



Multi-field modelling of hydride forming metals Part II: Application to fracture



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ABSTRACT

In Part I of the present article, we formulated a continuum-based computational model for stress- and temperature-directed diffusion of hydrogen in metals that form brittle binary hydrides, such as Zr and Ti alloys. Among the space–time dependent parameters calculated by the model are the volume fraction and the mean orientation of hydride precipitates. These parameters are of importance for quantifying the embrittlement of hydrided materials. In this second part of the work, we use measured data for the strength and toughness of hydrided Zr alloys to correlate the local fracture properties of the two-phase (metal + hydride) material to the aforementioned parameters. The local fracture properties are used as space–time dependent input to a cohesive zone type submodel for fracture, which is fully integrated with the hydrogen transport model from Part I. The complete model is validated against fracture tests on hydrogen-charged Zr–2.5%Nb, a material used in nuclear reactor pressure tubes. More precisely, we study local embrittlement and crack initiation at a blunt and moderately stressed notch, resulting from gradual accumulation of hydrides at the notch during temperature cycling. We also simulate tests on crack initiation and growth by delayed hydride cracking, a subcritical crack growth mechanism with a complex temperature dependence. From the results of the simulations, we conclude that the model reproduces many observed features related to initiation and propagation of hydride induced cracks in the Zr–2.5%Nb material. In particular, it has the capacity to reproduce effects of the material's temperature history on the fracture behaviour, which is important for many practical applications.

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1. Introduction

A finite-element based multi-field continuum model, accounting for the interaction between mechanical behaviour and hydrogen behaviour in hydride forming metals, was formulated in Part I of this paper [1], in which the model was also validated against experiments on hydrogen transport, metal-hydride phase transformation and stress-directed orientation of hydride precipitates. In this second part of the paper, we describe the cohesive zone model used for fracture of the hydrided material in detail and demonstrate the model's capacity to reproduce initiation and propagation of hydride induced cracks in a particular zirconium alloy.

As already touched upon in Part I, zirconium and titanium alloys may become significantly embrittled by the precipitation of binary metal hydrides. Of particular concern are precipitates of face-centered cubic (fcc) δ -hydride, which are platelet-shaped and contain 0.61–0.65 at% hydrogen [2]. For a given temperature, the degree of embrittlement depends on the volume fraction, ori-

entation, size and distribution of the δ -hydride precipitates. In regard to mechanical properties for the hydrided material, the hydride precipitates affect primarily the fracture toughness and the total elongation, i.e. the plastic strain to failure in tension. However, if the material contains hydride platelets oriented such that their normals are parallel to the loading direction, also the yield strength and ultimate tensile strength (UTS) are degraded [3].

Several mechanisms contribute to hydride-induced embrittlement of Zr and Ti alloys [3]: At low temperature and sufficiently high hydride concentrations, the embrittlement is mainly due to hydride fracture, i.e. cracks propagate through a network of interconnected hydrides, which provide a brittle crack path through the material. Hydrides precipitate preferentially, but not exclusively, on grain boundaries, which means that the hydride network morphology is affected by the grain structure of the metal. Consequently, the hydride volume fraction required to form a continuous network of hydrides, through which brittle fracture can take place, depends on the microstructure and thus on the thermo-mechanical manufacturing route for the material: It has been shown that manufacturing routes leading to finer grain structures generally produce materials that can accommodate a larger hydride fraction without loss of ductility [4,5]. The threshold hy-

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hydride volume fraction for formation of a continuous hydride network in α -phase Zr and Ti alloys is typically in the range of 0.03–0.05 [6–8]. However, continuous brittle crack paths through hydrides can be formed at even lower hydride fractions, if the hydrides are preferentially oriented. The direction of loading in relation to the orientation of the platelet-shaped δ -hydride precipitates is therefore very important for crack propagation in a brittle manner.

At temperatures above approximately 400–450 K, the metal matrix generally yields before the δ -hydrides fracture [9], which means that brittle fracture through a network of hydrides becomes unlikely. Hence, at low hydride concentration and/or elevated temperature, the hydride-induced embrittlement is generally not caused by hydride fracture. The embrittlement is instead attributed to either of two effects, pertaining to irradiated and unirradiated materials, respectively. In Zr and Ti alloys that have been exposed to high energy radiation, plastic deformation usually takes place in dislocation channels with limited extension, due to the high density of radiation induced lattice defects [10]. Plastic deformation may therefore be hindered even by a moderate concentration of hydride precipitates [11]. In unirradiated materials, dislocation movements takes place more uniformly, and plastic deformation is therefore not so easily hindered by sparsely located hydrides. In this case, the embrittlement is attributed to initiation and link-up of voids in the material, promoted by hydride precipitates [12–14]. Nucleation and growth of voids reduce the macroscopic ductility of the material, even though the solid material between the voids possesses significant ductility. The fact that different embrittling mechanisms come into play, depending on the hydride concentration, hydride orientation, temperature, radiation dose and stress state in the material, makes modelling of the embrittlement difficult. There are also differences between materials, e.g. in alloy composition and microstructure, which further complicate the picture.

