〈技術資料〉

量子力学による金属腐食論（VII報）
－Hopfield理論による電子移動確率－
Metal Corrosion Theory by Quantum Mechanics. VII
－ Electron Transfer Probability by Hopfield's Theory －

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Abstract

A series of papers discusses a metal corrosion theory by using quantum mechanics, especially electron transfer theory during corrosion process. I have already proposed the theoretical equation by which we can calculate the value of corrosion current density, in the earlier papers, Landau – Zener theory was theoretically derived. By using Landau – Zener theory, Fermi's golden rule can be derived theoretically. In the last paper, by using Fermi's golden rule and Heisenberg's uncertainty principle and Marcus theory, I calculated the corrosion current density of iron. However, the value was higher than the measured value. This discrepancy between the calculated value and the measured value mainly due to selection method of density state function. In order to calculate exact corrosion current density, we need to select the density state function of donor and acceptor, that is, we need to use Hopfield's formula. In this paper, Hopfield formula will be derived theoretically by using Quantum mechanics. In the next paper, the theoretical formula of corrosion current density will be derived by using Hopfield theory.

1.　はじめに

これまでの、および今後の一連の報告は、量子力学を用いて金属の腐食電流密度を理論的に算出できる理論式を誘導することを目的として

いる。先の報告（量子力学による金属腐食論（VI報））において、過去の報告で誘導したLandau – Zener理論からフェルミの黄金律を誘導し、さらに不確定性原理やマーカス理論を用いた腐食電流密度の推定を行った[1-6]。その結果、これらの推定値は実測値よりも大きな値となり、正確な腐食電流密度を計算するためには、筆者の提案した理論式を用いる必要があることを述べた[6]。そして、上記のフェルミの黄金律や不確定性原理を用いた計算方法がドナーかア