Electrochemical Studies and Molecular Dynamics Simulation of the Interaction between Accelerators and Cu Surface During the Electroplating Process

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Accelerators are crucial for electroplating in the electronics industry. In this research, the electrochemical behavior of two accelerators, 3-(benzothiazolyl-2-mercapto)-propyl-sulfonic acid sodium salt (ZPS) and bis(3-sulfopropyl) disulfide (SPS), during Cu electrodeposition was analyzed using electrochemical techniques. Meanwhile, the adsorption behavior of the two accelerators on Cu(111) was also studied using molecular dynamics (MD) simulation, which predicts the preferable reaction sites for nucleophilic or electrophilic attack and the corresponding interactions based on density functional theory. The MD results showed that ZPS could be adsorbed on the Cu(111) firmly through the thiouronium group and a benzothiazolyl group, whereas the SPS was adsorbed through the thiouronium group. Moreover, the accelerating efficiency of these two accelerators was closely related to the frontier molecule orbital density distributions and Fukui indices.

Keywords: copper electroplating; electrochemistry; MD simulation; ZPS; SPS

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