Materials Science & Engineering Dissertation Defense

Passivation and Dissolution of Alloys

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Abstract

The passivity of metals and their alloys is a phenomenon of vast importance as it prevents many construction materials from rapid deterioration. Alloying with a sufficient quantity of passivating elements (Cr, Al, Si), typically in the range of 10% - 20%, is commonly employed to improve the corrosion resistance, owing to the formation of a passive oxide film with a thickness of few nanometers. Here, a theoretical model is suggested for the initial stage of the passive film formation and quantitative validation of its assumptions and predictions on the passivation behaviors of three corrosion-resistant binary alloys, Fe-Cr, Ni-Cr, and Cu-Rh alloys is displayed.

The percolation model relates alloy passivation to site percolation of the passivating elements in the alloy matrix and is developed considering 2D-3D cross-over effects of percolation in the thin film and the impact of atomic configuration on the percolation threshold. In the initial passivation stage of the studied alloys, Fe/Ni/Cu is selectively dissolved and distributed in the electrolyte, destroying the passive network built up by Cr/Rh oxides and undercutting isolated Cr/Rh oxide nuclei. The only way to form a protective passive film is that the concentration of Cr/Rh is high enough to realize site percolation within the thickness of the passive film or the depth that has been dissolved in. The theoretical description, given by the model, on the relation between the Cr/Rh composition in the alloys and the dissolved depth is examined via experiments and simulations. Meanwhile, the initial passivation stage scenario is verified with the dissolution selectivity measured by the inductively-coupled plasma mass spectrum (ICP-MS). The influence of cluster size on the electrochemical behavior of constituent elements is addressed by density functional theory (DFT) simulations. On the other hand, the impact of the atomic configuration parameter, Warren Cowley short range order (WC SRO) parameter, on the percolation threshold is simulated by the Monte Carlo renormalization group (MC-RNG) methods. Based on the WC SRO parameter of alloys disturbed with different heat treatment, the passivation behaviors of these alloys could be predicted, which is compared with experimental results. In this work, the percolation model shows a decent application in the examined alloy systems and is expected to provide some implications to the design criteria in alloy design for enhanced corrosion resistance when considering the alloy parameters like composition and atomic configuration.

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