PREDICTING HYDROGEN EMBRITTLEMENT OF STAINLESS STEELS USING PHYSICS-BASED MACHINE LEARNING

Michael C. Gao, National Energy Technology Laboratory
michael.gao@netl.doe.gov
William Trehern, National Energy Technology Laboratory/Leidos
Shun-Li Shang, Pennsylvania State University
Zi-Kui Liu, Pennsylvania State University

Key Words: Hydrogen embrittlement, machine learning, first-principles density functional theory, CALPHAD

Hydrogen, even in small amounts, can cause severe degradation to mechanical properties of metals, known as hydrogen embrittlement (HE), such as the loss of ductility and fracture toughness. Despite many decades' studies in HE of metals and various proposed mechanisms and models, to date a comprehensive understanding of HE is still lacking. This is mainly because HE involves the interplay among thermodynamics, kinetics, mechanical behavior, and microstructure as well as environment. In this work, a large dataset of high-quality literature data on HE in stainless steels is first developed and visualized. Multiscale modeling using first-principles density functional theory and CALPHAD is performed to provide physical insight into HE mechanisms. Important properties are predicted, including intrinsic ductility via computing unstable stacking fault energy and surface energy, H adsorption energy and H diffusivity. Based on high-fidelity experimental and synthetic data of stainless steels, multiple machine learning models are trained and then tested including random forest, XGBoost and neural networks. Key descriptors important to HE in stainless steels are identified and ranked based on the importance to the model. Approaches for improving HE resistance of stainless steels via new alloy discovery with optimal microstructure will be discussed.