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Accurate Atomistic Study on Hydrogen Solubility in α-Iron at High H_2 Pressures

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ABSTRACT

Hydrogen dissolves in most metallic materials and causes hydrogen embrittlement (HE). This is particularly relevant to iron, a widely used material in engineering applications, which can degrade when exposed to high-pressure hydrogen gas under high temperature. As the hydrogen concentration is a primary factor controls defects properties in metals [1], it is crucial to understand the hydrogen solubility under high H_2 pressure, but this aspect remains unclear. At low H_2 pressures, the solubility of hydrogen can be predicted using Sieverts' law [2], which states that the solubility increases proportionally to the square root of H_2 partial pressure. However, when the pressure is high, the failure of Sieverts' law is expected due to the molecular interaction of H_2 [3]. Due to the extremely small size of hydrogen, it is hard to make direct observation. Therefore, in this research, the temperature-dependent solubility of α-iron at different H_2 pressures has been calculated by using molecular dynamics (MD) simulations, with highly accurate machine learning potential [4] based on density functional theory results for iron and hydrogen binary system. Our findings reveal that under moderate hydrogen pressures, the solubility of hydrogen in α-iron follows a modified Sieverts' law, where the hydrogen solubility is proportional to the hydrogen fugacity. However, at higher hydrogen concentrations over 1000 ppm, deviations from the modified Sieverts' law occur due to hydrogen-induced volume expansion and interactions between atomic hydrogen.

KEYWORDS

Hydrogen solubility; α-iron; molecular dynamics; machine learning potential

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