Multiscale Simulation and Experimental Characterization of Epoxy/Polyaniline Nanocomposite Coatings – Towards the Rational Design of Nanocomposite Coatings Used in Corrosion Protection

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Corrosion of mild steel causes massive costs due to inspection, maintenance and repair each year. Currently, for corrosion protection conductive polymers are of great interest. The most studied polymer is Polyaniline (PANI) since it is easy to synthesize and can be prepared either chemically or electrochemically [1]. The conductivity of PANI is controlled through protonation leading to an increase in conductivity (doping) and de-protonation (de-doping) causing a decrease in conductivity [2]. The electrochemical properties and performance as corrosion inhibitor are significantly influenced by the choice of doping agent [3]. Blends of PANI and epoxy resin have shown promising corrosion inhibition properties [4], [5], [6].
Despite the large number of studies on PANI and PANI containing coatings for the corrosion protection of mild steel, the mechanisms of action, influence of the doping agent and failure of the anticorrosive properties have not yet been fully understood. Therefore, we employ a combination of theoretical and experimental methods for the investigation of epoxy/PANI nanocomposites doped with different doping agents. Simulations ranging from atomistic scale to macroscale should allow to investigate the charge-transfer reactions taking place at the steel-coating interface, the role of doping agents and ferric oxide type at the interface in electron transfer reactions and interfacial adhesion (atomistic scale – first principle quantum mechanical (QM) and molecular dynamics (MD) simulations) as well as the role of surface morphology and cracks (macroscale – Finite Element (FE) modeling) in corrosion protection and failure of the coating. The results of simulations are benchmarked against experimentally determined electrochemical properties, surface morphology, interfacial energy and adhesion.
The results will point-out the factors crucial for the success or failure of employing an epoxy/PANI nanocomposite coating for the corrosion protection of mild steel. The knowledge on the electrochemical processes occurring at the metal-coating interface will not only be important for corrosion science, but also for the application of PANI in electrochemical sensors, capacitors, solar energy conversion or rechargeable batteries.

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