THE INTERACTION BETWEEN METALS (AG, CU) AND SEMICONDUCTING MINERALS (MOLYBDENITE)

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In order to understand the adsorption mechanism of metal atoms to semiconducting surfaces, we have studied the adsorption of Ag and Cu on molybdenite and the surface diffusion of these adsorbates. Our STM images show that adsorption islands of a characteristic size (2 nm for Ag on MoS2, 8-10 nm for Cu on MoS2)are formed. These islands tend to diffuse around on the (001) surface, suggesting that the Cu-S bond is weak. Surface diffusion is only hindered once individual islands start to coalesce. By applying quantum mechanical approaches, it is possible to calculate the electron transfer between the mineral surface and the metal atom as well as the adsorption energy as a function of surface coverage. In addition, our calculations indicate that one monolayer of silver would get warped on the molybdenite (001) surface. A lot of this stress is released by successively removing part of this monolayer. The best results in terms of a combination of high coverage and the least possible stress was obtained with Ag islands with seven atoms in diameter which exactly agrees with the experimentally observed islands with a diameter of 2 nm. UPS results also suggest that a specific new state is formed which may describe the Ag-S bond that does not occur in pure silver or molybdenite.This study shows how the combination of experimental and molecular modelling techniques are useful tools to understand the nature of the metal to sulfide bond. Further, insights may be gained concerning the natural association of certain metals with sulfides.