In addition to the aforementioned embrittling effects, which may cause critical (unstable) fracture in hydrided Zr and Ti alloys, precipitation of hydrides may also challenge the structural integrity through slow, subcritical fracture mechanisms [3]. This is because hydrogen in solid solution diffuses towards regions with high hydrostatic stress, which over time may lead to local hydride formation ahead of stress-concentrators, such as flaws and cracks. Ultimately, the locally embrittled and stressed region may fail, leading to a short (few tens of microns) increment of crack growth. The process then repeats itself, thus giving rise to stable crack growth, the rate of which is basically controlled by the rate of hydrogen diffusion to the peak stress region. This subcritical fracture mechanism is known as sustained load cracking (SLC) for titanium alloys [15] and as delayed hydride cracking (DHC) for zirconium alloys [16]. It has been responsible for failure of Ti alloy components in aircrafts [17] and Zr alloy components in chemical plants and nuclear power reactors [18].

As with other environmentally assisted crack growth mechanisms, the crack growth rate under SLC or DHC is strongly dependent on temperature and stress intensity. The temperature dependence is complex, since the crack growth rate is affected not only by the current temperature, but also by the temperature history of the material [16]. The typical relation between crack growth rate and stress intensity for DHC in zirconium alloys is illustrated in Fig. 1. The indicated numbers for crack growth rate and stress intensity are typical values for temperatures around 550 K.

At stress intensities below a certain threshold, K_{IH} , the crack does not grow, even though hydrides may form ahead of the crack front. In this case, the tensile stress and/or the size of the hydrided region ahead of the crack front are insufficient for local fracture to occur. For stress intensities above K_{IH} , the crack grows, and three

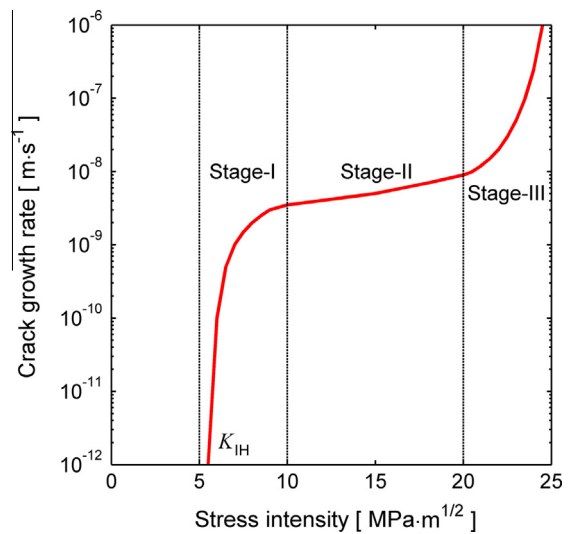


Fig. 1. Typical relation between crack growth rate and stress intensity for delayed hydride cracking (DHC) in zirconium alloys at 550 K; see e.g. [16] and references therein. K_{IH} is the threshold stress intensity for DHC, below which the crack growth rate becomes vanishingly small.

distinct regions, or stages, can be identified. In stage I, the crack growth rate is very sensitive to the stress intensity. In stage II, the growth rate does not change significantly with increasing stress intensity. This trend is broken in stage III, where the applied stress intensity approaches the material's fracture toughness, and initiation of unstable fracture is imminent. From an engineering point of view, the two most important parameters for DHC or SLC in a specific material are the threshold stress intensity factor, K_{IH} , and the stage-II crack growth rate.

In the following, we make use of various mechanical tests on hydrided zirconium alloys to validate the computational model from Part I [1]. Details of the cohesive zone fracture model and how it is linked to the calculated distribution of hydride precipitates in the material are first given in Section 2. In Section 3, we present and discuss results from validation of the model against mechanical tests reported in the literature. The intention is to assess the capacity of the model to reproduce initiation and propagation of hydride induced cracks. Section 4 discusses the strengths and weaknesses of the presented modelling approach in light of the results from Section 3. Conclusions are drawn in Section 5, where also suggestions for model improvements and further work are given.

2. Cohesive zone fracture model

As explained in Part I [1], we model initiation and propagation of cracks by embedding a decohesion law for the material within a specific kind of finite elements. Fracture is thus regarded as a gradual process, which takes place in a finite-size region ahead of the crack front, where separation of the material is resisted by cohesive tractions; see Fig. 4 in [1]. In the following subsections, we will focus on the applied decohesion law, which is the mathematical relation between the cohesive tractions and the separation of the material. The decohesion law utilized depends on the local state of the material at the crack front, and in particular, on the concentration and orientation of hydride precipitates.

2.1. Decohesion law

In Appendix B to [1], we showed that the local cohesive tractions at the crack front, T'_i , can be related to the local displacement jumps across the crack plane, w'_j , through

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