Short Communication

Bis-(3-sulfopropyl) Disulfide Acceleration of Copper Electrodeposition via Molecular Dynamics and Quantum Chemical Calculations

Fuliang Wang^{1,2}, Yuping Le^{1,2,*}

¹ School of Mechanical and Electrical Engineering, Central South University, Changsha 410083, China

² State Key Laboratory of High Performance Complex Manufacturing, Changsha 410083, China

*E-mail: leyuping1@163.com

doi: 10.20964/2020.06.11

Received: 6 June 2019 / Accepted: 4 December 2019 / Published: 10 May 2020

Bis-(3-sulfopropyl) disulfide (SPS) is commonly used as an accelerator for copper electroplating in through-silicon via and printed circuit board fabrication. However, detailed SPS accelerator dynamics have not yet been fully studied. In this study, the adsorption behavior and accelerator dynamics of SPS on a copper surface were studied by using molecular dynamics and quantum chemical calculations. The natural atomic charges, molecular properties, distributions of frontier molecular orbitals, and Fukui indices were obtained. According to the simulations, the SPS reaction cycle on a copper seed layer surface was proposed. In this cycle, the SPS adsorbed on the cathode is attacked by H^+ , Cl^- , and the oxygen anion of $-SO_3H$, obtains an electron from the cathode, and breaks into two 3-mercaptopropane-1-sulfonic acid (MPS) molecules. Subsequently, two free MPS dimerize into an SPS, releasing an electron to reduce Cu^{2+} into Cu^+ . Through this SPS reaction cycle, electrons on the copper seed layer surface (cathode) are transferred to Cu^{2+} to yield Cu^+ , thereby accelerating the deposition process.

Keywords: Bis-(3-sulfopropyl) disulfide, MD simulation, Quantum chemical calculations, HOMO, LUMO.

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