

Modeling of Inhibitor Release from Organic Coating Using Finite Element Method in Assisting in the Multifunctional Organic Coating Design

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Summary: Several strategies for the control of solubility and delivery of inhibitors in organic coatings are being explored in a DoD MURI. One method uses anion-exchanging hydrotalcites (HTs). Buchheit et al. have demonstrated the inhibition of AA2024-T3 corrosion by the migration of VO^{3-} released from a HT.

The mode of corrosion protection envisioned is for HTs to reside at a metal surface as a conversion coating or as a pigment in the primer coating. In the presence of an attacking solution, HT anion exchange will release of an inhibiting anion into the solution and absorb and immobilize the attacking ion or ions. This study extends the early crevice corrosion modeling work to inhibitor release/aggressive anion capture from/to HT in epoxy coatings. The kinetics of the bare Al alloy were determined from separate electrochemical measurements. Similarly inhibitor release kinetics and diffusion parameters were assumed based on measurements on virgin epoxy films.

The objectives of this study are:
1) Develop a computational model for the inhibitor release and transport within and from the hydrotalcite coating system to assist in the design of the multifunctional coating system with the encapsulated inhibitors. The model and source code will be also released via <http://www.virginia.edu/cese/research/crevicer/>.

2) Study the influence to the corrosion inhibition of: inhibitor release rate, inhibitor loading, polymer resins, chloride gettinger rate, scratch size, water layer thickness, NaCl concentration.

This modeling study is associated with another experimental study of release and transport of chemical species within and from functional coatings.

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