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How to separate a grain boundary? The effect of hydrogen environment

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Abstract

This research belongs to Project 1 in the roadmap of hydrogen material compatibility division: physical descriptions of hydrogen-materials interactions, which is focused on elucidate mechanisms and formulate physical descriptions for hydrogen-materials interactions and hydrogen-induced degradation in structural metals to inform alloy development and predictive crack propagation models.

The mechanism of hydrogen on metal mechanical properties remains a topic of debate. There is still lack of understanding on the formation mechanism, evaluation method, and the predictive framework of this intergranular fracture, and more efforts are required. Recently, cell dislocation structures formed by hydrogen-enhanced local plastic deformation beneath the fracture surface are found to be one of the most important factors in the formation of intergranular fracture. However, the dislocation emission and dislocation-grain boundary interaction in the formation process of intergranular fracture is still unknown.

By using a density functional theory based empirical potential, the interface energies of 50 types of Fe grain boundaries and free surfaces were calculated in thermodynamic equilibrium with hydrogen-poor and hydrogen-rich environments. We extended the classical model for calculating the ideal work of separation with solute atoms to a level that distinguishes every trapping site on the interface. All possible trapping sites for hydrogen were addressed to create a series of initial Fe-H configurations, and this approach gives energies for estimating the lowest-energy structures at different hydrogen chemical potentials (or pressures). Hydrogen atoms in grain boundary have higher trapping energy and more *unsafe* trapping sites than in free surface, coverage of hydrogen on grain boundary is always unsaturated under conditions of limited hydrogen chemical potential. The decrease in separation work at pressures lower than 1000 atm, which are the conditions used to experimentally investigate hydrogen embrittlement, was calculated to be only half the magnitude of the decrease at the hydrogen-rich condition used in the classical model. The generous model proposed here resolves the discrepancies between previous theoretical work and experimental results, and stresses the important role of other defects around grain boundary.

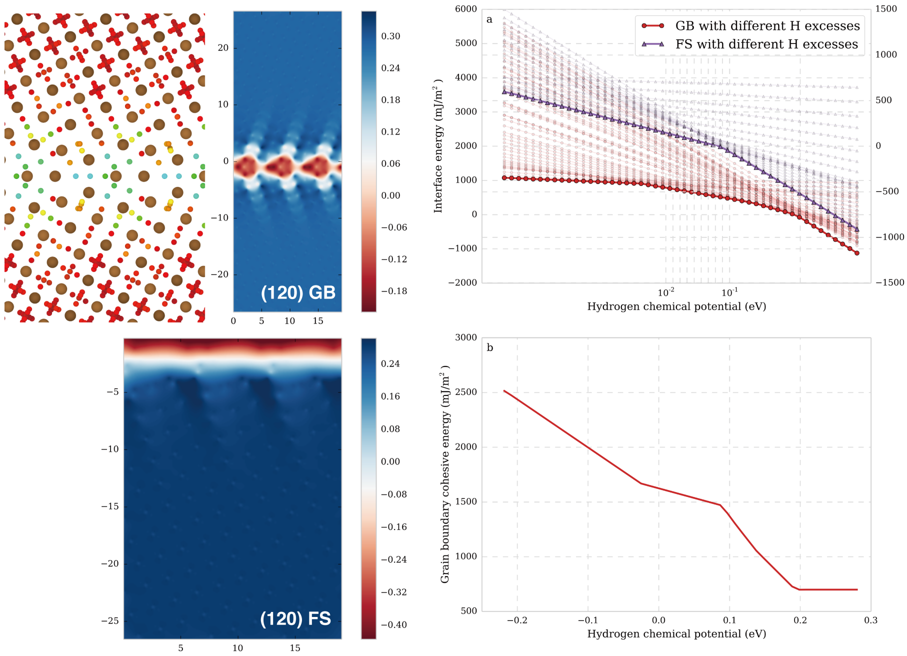

Figure 1 The trapping site map of hydrogen atoms (left) and the variation of interface energy as a function of hydrogen chemical potential.