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Dagdag, O.[a] , Hsissou, R.[a] , Berisha, A.[b] , Erramli, H.[c] , Hamed, O.[d] , Jodeh, S.[d] , El Harfi, A.[a]

Polymeric-Based Epoxy Cured with a Polyaminoamide as an Anticorrosive Coating for Aluminum 2024-T3 Surface: Experimental Studies Supported by Computational Modeling

(2019) *Journal of Bio- and Tribo-Corrosion*, 5 (3), art. no. 58, .

DOI: 10.1007/s40735-019-0251-7

[a] Laboratory of Agroresources, Polymers and Process Engineering, Department of Chemistry, Faculty of Science, Ibn Tofail University, BP 133, Kenitra, 14000, Morocco
[b] Department of Chemistry, Faculty of Natural and Mathematics Science, University of Pristina, Pristina, 10000, Serbia
[c] Laboratory of Materials, Electrochemistry and Environment, Department of Chemistry, Faculty of Sciences, Ibn Tofail University, Kenitra, Morocco
[d] Department of Chemistry, An-Najah National University, P. O. Box 7, Nablus, Palestine

Abstract
The present research focused on a coating formulation for aluminum surface 2024-T3 to protect it from corrosion. The formulation consisted of a polymeric epoxy resin-coated bisphenol A diglycidyl ether (DGEBA) cured with a polymeric polyaminoamide. The coated aluminum 2024-T3 was tested in a harsh environment of electrolyte solution (3 wt% NaCl solution) to simulate the harsh marine environment. The coated sample was evaluated by Electrochemical Impedance Spectroscopy (EIS). Under these conditions, a very high impedance (Z) value was obtained; even after exposure for a period longer than 4392 h, the performance was still acceptable. Surface morphological study of metallic specimens before and after exposures to the simulated marine environment (3 wt% NaCl) was carried out using scanning electron microscopy (SEM). The results indicate that the DGEBA-polyaminoamide (DGEBAAA) performed as an excellent barrier for Al surface. The results were combined by several modeling approaches involving molecular dynamics simulation (MD), Monte Carlo methods (MC), and the electronic density functional theory (DFT) computations to explore the adhesion forces between the DGEBAAA and the aluminum surface. The computational MD, MC, and DFT studies were executed in aqueous media. Computational results further evidenced the stronger DGEBA-aminoamide adhesion onto the aluminum 2024-T3 even in a wet environment. © 2019, Springer Nature Switzerland AG.

Author Keywords
AA2024-T3; Coating; DFT; DGEBA-polyaminoamide; EIS; MD and MC simulation

Index Keywords
Adhesion, Aluminum corrosion, Coatings, Computation theory, Corrosion resistant coatings, Curing, Density functional theory, Electrochemical corrosion, Electrochemical impedance spectroscopy, Electrolytes, Epoxy resins, Molecular dynamics, Monte Carlo methods, Scanning electron microscopy, Sodium chloride; AA2024-T3, Anti-corrosive coatings, Bisphenol-A-diglycidyl ethers, Computational results, Electrolyte solutions, MC simulation, Molecular dynamics simulations, Polyaminoamide; Aluminum coatings

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Publisher: Springer International Publishing

ISSN: 21984220
2-s2.0-85066144220
Document Type: Article
Publication Stage: Final
Source: Scopus