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Molecular Dynamics Simulations of the Hydrogen Embrittlement Base Case: Atomic hydrogen in a defect free single crystal

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ABSTRACT

While significant research has been conducted on the various mechanisms of hydrogen embrittlement, there remains a lack of quantitative understanding on the effect of atomic hydrogen concentration on mechanical properties. Previous experimental work suggests that an increased hydrogen concentration will degrade both the elastic modulus and yield stress. However, experimental samples often contain other atomistic defects that make it difficult to determine the role hydrogen alone plays on material behaviour. Further, experimental studies are often unable to directly quantify the effect of hydrogen concentration on modulus. Therefore, the purpose of this study was to use molecular dynamics simulations to quantify the effect of interstitial hydrogen on the mechanical properties of perfect single crystal alpha iron during loading. Results demonstrated the potential type used significantly affected predicted results. The EAM potential for Fe-H systems was selected as it accurately predicted both the hydrogen free modulus and diffusion coefficient of hydrogen in iron. Atomic hydrogen between 0.5 - 5% was shown to linearly degrade the elastic modulus and stress to initiate dislocations at all temperatures considered. Increasing hydrogen concentration was shown to promote the formation of dislocations at a lower stress, resulting in a higher density of dislocation and shorter slip distances. Through demonstrating the effect of atomic hydrogen alone, without other atomistic defects, this study provides a foundation for better understanding the role of hydrogen on the degradation of mechanical properties during loading.

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