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Formation Energies and Electronic Properties of Vanadium Carbides Found in High Strength Steel Alloys KRISTA LIMMER, JULIA MEDVEDEVA, Missouri University of Science and Technology — Carbide formation and stabilization in steels is of great interest owing to its effect on the microstructure and properties of the Fe-based alloys. The appearance of carbides with different metal/C ratios strongly depends on the carbon concentration, alloy composition as well as the heat treatment. Strong carbide-forming elements such as Ti, V, and Nb have been used in microalloyed steels; with VC showing an increased solubility in the iron matrix as compared with TiC and NbC. This allows for dissolution of the VC into the steel during heating and fine precipitation during cooling. In addition to VC, the primary vanadium carbide with cubic structure, a wide range of non-stoichiometric compositions VCy with y varying from 0.72 to 0.88, has been observed. This range includes two ordered compounds, V8C7 and V6C5. In this study, first-principles density functional theory (DFT) is employed to examine the stability of the binary carbides by calculating their formation energies. We compare the local structures (atomic coordination, bond distances and angles) and the density of states in optimized geometries of the carbides. Further, the effect of alloying additions, such as niobium and titanium, on the carbide stabilization is investigated. We determine the energetically preferable substitutional atom location in each carbide and study the impurity distribution as well as its role in the carbide formation energy and electronic structure.

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