Corrosion Modeling: Continuum and Molecular Dynamics

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EXTENDED ABSTRACT

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INTRODUCTION

Simulating reaction dynamics across length and time scales has been a grand challenge in materials science and engineering. Electrochemical reactions, including those relavant to corrosion, are particularly formiable since they envolve interactions among various chemical species, both in liquid and solid phases. Our work is aimed at outlining key dynamical parameters bridging chemical reactions at diferent length and time scales. In the atomistic scale, autonomous basin climbing method offers a solution to simulate reactions spanning over a long time period. In combination with the techniques of kinetics Monte Carlo, time of a reaction can be calculated. Here, we demonstrate the success of applying to the autonomous basin climbing and kinetic Monte Carlo approaches to predict diffusion mechanisms in a dilute Ni-Al system. The simulation results will be compared to an experimental data. In the larger scale, the diffusion of ions and chemical reactions at the electrodes are modeled by a set of kinetic equations. The coupled system of equations stems from diffusion in the aqueous liquid and the degree of reactions at the solid-liquid interface. A multiphysics solver can be then applied in order to determine or visualize physical processes in the electrochemical reactions.