EFFECT OF HYDROGEN ON PHASE STABILITIES IN STEELS

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Hydrogen embrittlement (HE) is a persistent mode of failure in advanced high-strength steels. During the service life of these steels phase transformations occur and are a key element that determines their response to the service loads. Thus, the investigation of the role of hydrogen atoms in the relative stability of the phases present and forming in steels is of great interest.

In this work, we studied the role of hydrogen on the relative stability of the fcc/bcc/hcp phases using the ab initio thermodynamics. The results indicate that at low hydrogen chemical potentials the stability of the fcc phase, which can be representative of retained austenite (RA) in steels, is slightly enhanced by the presence of hydrogen atoms. In contrast, at high hydrogen chemical potentials the bcc phase is stabilized by H. Moreover, since the excess volume of the hydrogen-rich bcc phase is significantly larger than that of the fcc phase, the presence of a stress field can change the relative stability of these phases in the coexistence regions of the phase diagram. This feature is particularly important for cyclic loading conditions: during loading cycles forward and reverse phase transformations occur and the hydrogen released by these transformations can damage the material.