

Surfactant molecules to promote removal of cadmium ions from solid surfaces: A complementary experimental-simulation study

María del Alba Pacheco Blas^a, Margarita Rivera^b, Héctor Domínguez^a

^aInstituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México, México Cd.Mx., 04510

^bInstituto de Física, Universidad Nacional Autónoma de México, México Cd.Mx., 04510

`maria.pacheco@ciencias.unam.mx`

Abstract

Due to its high toxicity heavy metals are a global problematic of high concern. Sodium dodecyl sulfate (SDS) was used to interact with cadmium ions to demonstrate the efficiency of surfactant molecules to promote desorption from solid surfaces. Scanning electron and atomic force microscopy were employed to study desorption of cadmium ions from highly oriented pyrolytic graphite (HOPG), as a model to understand the removal of metallic ions from carbon substrates. Contact angle measurements were carried out to investigate the wettability behavior of the surfactant on the contaminated surface. The desorption mechanism from a microscopic level was studied by using molecular dynamic simulations. Density profiles, pair correlation functions and diffusion coefficients were analyzed to determine the cadmium-surface interaction in the presence of surfactant molecules to improve ion detachment. Simulations showed that surfactant molecules moved in between the adsorbed cadmium ions and the graphite surface pushing up the metallic groups to improve metal desorption. The experimental and simulation results agree with atomic absorption spectroscopy results.

Keywords

Cadmium desorption by surfactants, Microscopic techniques, Contact angle, Molecular dynamics simulations