

ACEX2019

13th International Conference on Advanced Computational Engineering and Experimenting
ATHENS (Greece) from 1-5 July, 2019

Comprehensive Experimental and Computational Screening of Magnesium Dissolution Modulators (Inhibitors and Promoters)

Sviatlana V. Lamaka

*Magnesium Innovation Centre - MagIC,
Helmholtz-Zentrum Geesthacht (HZG), Germany*

This work presents the results of a systematic search for magnesium dissolution modulators that were employed either as *corrosion inhibitors* intended for protecting magnesium employed for structural applications or as *additives for tailored dissolution* of magnesium anode for Mg-air battery application [1-4]. The ability to form complexes with Fe^{n+} and Mg^{2+} was considered when choosing the compounds for experimental screening [2,3]. The extensive database gathered the influence of a large number of organic/inorganic compounds on behaviour of Mg materials in aqueous electrolytes. A number of new corrosion inhibitors was discovered with efficiency exceeding that of chromate. Inhibiting efficiency of multiple compounds was found to be dependent on the alloy specification. Dissolution modulators relevant for Mg-air battery or for bio-medical applications are also highlighted. Examples will be given how the discovered inhibitors can be incorporated into the protective coatings.

At the same time, we realized that the field of potential magnesium dissolution modulators is huge, containing several millions of individual compounds. This makes it impossible to test all promising compounds and gather out a detailed atomistic understanding of the inhibition mechanisms for each dissolution modulator. Instead, a concept is being developed (combining experimental, machine learning, DFT calculations and molecular dynamics tools) to enable *in silico* prediction of inhibition and dissolution promoting properties of compounds that have not been tested experimentally.

[1] D. Höche, C. Blawert, S.V. Lamaka, N. Scharnagl, C. Mendis, M.L. Zheludkevich. The effect of iron re-deposition on the corrosion of impurity-containing magnesium. ***Phys. Chem. Chem. Phys.***, 18 (2016) 1279-1291.

[2] S.V. Lamaka, D. Höche, R.P. Petrauskas, C. Blawert, M.L. Zheludkevich. A new concept for corrosion inhibition of magnesium: Suppression of iron re-deposition, ***Electrochemistry Communications***, 62 (2016) 5-8.

[3] S.V. Lamaka, B. Vaghefinazari, D. Mei, R.P. Petrauskas, D. Höche, M.L. Zheludkevich. Comprehensive screening of Mg corrosion inhibitors, **Corrosion Science**, 128 (2017) 224-240.

[4] D. Höche, S.V. Lamaka, B. Vaghefinazari, T. Braun, R.P. Petrauskas, M. Fichtner, M.L. Zheludkevich, Performance boost for primary magnesium cells using iron complexing agents as electrolyte additives, **Scientific Reports**, 8 (2018) 7578.