration at the outer boundary of the grain aggregate
C_I grain interior hydrogen concentration
D_L diffusivity of hydrogen
Ω partial volume of hydrogen

1. Introduction

It is well established that the macro-mechanical properties of polycrystalline materials are determined by its microscale characteristics such as grain size and grain boundary type. This gives rise to the concept of grain boundary engineering (GBE) (Kobayashi et al., 2012) which has been widely applied in the development of high performance structural and functional polycrystalline materials. A premise for GBE is to get systematic knowledge on how the material property is influenced by variation of a specific feature of grain, which can be done both numerically (Pezzotta et al., 2008; Li et al., 2009; Jothi et al., 2014) and experimentally (Cheung et al., 1994; Lehockey and Palumbo, 1997; Shimada et al., 2002).

A typical application of GBE is found in hydrogen embrittlement study of nickel based alloys which are prone to hydrogen degradation while possessing acceptable corrosion resistance and high strength (Stenerud et al., 2015). Bechtle et al. (2009) proved that the fracture toughness in hydrogen environment is enhanced in pure nickel with higher fraction of special grain boundaries. Kobayashi et al. (2012) applied the GBE technique based on fractal analysis for control of segregation-induced intergranular brittle fracture in polycrystalline nickel. Oudriss et al. (2012) investigated the effects of grain characteristics on hydrogen diffusion and trapping in pure nickel. In the numerical aspect, Wei and Anand (2004) investigated the grain boundary sliding and separation by modelling the grain interior with a crystal-plasticity model and the grain boundary with the cohesive zone model. Li et al. (2009) developed a phase mixture based finite element model to study the deformation behavior of polycrystalline nickel where the grain interior is assigned with orthotropic elasticity and the grain boundary with viscoplasticity. Jothi et al. (2014) studied the influence of grain boundary misorientation on hydrogen embrittlement in bi-crystal nickel by combining the stress analysis and transient hydrogen diffusion analysis. Most recently, Alvaro et al. (2015) simulated the nanomechanical testing performed on the nickel cantilever beam where the grain interior is assigned with orthotropic elasticity and the grain boundary modelled with the cohesive zone technique.

In real life, the grain structure is characterized by specific arrangements of the atoms, which is far more complicated than that captured by a continuum material model. The continuum level simulation, however, is still favorable considering its realistic length scale and time scale. Actually, such methodology has proven to be a powerful tool in revealing the influence of a specific grain feature with good accuracy compared to the experimental results (Pezzotta et al., 2008; Li et al., 2009). The grain misorientation angle is parameterized in (Jothi et al., 2014) illuminating its effect on the mechanical response and hydrogen diffusion, which provides information for GBE. In (Alvaro et al., 2015) the cohesive zone framework with its parameters calibrated via the atomistic calculation proves a successful tool in simulating the experimental results.

Jothi et al. (2014) reported in their parametric study on the continuum level that the grain misorientation has significant influence on the mechanical response as well as the hydrogen diffusion in bi-crystal nickel, for instance, maximum opening stress as well as maximum local hydrogen concentration were observed in the cases with misorientation angles $15° < \theta < 45°$. In that study, however, the actual failure behavior could not be observed since neither damage evolution law nor a failure criterion was attributed. Further, the size effect could not be captured since only the elasticity model was considered.

In the present work, a complete continuum framework for simulating hydrogen embrittlement in a four-grain nickel aggregate is developed based on the so-called three step hydrogen informed cohesive zone technique (Olden et al., 2008). The grain interior is modelled with orthotropic elasticity (Li et al., 2009;