Specific Adsorption of Halide Ions on Iron Surface: A Combined Electrochemical and Monte Carlo Simulation Investigation

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The specific adsorption effect of halide ions (i.e., Cl⁻, Br⁻, I⁻) on the surface of mild steel in acid media has been explored by electrochemical and Monte Carlo simulating methods. The electrochemical impedance spectroscopy (EIS) and Tafel polarization results demonstrated that the mild steel was protected from corrosion to some extent when KX (X=Cl, Br, I) exist. The absorption strength was determined by calculating a customized parameter, namely, adsorption efficiency, which suggest that absorption ability, in descending order of magnitude, was I⁻, Br⁻, and Cl⁻. Moreover, Monte Carlo simulation was employed to look for the most stable adsorption configurations of halide ions onto Fe(110) surface. Our experimental findings were in accordance with the theoretical analysis.

Keywords: Halide ions, Specific adsorption, Iron surface, Electrochemical, Monte Carlo simulation

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