Expedient screening of magnesium corrosion modulators: combining high-throughput multi-well exposure, topographical volume loss quantification, image analysis and predictive machine learning modeling

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Abstract In this work, we demonstrate a new approach to expedient discovery of magnesium corrosion inhibitors and accelerators. We start with high-throughput experimental multi-well exposure, similar to that previously shown in [1]. Unlike the previous work, we quantify the corrosion impact by topographical volume loss using a laser profilometer. Over 240 individual organic chemical compounds were tested for the AZ31 alloy, generating ca.1000 corrosion imprints. The inhibition efficiency, as well as inhibition power [2] and symmetrized inhibition efficiency [3] of corrosion modulators was determined by profilometric analysis after corrosion exposure. It was further validated by traditional weight loss analysis. Along with this, we analysed the optical images of corrosion imprints generated during multi-well exposure. The developed convolutional neural network used optical images as input and predicted the volume loss based on those images. The model was effectively trained and it could be demonstrated that deep learning approaches can be successfully implemented for corroded surfaces. Corrosion inhibition values for individual chemical compounds quantified either by profilometric or image analysis were then used to train a quantitative structure-property relationship model for predicting corrosion inhibition performance of yet untested compounds. An active learning workflow was then developed to accelerate the discovery of potentially effective inhibitors among thousands of commercially available chemical compounds. This new approach can be

easily automated and upscaled, and as such is of great importance for promoting the discovery of corrosion inhibitors for various metallic materials.

Keywords magnesium, corrosion inhibition, high-throughput testing, machine learning, image analysis, organic corrosion inhibitors

References

[1] P.A. White, G.B. Smith, T.G. Harvey, P.A. Corrigan, M.A. Glenn, D. Lau, S.G. Hardin, J. Mardel, T.A. Markley, T.H. Muster, N. Sherman, S.J. Garcia, J.M.C. Mol, A.E. Hughes, A new high-throughput method for corrosion testing, Corrosion Science, 58 (2012).

[2] A. Kokalj, M. Lozinšek, B. Kapun, P. Taheri, S. Neupane, P. Losada-Pérez, C. Xie, S. Stavber, D. Crespo, F.U. Renner, A. Mol, I. Milošev, Simplistic correlations between molecular electronic properties and inhibition efficiencies: Do they really exist?, Corrosion Science, 179 (2021).

[3] A. Kokalj, C. Xie, I. Milošev, D. Crespo, How relevant are molecular electronic parameters for predicting corrosion inhibition efficiency: imidazoles as corrosion inhibitors of Cu/Zr materials in NaCl solution, Corrosion Science, 193 (2021).