

Illuminating the chemo-mechanics of hydrogen enhanced fatigue crack growth in aluminum alloys



R.J. Zamora^a, K.L. Baker^b, D.H. Warner^{a,*}

^a School of Civil and Environmental Engineering, Cornell University, Ithaca, NY 14853, USA

^b Institute of Mechanical Engineering, Ecole Polytechnique Federale de Lausanne, Lausanne CH-1015, Switzerland

ARTICLE INFO

Article history:

Received 20 December 2014

Revised 9 August 2015

Accepted 15 August 2015

Available online 29 August 2015

2010 MSC:

00–01

99–00

Keywords:

Fatigue

Hydrogen embrittlement

Multi-scale modeling

Atomistic simulation

ABSTRACT

The presence of elemental hydrogen is known to accelerate fatigue crack growth in aluminum alloys. However, a direct link between experimental data and the governing atomistic mechanisms has remained elusive. Here we present a series of computational studies, across multiple length scales, directly linking an atomistic mechanism to experimental data for a specific aluminum alloy. Starting with an ab initio investigation of hydrogen bonding near the (111) aluminum surface, we quantify the effects of hydrogen surface impurities on slip and decohesion. We then modify an aluminum-only interatomic potential to reproduce ab initio trends by strategically shielding critical surface bonds in accordance with the environmental exposure level. The strategic shielding approach is used within a coupled atomistic-continuum discrete dislocation framework to predict the effect of hydrogen on near threshold fatigue crack growth rates. The predicted trends agree with published experimental data, suggesting that hydrogen enhanced surface deformation is a key failure mechanism for aluminum alloys in humid environments.

© 2015 Acta Materialia Inc. Published by Elsevier Ltd. All rights reserved.

1. Introduction

When an aluminum alloy is cyclically loaded (fatigued) at low loads in a controlled environment, an increase in humidity will significantly decrease the time to failure [1–3]. This is especially true when an edge crack is present on the surface of the loaded material. In this case, the exposed metallic surface at the advancing crack-tip is free to react with water and oxygen molecules in the air, a reaction which generates atomized hydrogen impurities in addition to an oxide film [4]. The presence of atomized hydrogen is experimentally linked to enhanced crack growth rates, a process commonly referred to as hydrogen assisted cracking (HAC) [3].

During a typical high cycle fatigue test, the relationship between the crack growth rate (da/dN) and the environmental exposure level (P/f) follows the general trend illustrated in Fig. 1. The exposure level, defined as the atmospheric pressure of water vapor (P) divided by the loading frequency (f), approximately describes the amount of water vapor available to react with the aluminum surface at the crack-tip per loading cycle. As stated, the H_2O –Al interaction is known to produce atomized hydrogen impurities, making P/f also proportional to the crack-tip hydrogen

concentration. Depending on the value of P/f , the crack growth behavior can be classified into one of three general regimes: (i) below the exposure threshold (T_{Exp}), the growth rate will be unaffected by exposure. (ii) Between T_{Exp} and the saturation threshold (T_{Sat}), the growth rate will increase proportionally with exposure. (iii) Above T_{Sat} , the growth rate will either plateau or continue to increase at a lower rate before reaching a plateau [2,3].

Here, we will focus on regime (ii), where da/dN is expected to increase proportionally with the environmental exposure level. In this regime, we assume that the surface near the crack-tip is not fully covered by an oxide [2,3], allowing for a range of possible surface coverages below the level of passivation. In the simulations discussed here, we consider only aluminum–hydrogen interactions, and leave the chemo-mechanical effects of oxide coverage for future study.

While HAC is often used to describe accelerated crack growth at exposure levels above T_{Exp} , the exact chemo-mechanical origins are rarely agreed upon. In the literature, HAC is often assumed to occur by mechanisms like hydrogen enhanced decohesion (HEDE) [5–7], in which impurities reduce surface energies and encourage decohesion, or by adsorption induced dislocation emission (AIDE) [8] and hydrogen enhanced localized plasticity (HELP) [9,10], in which impurities encourage dislocation emission and mobility. Although each of these mechanisms has been supported by one or both

* Corresponding author.

E-mail address: dhw52@cornell.edu (D.H. Warner).

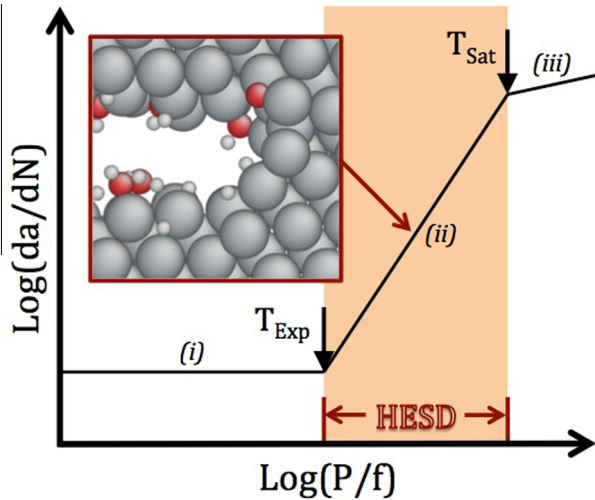


Fig. 1. Typical high cycle fatigue crack growth behavior expected for an Al-alloy over a range of environmental exposure levels. Here, we propose that hydrogen enhanced surface deformation (HESD) must be (at least partially) responsible for the proportional increase in da/dN as a function of P/f between the exposure (T_{Exp}) and saturation (T_{Sat}) thresholds (the highlighted area). Detailed descriptions of exposure regimes (i–iii) are presented in the text. The inset shows an HESD susceptible crack-tip system. Here, the crack-tip is not yet “saturated” by oxide formation, and an atomized hydrogen concentration is present on the surface. Large (dark-gray) atoms are aluminum, medium (red) atoms are oxygen and small (light-gray) atoms are hydrogen. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

theoretical and experimental studies [7,11,10,12], none has been explicitly used to predict experimental data within a physics based model.

