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Photoelectric polarization and quantum-chemical data about electrochemical films formed in perchlorate alcohol solutions

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The work is held to investigation of alcohol solvent role in the mechanism of electrochemical films formation on the transition metals. Photoelectric polarization data in situ allowed to find that structure and mechanism of the surface layer growth is determined by donor-acceptor interaction between d-metals surface states and dipoles of solvent. They are associated to neutral adsorption-electrochemical complex [MeOHR]0 on the surface of anode. The stoichiometry of films is defined by defects concentration in the crystal lattice formed phase. The states of the crystal field are contributing to the bonding. The results of quantum-chemical modeling of surface complex and anion in individual and coordinated state showed that anion ClO4- was a component of outer-sphere for surface complex.

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