Hydrogen-carbide interactions in steels: Ab-initio combined with experiment

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The development of advanced high-strength steels is in high demand because of its
wide scale applications. One of the promising candidate in this regard is the austenitic
Fe-Mn-Al-C steels which exhibit interesting mechanical properties such as exceptional
combination of high strength and ductility along with low density and high corrosion
resistance. The excellent mechanical properties of these steels are mainly attributed to
the microstructure features that correlate with deformation mechanisms and strongly
depend on the amount of Al in the material. An Al content higher than 6 wt.% in these
alloys promotes precipitation of regularly arranged nano-sized κ carbides during
annealing. There are conclusive experimental evidences of these precipitates playing a
crucial role in the strengthening of the Fe-Mn-Al-C steels. Our aim is to validate the
experimental finding by employing density functional theory (DFT) to investigate the
role played by the κ carbide in these Al-rich steels. Since the strengthening effects undergo
modifications depending on the stoichiometry of the carbide, we initiate our study by
performing a detailed analysis of the stoichiometry of these carbides. Our DFT
investigations reveal a deviation from stoichiometry for both Al and carbon in κ carbide
which is confirmed by atom probe tomography (APT) technique. One of the reasons
behind the off-stoichiometry is found to be the elastic strains posed by the coherent
interface between the carbide and the matrix. Furthermore, the off-stoichiometry is
found to be decisive in quantifying the amount of hydrogen in these steels as the carbon
vacancies inside the carbide as well as in the interface act as traps for hydrogen. Our
study, thus, not only explains the off-stoichiometry but also sheds light on the efficient
ways of controlling diffusive hydrogen in these steels thereby making them suitable for
automotive applications.