Here, we have used electronic structure calculations to confirm that atomic hydrogen can generally weaken metallic bonding, accelerate both cleavage and dislocation slip at an exposed aluminum surface, a process that we will refer to as hydrogen enhanced surface deformation (HESD). Following this hypothesis, we used direct atomistic simulations to demonstrate that the underlying bond weakening effect responsible for the HESD mechanism accelerates the rate of fatigue crack growth in a manner consistent with experimental results. The atomistic simulations were performed using a concurrently coupled atomistic-discrete dislocation multiscale modeling framework, the bond shielding approximation developed here, and a well established empirical potential for pure aluminum.

2. Hydrogen binding at an aluminum surface

To quantify the effects of near surface hydrogen impurities on slip and decohesion, we started by identifying the most probable atomic sites for hydrogen to reside (i.e. we calculated the binding energies of near-surface interstitial lattice sites). Considering the fact that a crack-tip is essentially a free surface, we approximated the binding energy landscape of atomized hydrogen impurities at an aluminum crack-tip by considering a variety of interstitial sites near the (111) surface. Using the Kohn–Sham density functional theory (KS-DFT) approach [13], we determined a range of possible binding energies (E_B^H) by:

$$E_B^H = \left[E_{DFT}^{H+Al} - \left(E_{DFT}^{Al} + E_{DFT}^H \right) \right]. \quad (1)$$

Here, E_{DFT}^H is the energy of an isolated hydrogen atom, E_{DFT}^{Al} is the energy of the pure (111) surface and E_{DFT}^{H+Al} is the energy of the (111) surface with an adsorbed hydrogen atom.

All KS-DFT calculations were performed within the vienna ab initio simulation package (VASP) [14], utilizing PAW pseudopotentials in conjunction with the PBE exchange–correlation approximation at a plane wave energy cutoff of 450 eV. All k -point meshes were scaled to match a $15 \times 15 \times 15$ Monkhorst–Pack grid for a primitive fcc unit cell. Only one k -point was used in directions with vacuum. Equilibrium geometries were obtained by relaxing atoms to a force tolerance of 20 meV.

To obtain the binding energy results summarized in Fig. 2, a simple orthogonal supercell was used, consisting of 108 aluminum atoms, with the cell vectors being approximately 9.7 Å in the $[11\bar{2}]$ direction, 8.4 Å in $[1\bar{1}0]$ and 20.7 Å in $[111]$. To introduce a free surface, the $[111]$ cell vector was extended by an additional 15.0 Å, effectively creating a slab geometry with vacuum separating (111) and $(\bar{1}\bar{1}\bar{1})$ surfaces. This simulation geometry will be referred to as the *orthogonal* periodic surface cell. To capture realistic lattice spacing perturbations at the surface, the atoms within the five outermost (111) planes were allowed to relax on one side of the slab. Standard convergence tests (with 50 meV/atom criteria) were used to determine both the vacuum distance and the number of surface planes to relax. Although relaxing three surface planes resulted in accurate binding energies for interstitials confined to the outermost (111) plane, the relaxation of five surface planes was used to allow deeper interstitial sites to be characterized.

Due to the periodic nature of the simulation supercell, the presence of a single hydrogen atom results in a planar impurity concentration of about $0.0082/\text{Å}^2$, or about 8.3% monolayer surface coverage. Systematic convergence testing revealed that such an impurity concentration accurately predicts isolated binding energies within an approximate energy tolerance of 50 meV/atom.

Overall, the binding energy predictions agree with other ab initio work [15,11], supporting the popular wisdom that an isolated hydrogen impurity will most likely occupy a surface position in the absence of unsaturated sub-surface vacancies and dislocation cores. Furthermore, considerations of biaxial and uniaxial strain were not found to significantly change the favorability of the free surface over sub-surface sites. Therefore, the energetic favorability of hydrogen ingress does not seem to depend strongly on the elastic stress state near the surface.

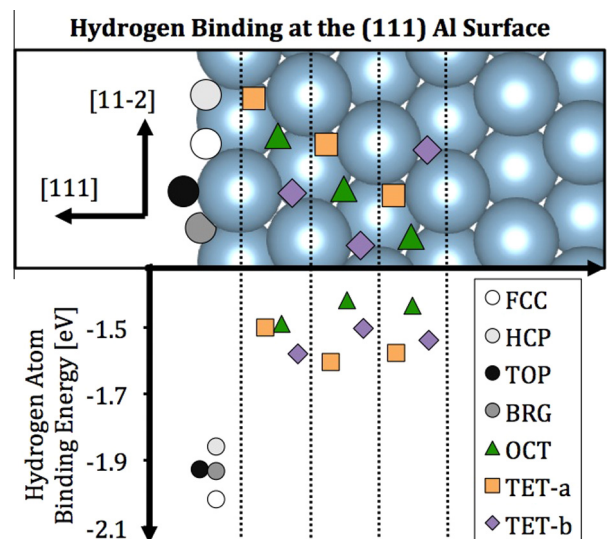


Fig. 2. Binding energies (E_B^H) for a variety of isolated interstitial hydrogen impurity sites at the (111) aluminum surface, according to Eq. (1). All calculations were performed using the PAW-PBE Al and H pseudopotentials in VASP [14].

Download English Version:

<https://daneshyari.com/en/article/7879422>

Download Persian Version:

<https://daneshyari.com/article/7879422>

[Daneshyari.com](https://daneshyari.com)