**QUANTUM-CHEMICAL ANALYSIS OF ELECTROCHEMICAL PROCESSES INVOLVING COPPER IONS AND MALEIC ACID**

The qualitatively new stage of development of electrochemistry is associated with actual problems of modern technology, which are based on the usage of nanosystems in the production of new functional materials [1, 2]. The basic problem of nanotechnology is insufficient development of theoretical ideas regarding the behavior of individual particles and structures in the range of micro- and nanosize. The main problem is the absence of a unified theory of action of surfactants on electrode processes in solutions of metal ions. This is due to the fact that the information concerning the influence of additives on the electrode process has been mainly associated with their impact on individual stages. It seems to be extremely difficult to separate the effects of surfactants on the particular stage using experimental electrochemical methods, because all the stages of discharge and crystallization of metals mutually affect each other. Some progress can be achieved in this case by combining experimental methods with quantum-chemical modeling.

The aim of this work was to study the influence of maleic acid (MA) on the electrode processes that accompany electrodeposition of copper from an aqueous solution using theoretical quantum-chemical method. Copper aqua complexes (Cuz, where z = 0, +1, +2) and polyligand complexes with MA have been chosen as the object of research. Modeling of possible structures has been performed using B3LYP functional.  Solvation effects have been taken into account using polarization continuum model. Wachters+f basis set has been used for copper atoms and 6-311G(d,p) basis set has been used for hydrogen and oxygen atoms.

In previous experiments, it has been found out that yellow complexes of Cu+ accumulate in the anodic space of electrochemical cell during the electrolysis of the solution containing 0.1 mol/L CuSO4 and 0.1 mol/L MA. They mix with the source electrolyte and produce a green-colored solution. On the other hand, no change of color has been observed in the cathodic space of the cell. The electrochemical copper deposit obtained on the cathode has fine-crystalline structure [3].

Based on the research findings the theoretical possibility of formation of copper σ- and π-complexes with MA has been found. Thus, oxygen atoms from carboxyl groups, as well as the C=C fragment of the MA molecule can act as complexation centers. However, the fact that hydrophilic COO– and COOH groups in the solution are surrounded by several layers of water molecules is a significant complication in the first case. Considering the experimental observations we can suggest the following mechanism of anodic process. At the first stage MA adsorbs chemically on the copper anode through the formation of π-bonds between surface copper atoms and C=C fragments of MA. At the second stage electron detachment causes formation of Cu+ π-complexes, where these π-bonds are preserved. The resulting Cu+ π-complexes with MA are stable enough and they can be detected visually. The saturated analog of MA – succinic (dicarboxylic) acid, has not exhibited the ability of formation similar colored Cu+ complexes – under the same conditions.

**References:**

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