Investigation of Migration-Dissolution Kinetics and Corrosion Prediction of Copper Alloys under Seawater Pressure

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Abstract In the deep-sea environment with under various seawater pressures, the microstructural evolution and stress-coupled failure of copper alloys are key factors contributing to their accelerated corrosion [1,2]. This study focuses on two copper alloys including manganese-aluminum bronze (MAB) and nickel white copper (B10), commonly used in ship propellers and seawater pipelines. By combining simulations with experiments, the alloy structure models with atomic surface segregation and stress-coupling models under various seawater pressures were established. The failure mechanisms were systematically studied under pressures ranging from 0.1 to 10 MPa, and the corrosion rates were predicted. Density functional theory (DFT) calculations revealed that seawater pressure significantly affects the structural stability of the alloys, with the corrosion dissolution process being controlled by a multi-step coupling of copper atom migration and dissolution energy barriers [3,4]. The LST (Linear Synchronous Transit) / QST (Quadratic Synchronous Transit) method was used to identify the transition state structures of surface atom migration and dissolution paths under deep-sea conditions, providing quantitative analysis of the migration-dissolution activation energy barriers in the alloys [5-7]. With the seawater pressure increasing, the formation energy of copper vacancies and the migration-dissolution activation barriers decrease, leading to a significant acceleration of the dissolution rate. Molecular dynamics (MD) simulations further demonstrated that seawater pressure enhances the interaction between metal atoms and seawater molecules, accelerating the dissolution of Cu atoms [8-10]. The corrosion rate prediction models for MAB and B10 under static deep-sea pressure showed R^2 values of 0.996 and 0.995, with errors less than 5% in comparison with the tested values of corrosion rates, indicating the model accurately reflects the corrosion trend of copper alloys in the seawater environments. Through analyzing the mechanical effects of seawater on the alloy surfaces, atomic-level characterization and prediction of alloy structural evolution and corrosion behavior under varying seawater pressures were achieved.

Keywords Copper alloy, seawater pressure, failure dynamics, migration-dissolution activation energy barrier, corrosion behavior prediction

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