Density functional theory studies of effects of oxygen on grain boundary fracture in nickel

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Ni-based alloys are important structural materials for current and future reactor systems. However, they are susceptible to stress corrosion cracking (SCC). During SCC, grain boundaries in Ni-based alloys are oxidized, which can lead to intergranular fracture under residual stresses. In this work, density functional theory (DFT) calculations are conducted to understand the effect of oxidation on the grain boundary strengthen in Ni-based alloys. Grain boundaries of different characters are studied, including coherent twin, incoherent twin, and a few other high-angle grain boundaries. Oxygen is introduced at different sites near each grain boundary to study the effect of oxygen position on the grain boundary strength. In addition, the oxygen content at each grain boundary is varied and up to one monolayer of oxygen atoms are studied. The results show that oxygen embrittles all Ni grain boundaries but the magnitude depends on the grain boundary character. Grain boundary strength decreases linearly or nonlinearly with the oxygen content, depending on the boundary type. The mechanical and chemical contributions to the embrittlement are also evaluated for each grain boundary. It is found that the chemical contribution dominates the embrittlement potency.