



Cohesive zone simulation of grain size and misorientation effects on hydrogen embrittlement in nickel



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ABSTRACT

The size and misorientation effects on hydrogen embrittlement of a four grain nickel aggregate are studied with the help of hydrogen informed cohesive zone model. The grain misorientation angle is parameterized by fixing the lower grains while rotating the upper grains about the out-of-plane axis. Brittle failure of the grain aggregate is observed and nominal strength obtained. In the crack-free situation, the grain misorientation exerts an obvious weakening effect on the nominal strength, which is most pronounced at misorientation angles around 20°. Such trend applies to the pre-cracked situation but is much less pronounced. Both misorientation and pre-crack lead to size effect. The nominal strength shows a decreasing trend with the grain size, indicating that grain refinement tends to improve the load bearing capacity, which coincides with the observation in practice. Further, it is shown that the size effect diagram without hydrogen can be divided into three regimes. The conclusions apply to the case with hydrogen, except that the trend of the size effect curve can be affected by large grain sizes due to the longer absolute distance of hydrogen diffusion. These results provide guidelines for grain boundary engineering and for nanomechanical tests aiming at calibrating the intergranular decohesion parameters.

1. Introduction

Nickel alloys are often selected for subsea applications in critical components exposed to seawater and well fluid due to acceptable corrosion resistance and high strength [1]. These alloys, however, are prone to hydrogen embrittlement (HE), which is well recognized [2–5]: when exposed subsea, components made from nickel alloys are usually connected to the cathodic protection system which serves as a hydrogen source, part of the generated hydrogen will then adsorb on the surface and diffuse as atomic hydrogen into the metal thereby causing premature failure.

In order to alleviate the HE problem in metals, attempts from several perspectives have been reported. Ensinger [6] and Ćwiek [7] reported introducing external coating as hydrogen diffusion barrier to reduce the severity of HE; with the similar goal of limiting hydrogen uptake from the environment, surface treatment such as peening was reported to increase the resistance to HE [8]. Another category of research has focused on diffusion and redistribution after hydrogen enters the metal; it is generally assumed that the hydrogen population can be distinguished as diffusible and trapped (reversible and irreversible) according to the level of activation energy [9] and that only the diffusible hydrogen are responsible for HE. Therefore, the presence of strong traps could reduce the

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Nomenclature			
<i>HE</i>	hydrogen embrittlement	a_m	crack length corresponding to the nominal strength
<i>TSL</i>	traction separation law	$l_{c\#f}$	length of cohesive process zone at failure
E'	the effective Young's modulus	l_0	material length
$\sigma_{N,f}$	the nominal strength of the grain aggregate	L	grain size
σ_c	critical cohesive stress, or cohesive strength	η	ratio between l_0 and L
δ_c	critical cohesive separation	α_0	ratio between α_0 and L
σ_{yy}	the opening stress along the crack plane	α	ratio between α and L
r	true distance from the pre-crack tip	C_L	local hydrogen concentration
a_0	initial length of the pre-crack	C_B	outer boundary hydrogen concentration
a	current crack length	R	resistance to crack propagation

amount as well as the diffusivity of diffusible hydrogen, thus enhancing HE resistance of the component exposed to a given hydrogen source. Dadfarnia et al. [10] studied the hydrogen interaction with multiple traps and discussed the possibility to mitigate HE with this mechanism. Nagao et al. [11] reported that the introduction of nanosized (Ti,Mo)C precipitates improved the hydrogen resistance of a high-strength tempered lath martensitic steel by providing a high density of hydrogen traps. Olden et al. [12] and Ogita et al. [13] reported that the austenite phase in duplex steels could act as a sink and diffusion obstacle for hydrogen thereby affecting hydrogen redistribution and diffusion rate. All these studies agreed that the susceptibility to HE returns after saturation of strong trapping sites.

Grain boundaries are also potential trapping sites for hydrogen. Du et al. [14] performed first principle study where the mobility of hydrogen within the investigated grain boundaries was low compared to diffusion in perfect single-crystalline bulk, indicating hydrogen trapping effect. Oudriss et al. [15,16] performed experimental work on nickel showing that the grain boundaries with low misorientation ($\Sigma 1$) and a category of “special” boundaries ($\Sigma 3$ – $\Sigma 29$) are usually preferential areas for hydrogen segregation, which affects the hydrogen diffusion mechanism. On the other hand, it is recognized that other types of grain boundaries, e.g. the high-angle random boundaries considered as disordered phase, could serve as hydrogen path short-circuit thereby accelerating hydrogen diffusion [15–18]. The grain boundary effect on hydrogen diffusion is therefore two-folds and depends on the competition between these two mechanisms. In addition, the grain boundary character has obvious influence on the mechanical property of the material in the absence of hydrogen. Bechtel et al. [19] performed HE tests on nickel concluding that the special boundaries were intrinsically more resistant to fracture than random boundaries. Studies on the similar scope are seen in [20–23]. All these aspects of grain boundary effect need to be integrated into the design of HE resistant materials on the grain level, i.e. the grain boundary engineering. The concept of grain boundary engineering was proposed by Palumbo [24,25] as a redefinition of the idea of “grain boundary design and control” [26], and it has been widely applied in the development of high performance structural and functional polycrystalline materials in addition to HE [27,28]. A premise for grain boundary engineering 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 [14,20,29–31] and experimentally [15,16,19,32,33].

From a numerical aspect, atomic simulation approaches such as the density functional theory calculation and the molecular dynamics technique are increasingly popular considering that the grain structure in real life 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 and time scales. Actually, such methodology has proven a powerful tool in revealing the influence of a specific grain feature with good accuracy compared to the experimental results. Wei and Anand [34] investigated the grain boundary sliding and separation by modeling the grain interior with a crystal-plasticity model and the grain boundary with the cohesive zone model. Li et al. [30] 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. Most recently, Alvaro et al. [35] simulated the nanomechanical test performed on the nickel cantilever beam where the grain interior is assigned with orthotropic elasticity and the grain boundary modeled with the cohesive zone technique. The proper selection of micromechanism is fundamental for a continuum level simulation of HE, which determines the modeling technique and the applicability of the results. Two most well established HE mechanisms are the hydrogen enhanced decohesion (HEDE) model and the hydrogen enhanced localized plasticity (HELP) model [36]. The former claims that the presence of hydrogen reduces the cohesive strength of the lattice thus enhancing decohesion, and the latter claims that the presence of hydrogen enhances the mobility of dislocations thus enhancing localized plasticity. While these two mechanisms could act simultaneously in reality [37], we usually adopt only one of them as the underlying mechanism in the numerical simulation. In a continuum level simulation adopting the HELP mechanism, a hydrogen affected plasticity model is often implemented [38–40]. The simulation in the HEDE manner, on the other hand, employs usually the phenomenological decohesion model, e.g. the cohesive zone model whose parameters can be obtained from atomistic simulations [41–44].

Jothi et al. [45] parametrically studied the influence of grain boundary misorientation on hydrogen embrittlement in bi-crystal nickel by combining the stress analysis and the transient hydrogen diffusion analysis. They concluded that the grain misorientation has significant influence on the mechanical response as well as on the hydrogen diffusion, for instance, maximum opening stress and maximum local hydrogen concentration were observed in the cases with misorientation angles $15^\circ < \theta < 45^\circ$. In that study, however, the actual failure behavior could not be observed since neither an HE mechanism nor a corresponding failure criterion was attributed.

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