DEFECT-HYDROGEN INTERACTION IN AL ALLOYS: CHALLENGES AND BENEFITS REVEALED BY AB INITO CALCULATIONS

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Climate change motivates the search for light-weight materials for transportation and energy storage solutions. As one of the challenges, the deleterious effect of hydrogen on the mechanical properties of metallic alloys is known to reduce the applicability of metallic alloys, motivating the characterization and simulation of hydrogen-defect interactions in these materials. In this work, the interaction of hydrogen with planar defects in aluminium has been investigated by means of ab initio simulations.

On the one hand, two distinct types of GBs have been considered – the Σ11(113) [011] with a close-packed interface structure and the Σ5(210) [001] with a more open interface structure – in order to reveal the mechanisms governing the H segregation energetics. The investigations are afterwards extended to the impact of solutes in the Al alloy. Two scenarios are compared: Their segregation to the grain boundaries and their binding in precipitates. We therewith gained insights into the role of the solute size on the structural and chemical embrittlement in absence and presence of hydrogen. A thermodynamic assessment of the impact of solutes onto H chemisorption in the interfacial vicinity is provided by performing a high-throughput analysis for potential alloying candidates. The identified trends of the solute-H interactions are used to examine the relative importance of changes in hydrogen enhanced decohesion as a thermodynamic effect.

On the other hand, the interaction of hydrogen with defects can be beneficial for the formation of metal hydrides. To enhance the formation and stability of such often highly volatile hydrides we have consider a novel concept: tailoring and employing the negative pressure of microstructural and structural defects to enhance H solubility and thus hydride formation. Using systematic ab initio and atomistic simulations, we demonstrate that an enhancement in the formation of hydrides at the negatively pressurized crack tip region is feasible by increasing the mechanical tensile load on the specimen. The theoretical predictions have been used to reassess and interpret atom probe tomography experiments for a high-strength 7XXX-aluminium alloy that show a substantial enhancement of hydrogen concentration at structural defects near a stress-corrosion crack tip. Based on these insights we derive strategies for enhancing the capability of metals as H-storage materials.