Modelling of hydrogen-induced ductility loss in titanium-based hydrogen storage

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Abstract

One promising solution for decarbonisation is the use of hydrogen as energy carrier. Besides its exceptional advantages like high calorific value, better safety and non-existent harmful emissions, one major challenge is still hydrogen embrittlement of titanium alloys used as a hydrogen storage. In this work, a method is presented that can numerically model and determine a threshold concentration of hydrogen in solid solution responsible for a sudden ductile-to-brittle transition. The origin of this sudden loss of ductility lies in the segregation thermodynamics that is modelled together with an elastoplastic fracture mechanics model. Starting from experimental fracture mechanics test data, a meaningful coupling mechanism was found for the fracture mechanics cohesive zone model in the form of a segregation-modified cohesive energy that triggers an acceleration of crack extension above defined concentration values. It can be demonstrated that above a threshold of only few atomic percent hydrogen in the solid solution, the segregated hydrogen concentration exceeds 20 at.%. The current results present a mechanism that enables the modelling of the sudden ductility loss triggered by a segregation-affected crack energy expression in titanium alloys exposed to hydrogen. This method is not only applicable to other various materials but can also be a substantial benefit for the safety assessment of hydrogen storage devices.