Adsorption Behavior of 3-phenylacrylaldehyde on a Tin Surface during Electroplating

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The global and local activities of 3-phenylacrylaldehyde and 4-phenylbut-3-en-2-one, their adsorption behavior on a tin surface, and the electrodeposition mechanism of tin were studied using quantum chemistry calculations, molecular dynamics simulations, and electrochemical measurements. The results indicate that active sites bind to C, O, and H atoms resulting in the multi-center adsorption of molecules on tin surfaces via coordinate and feedback bonds. The adsorption activity of 3-phenylacrylaldehyde was superior to that of 4-phenylbut-3-en-2-one. Polarization curves and SEM observations indicated that the presence of 3-phenylacrylaldehyde not only enhanced the cathodic polarization of tin electrodeposition but also accelerated the nucleation rate of tin. The increased adsorption of 3-phenylacrylaldehyde on a tin surface in a methylsulphonate plating solution resulted in a bright electroplated coating.

Keywords: Quantum chemistry calculation; molecular dynamic simulation; 3-phenylacrylaldehyde; reactivity; absorption behavior

FULL TEXT

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