"Atomistic Modeling of The Impact of Hydrogen on Metals"

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The impacts of hydrogen on the mechanical behavior of metals have been studied for many years, and many models and theories have been proposed. However, many issues remain open due to the difficulty in the direct observation of hydrogen behavior in materials. Therefore, atomistic modeling and simulation are promising tools that can directly examine the hydrogen behavior and its impacts on the mechanical behavior of metals, such as plasticity, defect growth, and fracture. Therefore, a vast number of atomistic simulations have also been performed. However, the lack of reliable atomic interactions has limited atomic simulations to small-scale density functional theory (DFT) calculations or qualitative molecular dynamics (MD) calculations. To overcome this problem, we recently constructed a general-purpose artificial neural network interatomic potential (ANNIP) for the iron-hydrogen binary system based on a DFT-based training dataset. The ANNIP was successfully applied to quantitatively simulate and understand the essential phenomena dominating the hydrogen-induced degradation of metals, such as hydrogen diffusion at defects, hydrogen trapping/desorption at defects, hydrogen-assisted cracking at the grain boundary, hydrogen-accelerated defect motion, and so on.