Hydrogen charging stations, Hydrogen-fueled cars, Ultra-strength structural materials

Atomistic study of hydrogen effects on materials strength

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Abstract

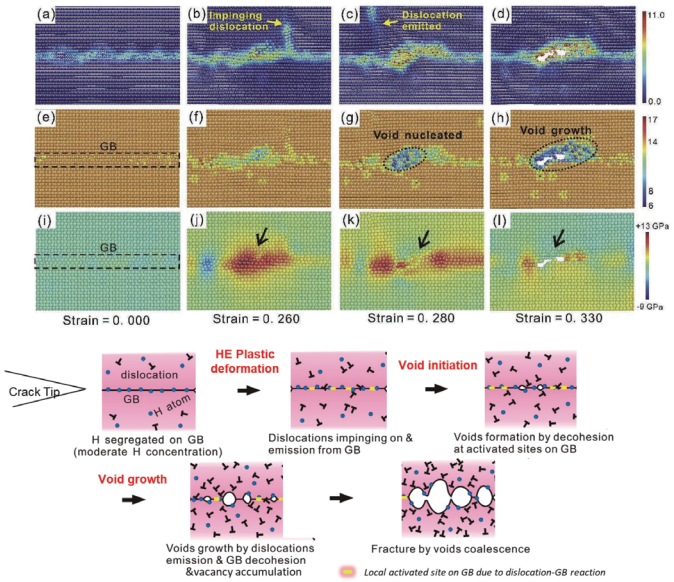
Hydrogen embrittlement has been known for a long time, and the phenomenon is particularly pronounced in advanced high-strength materials. In this study, we analyze the behavior of hydrogen atoms in materials undergoing deformation and fracture, which are extremely difficult to observe experimentally, by means of high-precision atomic simulations (molecular dynamics simulations) to clarify the atomistic details of the mechanism. Using neural networks, we have solved the problem of accuracy in the atomic interactions used in the atomic simulations, which have been the bottleneck for a long time in these simulations. We have made it possible to perform atomic-level simulations with unprecedented accuracy and scale.

Background & Results

Hydrogen embrittlement is an essential issue for the safe handling of hydrogen. Although many experimental and simulation studies have been carried out for more than half a century, they have remained unachieved due to the difficulty of direct observation of hydrogen and the difficulty of atomic simulations for the description of atomic interactions. In our study, the development of high-precision atomic interactions based on neural network has removed the bottleneck, solving the long-standing problem in hydrogen embrittlement research. In the future, we expect to establish material design guidelines for hydrogen-resistant materials and accelerate the development of a high performance hydrogen-resistant materials.

Significance of the research and Future perspective

The hydrogen embrittlement phenomenon has been studied for more than half a century and a number of theories have been proposed. However, the mechanism of hydrogen embrittlement remains unclear due to the difficulty in directly observing the hydrogen in materials. So far, research on hydrogen embrittlement has been conducted both experimentally and through atomic-level simulations. In experiments, the mechanism was inferred based on indirect data collected because direct observation of hydrogen is not possible. On the other hand, atomic simulations, such as molecular dynamics, can directly analyze the behavior of hydrogen in materials. Still, there was a problem in the accuracy and the computational cost for the expression of the atomic interactions, In this study, we have developed a neural network atomic interactions that is capable of machine learning the results of high-precision first-principles calculations to enable large-scale analysis while maintaining high accuracy, thereby allowing us to track the behavior of hydrogen with unprecedented accuracy. Through this research, the specific mechanism by which hydrogen strongly interacts with defects in materials, thereby accelerating defect motion and growth in materials undergoing the deformation and the fracture, has been clarified at the atomic-evel.



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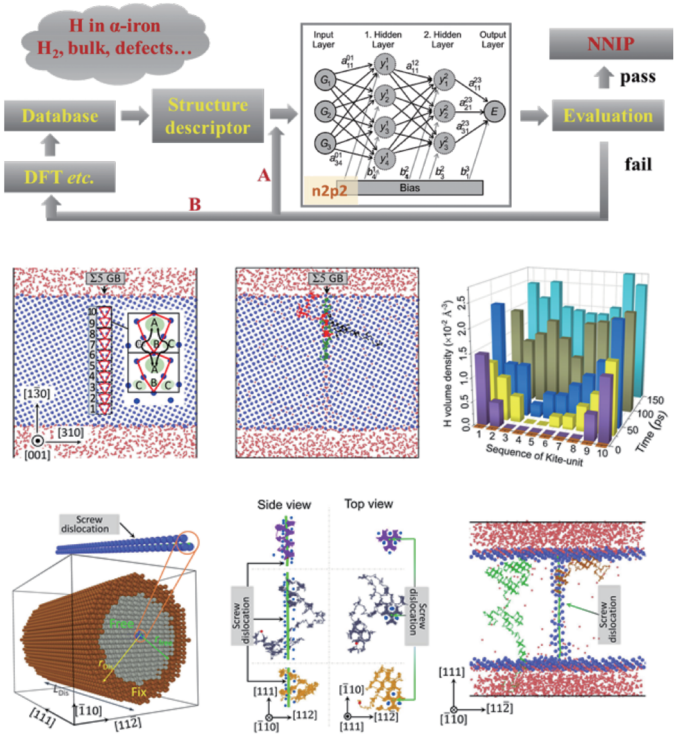

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Patent

Treatise

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Keyword hydrogen embrittlement, deformation and fracture, atomic simulation, machine learning