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Epoxy Resins and their Zinc Composites as Novel Anti-Corrosive Materials for Copper in 3% Sodium Chloride Solution: Experimental and Computational Studies †

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Abstract: The evaluation the anticorrosive performance of two macromolecular aromatic epoxy resins (ERs), namely, tetra glycidyl of ethylene dianiline (TGEDA), hexaglycidyl Tris (p-Ethylene Dianiline) Phosphoric Triamide (HGEDPAT), and their polymer composite reinforced with Zinc for copper corrosion in 3% NaCl by means of computational and experimental analyses. Anticorrosive property of the standards and composites was demonstrated using experimental and computational methods. Electrochemical results showed that HGEDAPT cured with methylene dianiline (MDA) showed better protection efficiency with optimum corrosion current density (icorr) value of 2.0 μcm^{-2} and the polarization resistance (R_p) value of 17,00 $k\Omega.cm^2$ than that of TGEDA-MDA having icorr value of 2.4 μcm^{-2} and the R_p value of 15.24 $k\Omega.cm^2$. The anticorrosive effect of TGEDA-MDA and HGEDAPT-MDA was evaluated in the presence of 5% zinc (Zn). Experimental results demonstrate that the presence of 5% of zinc in TGEDA-MDA and HGEDAPT-MDA formulations significantly enhanced their protection ability. The anticorrosive effect of different formulations followed the order: ER1 (TGEDA-MDA) (potentiodynamic polarization (PDP); 90% and electrochemical impedance spectroscopy (EIS) 92%) < ER2 (HGEDAPT-MDA) (PDP; 92% and EIS 93%) < ER3 (TGEDA-MDA-5%Zn) (PDP; 96% and EIS 97%) < ER4 (HGEDAPT-MDA-5%Zn) (PDP; 97% and EIS 98.5%). Density Functional Theory (DFT) study revealed that ER1 and ER2 interact with the metallic surface using donor-acceptor interactions in which electron-rich centers acted as the most favorable sites for the interactions. Molecular dynamics (MD) simulations studies suggest that ER1 and ER2 acquire flat or horizontal orientations, and their orientations on the metallic surface are largely influenced by the presence of zinc. Different experimental and computational studies are in good agreement.

Keywords: polymer composite; anticorrosive composite materials; zinc composite; copper; 3% NaCl; computational simulations.

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Conflicts of Interest

The authors declare no conflict of interest.