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A Novel Metal Physics Model for Hydrogen Adsorption and Absorption in Steels

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Extended Abstract

Recently, transportation of high-pressure hydrogen gas (H2) by steel pipelines have attracted wide attention. It is generally accepted that, without sufficient progress on infrastructure for safe, reliable, and large-scale H2 transportation, hydrogen economy will face significant barriers. Re-purposing existing gas pipelines will be key to developing a large-scale hydrogen economy and is even critical to achieve the net-zero emission target.

Safety of pipelines in hydrogen service has been a concern in terms of hydrogen embrittlement (HE) phenomenon occurring on steels. Different from extensive research work conducted in aqueous environments where the so-called "cathodic" hydrogen is generated and introduced into the steels, the environment where pipe steels are exposed in hydrogen pipelines is high-pressure hydrogen gas, where the hydrogen permeation occurs at a mechanism completely different from the "cathodic" hydrogen. The gaseous H2 must dissociate into atomic hydrogen (H), and the atomic hydrogen potentially enters the steels.

There are two possible mechanisms for generation and adsorption of H atoms on steel surface, i.e., spontaneous dissociation and dissociative adsorption. The thermodynamics of the two processes will be theoretically calculated based on free energy changes so that the principle for hydrogen atom generation in H2 pipelines will be determined. Furthermore, a metal physics model is developed to characterize the H adsorption (Hads) configuration on the steel surface. Effects of H adsorption site, H coverage and hydrostatic stress on H adsorption and absorption will be discussed. The crystalline lattice sites hosting absorbed H atoms (Habs) at subsurface of the steel are defined. Implications of the research outcomes on HE and its control for hydrogen pipelines are discussed.