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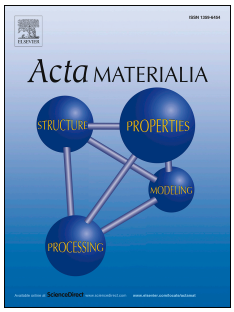

Ab initio simulation of hydrogen-induced decohesion in cementite-containing microstructures

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Ab initio simulation of hydrogen-induced decohesion in cementite-containing microstructures

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Abstract

In high-strength carbon steels suitable for use in the automotive industry, hydrogen embrittlement (HE) is a potential barrier to the widespread application of these materials. The behaviour of hydrogen within the most prevalent carbide, namely cementite, has been investigated via *ab initio* simulation. In order to examine possible decohesion effects of hydrogen on carbon steels, the binding and diffusion of hydrogen at the interface between ferrite and cementite has been examined. In order to understand the effect of hydrogen on the mechanical properties of carbon steels, simulated *ab initio* tensile tests have been performed on the ferrite-cementite bicrystal. The results of the tensile tests can be combined with thermodynamic considerations in order to obtain the expected hydrogen concentrations at such ferrite-cementite phase boundaries. We find that the effect of hydrogen on the cohesion of the phase boundary may be significant, even when the bulk hydrogen concentration is low.

Keywords: hydrogen embrittlement, *ab initio* simulation, carbon steels

1. Introduction

The phenomenon of hydrogen embrittlement (HE) has a significant influence on the mechanical stability of a wide range of metallic systems, and the embrittling behaviour frequently leads to catastrophic damage of metallic components. A frequent observation has been that high-strength metallic alloys are more susceptible to hydrogen damage, but there has been limited

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