Atomistic simulation of corrosion of Nickel in pure water using voltage equilibration electrochemical process

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Understanding the corrosion behavior of metals and alloys and the growth of passive films is of vital importance for both scientific research and engineering.

Multiscale modelling is more and more intensively used to investigate corrosion mechanism. However, taking into account the effect of electrochemical potential during atomistic simulation remains a real challenge for the modelling of corrosion processes. Many attempts have been made in this direction.

At the DFT level, the double reference method developed by Filhol et al. [1], set the electrochemical potential by adding (or removing) a non-integer number of electrons in the cell. However the use of this method to simulate the whole dynamical process of the growth of passive film on metals is not feasible due to computer resources limitation. For longer time and large model size, Kinetic Monte Carlo approach have been used with an applied constant potential resulting in electric field depending on the local thickness of the oxide film [2]. Another approach, based on reactive molecular dynamics simulation with an applied electric field have been also proposed [3]. Overcoming the limitations of this approach, a method based on the internal equilibration of atom's electronegativity have been proposed recently [4]. This method describes the electrochemical driving force resulting from the application of an external voltage to metallic electrodes.

Using this method, we have employed ReaxFF molecular dynamics simulations to study the anodic corrosion process of Nickel in pure water at different electrochemical potential. The dynamic interaction process between H2O and Ni surfaces with different orientations as well as the effects of thermal evolution of water molecules in contact with Ni surfaces have been investigated. We demonstrated that the application of external electrochemical potential increases the charge distribution of the metallic atoms at the surface and facilitates their dissolution into the electrolyte. The positively charging of Ni ions, driven by the induced electric field as shown in our previous study [3], lead to the dissociation of water at the active electrode surface. The percentage of Nickel dissolved and the oxide film thickness increases with the external voltage. The electrical current between the electrodes as a function of time during electrochemical reaction process is also computed.

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