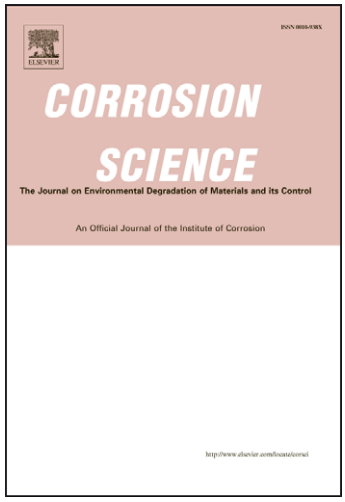

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The relation between adsorption bonding and corrosion inhibition of azole molecules on copper

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Abstract

Adsorption of plain azole molecules in protonated, neutral, and deprotonated forms on Cu(111) was characterized by density functional theory calculations. Both metal/vacuum and metal/water interfaces were considered and solvent effects were estimated by continuum solvation model. It is shown that chemisorptive bonding is by and large the strongest for deprotonated inhibitors. Only for imidazole the aqueous-phase adsorption free energy of the neutral form is comparable to that of deprotonated form. This suggests that for imidazole—because of its more basic nature—the neutral form and for triazole and tetrazole their deprotonated forms are the active species for inhibiting corrosion.

Keywords: A. Copper, B. Modelling studies, C. Interfaces, C. Acid inhibition, C. Neutral inhibition

1. Introduction

Azole molecules are known as efficient corrosion inhibitors [1–3]—substances that have the ability to remarkably slow down the corrosion of metals and alloys by decreasing the rate of corrosion processes. In our previous publication [4] the gas-phase adsorption of four azole molecules—imidazole, 1H-1,2,3-triazole, 1H-tetrazole, and pentazole—on Cu(111) and Al(111) surfaces has been characterized using density functional theory (DFT) calculations. We found that the molecules weakly adsorb in an upright geometry and the magnitude of adsorption energy uniformly decreases from imidazole to pentazole—a trend explainable in terms of molecular electronegativity and chemical hardness. However, with respect to corrosion and its inhibition, the solid/water interface is far more appropriate to consider than the solid/gas (or solid/vacuum) interface. It should be noted that in aqueous systems the metallic surfaces of copper are present only under acidic conditions, whereas in near neutral conditions copper is covered by thin Cu_2O oxide films [5, 6]. In this context it is also

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