ASSESSMENT OF HYDROGEN EMBRITTLEMENT BEHAVIOR IN AL-ZN-MG ALLOYS BY MULTI-MODAL 3D IMAGE-BASED SIMULATION

Hiro Fujihara, Kyushu University
fujihara@mech.kyushu-u.ac.jp
Hiroyuki Toda, Kyushu University
Kenichi Ebihara, Japan Atomic Energy Agency
Masakazu Kobayashi, Toyohashi University of Technology
Kazuyuki Shimizu, Iwate University
Akihisa Takeuchi, Japan Synchrotron Radiation Research Institute
Masayuki Uesugi, Japan Synchrotron Radiation Research Institute

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Recent first-principles calculations have reported that the interface between $MgZn_2$ precipitate and aluminum spontaneously debonds without stress when the hydrogen concentration at the interface reaches 10^{26} atoms H/m^3, and proposed this as a new mechanism of hydrogen embrittlement on a nanoscopic scale in Al-Zn-Mg alloy. Since hydrostatic stress, which act as a driving force for hydrogen diffusion, is to be high ahead of a crack tip, the precipitate debonding behavior could occur in a such region and it can cause eventually macroscopic fracture as hydrogen embrittlement. The local hydrogen accumulation behavior under stress must be investigated to determine if there is a correlation between nanoscopic hydrogen-induced debonding and macroscopic HE fracture behavior. In the present study, to investigate local hydrogen accumulation in the region associated with hydrogen embrittlement, particularly at the precipitate interface, the multi-modal three-dimensional (3D) image-based simulation combining a crystal plasticity finite element method and hydrogen diffusion simulation was conducted. The experimental and image-based simulation results could be directly compared, and hydrogen embrittlement behavior was interpreted based on the simulated hydrogen accumulation behavior in actual hydrogen embrittlement region.

Intergranular cracks initiated from the specimen surface, then they transitioned to quasi-cleavage cracks. The 3D image-based model was built based on the 3D microstructure. Heterogeneous stress and strain distribution appeared due to the difference in deformation resistance of each grain (Fig. 1a). The hydrostatic stress was elevated to more than 2 GPa in the vicinity of the intergranular crack tip. Hydrogen was accumulated corresponding to the distribution of hydrostatic stress (Fig. 1b). The hydrogen concentration increased to more than twice the initial concentration in a region limited within 5 μm from the crack tip, and the maximum hydrogen concentration reached 5 times the initial hydrogen concentration at the crack tip.

The hydrogen partitioning behavior caused by hydrogen accumulation under stress was evaluated. Accumulated hydrogen was mainly repartitioned to the vacancy and precipitate interface near the crack tip. The hydrogen occupancy of the semi-coherent interface of the precipitate is increased locally in the vicinity of the crack tip, and reached almost 1.0, which is the criterion of hydrogen-induced debonding behavior. The crack propagated into the region where the hydrogen occupancy of the $MgZn_2$ precipitate interface was higher than 0.6 (Fig. 2). The interfacial cohesive energy of the $MgZn_2$ precipitate might reduce by more than 60% compared to the initial state. This result agrees with the proposed mechanism that the nanoscopic hydrogen-induced debonding behavior of the $MgZn_2$ precipitate interface causes hydrogen embrittlement. It would appear that hydrogen embrittlement in the Al-Zn-Mg alloy was dominated by dynamic hydrogen partitioning to the $MgZn_2$ precipitate interface.

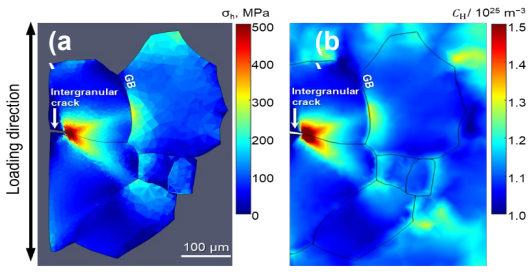

Figure 1 – The distribution of (a) hydrostatic stress and (b)

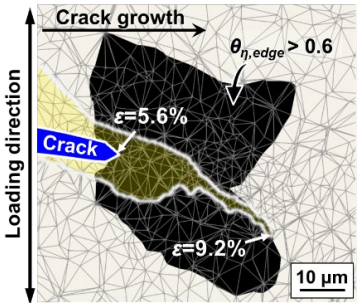

Figure 2 – Hydrogen occupancy distribution at the intergranular crack tip