Integrated computation of corrosion: Modelling, simulation and Applications

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Abstract In the last decade, integrated computation of corrosion has made significant progress towards the atomic-scale clarification of corrosion mechanisms and computer-aided designing of advanced materials with excellent corrosion resistance. We focuses on the theoretical calculation methods and developing tendency in corrosion study, and some specific applications are presented. First-principle calculations combined with molecular dynamics method, peridynamic theory and finite element method provide multiscale models to investigate micromechanisms of stress corrosion cracking and hydrogen-induced cracking. Calculations of passivity and passive film breakdown are elaborated through point defects diffusion and its correlation of the energy level degeneracy. Some vital kinetic parameters for metal electrode are estimated by combining first-principle calculations with electrochemical impedance spectroscopy analysis. Moreover, the artificial intelligence technology is pointed out how the computer can pave the way of predicting corrosion degrees as well as designing new corrosion resistant materials. To get better and efficient development of integrated computation of corrosion, extensive cooperation and powerful data infrastructure are needed by stronger collaboration in the future.

Keywords Model Corrosion; Computation; Modelling; Degradation evaluation

Reference

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