Corrosion-resistant Mg alloy design through high-throughput simulations and machine learning

Hong Zhu[1], Gaoning Shi[1], Jieqiong Yan[1], Xinchen Xu[1], Yaowei Wang[1], Tian Xie[2], Xiaoqin Zeng[2]

[1]*University of Michigan−Shanghai Jiao Tong University Joint Institute, Shanghai Jiao Tong University, 800 Dongchuan Road, Shanghai 200240, China*

[2]*School of Materials Science and Engineering, Shanghai Jiao Tong University, 800 Dongchuan Road, Shanghai 200240, China*

Presenter's e-mail address: hong.zhu@sjtu.edu.cn

Abstract

Magnesium alloys as the lightest engineering metals have the potential to be widely used in transportation etc, but the bad corrosion resistance has limited the further applications. To overcome the limitations of traditional experimental trial-and-error approach in corrosion research, the ab-initio method to predict the polarization curves for galvanic corrosion of multi-phase Mg alloys has been established. To accelerate the screening of Mg alloy systems with better corrosion resistance, the corrosion materials genome have been further developed by combining the high-throughput-simulations and machine learning methods. The important surface atomic features have been also uncovered in terms of reducing the cathodic hydrogen evolution and anodic Mg dissolution kinetics, which have successfully guided the experimental development of corrosion-resistant Mg alloys.

Keywords High-Throughput Simulations, Materials Genome Initiative, Corrosion Property, Machine Learning

Reference

[1] Yan, J.; Xu, X.; Shi, G.; Wang, Y.; Guan, C.; Chen, Y.; Yang, Y.; Ying, T.; Zhu, H.; Tang, Q.; Zeng, X. The Anodic Dissolution Kinetics of Mg Alloys in Water Based on Ab Initio Molecular Dynamics Simulations. Materials Genome Engineering Advances 2024, e47.

[2] Wang, Y.; Tang, Q.; Xu, X.; Weng, P.; Ying, T.; Yang, Y.; Zeng, X.; Zhu, H. Accelerated Discovery of Magnesium Intermetallic Compounds with Sluggish Corrosion Cathodic Reactions through Active Learning and DFT Calculations. Acta Materialia 2023, 255, 119063.

[3] Wang, Y.; Xie, T.; Tang, Q.; Wang, M.; Ying, T.; Zhu, H.; Zeng, X. High-Throughput Calculations Combining Machine Learning to Investigate the Corrosion Properties of Binary Mg Alloys. Journal of Magnesium and Alloys 2022, 12 (4), 1406–1418.

[4] Luo, Z.; Xu, J.; Wang, Y.; Xie, T.; Zhu, H.; Ying, T.; Li, D.; Wang, L.; Zeng, X.; Wolverton, C.; et al. Theoretical Analysis of the Galvanic Corrosion Behavior of Mg-Ge Binary Alloy. Journal of The Electrochemical Society 2019, 166 (13), C421–C427.