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Corrosion resistant magnesium alloy design based on the First-principles calculation.[1] YAOWEI WANG, TIAN XIE, XIAOQIN ZENG, HONG ZHU, Shanghai Jiao Tong University — Second phase strengthening has been widely used in alloys designs, many of which however have been reported to enhance the galvanic corrosion of magnesium alloys. However, up to now, a repeatable method to predict corrosion current density and potential still needs to be explored. In this study, a semi-empirical model was proposed based on the mixed potential theory and first principles calculation to analyze the galvanic corrosion of the alloys. Our model is further validated in the case of Mg-Ge alloys, which is composed of anode Mg matrix and cathode Mg2Ge second phase. The estimated exchange current of the hydrogen evolution upon Mg2Ge is about 3 orders of magnitude smaller than that on pure Mg, indicating the depressed galvanic corrosion of the Mg-Ge alloys is the simultaneous result of the low hydrogen exchange current upon Mg2Ge. Moreover, some typical intermetallics, such as MgZn2 and MgSc, were selected to compare the different corrosion properties of the alloys, which is in close agreement with the experimental observations. Our model is capable of predicting the galvanic corrosion behavior and provide a promising perspective for designing better corrosion-resistant alloys.

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