Atomistic Modeling of High Temperature Corrosion in Stainless Steel Alloys

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Stainless steel components in internal combustion engines are subjected to temperatures upwards of 800 °C and corrosive gases from the combustion process. These environmental factors, when paired with constant cyclic loading, increase the risk of failure by stress corrosion cracking (SCC). This leads engine manufacturers to make conservative choices in their materials selection which ultimately increases the cost to consumers. The purpose of this study is to investigate the surface energies, point defect formation energies, and defect migration energies via Density Functional Theory (DFT) calculations. We have determined the effects of compositions varying from the pure Fe to the alloys with a high concentration of Cr. In addition to their intrinsic interest, the results of these calculations will be passed forward to phase field models of corrosion and ultimately the engineering scale.

Keywords: Combustion, Corrosion, Density Functional Theory, Stainless Steel Alloys