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Investigation of surface stability and interaction of thionocarbamate collectors on pentlandite (Fe5Ni4S8) mineral

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Abstract
Pentlandite is the primary source of nickel as well as a major carrier of platinum group elements (PGEs). Nickel mining is popular in many nations, contributing to a variety of industrial applications such as stainless steel, coinage, and rechargeable batteries, which contribute to the ever-increasing demand for nickel, which is expected to run out by 2030. The flotation in pentlandite and nickel ore has always been performed using various collectors such xanthates, dithiophosphate and dithiocarbamate. Density functional theory computational method was used to determine the most stable surface and the preferred cleavage of Fe5Ni4S8. The bulk structure was determined by cluster expansion. The (100), (001), (110), (101), (111), (211) and (112) surface were cleaved from the relaxed bulk structure and their surface energies were computed. It was found that the (001) surface gave the lowest positive surface energy and therefore the most stable surface. Moreover, the reconstruction of the (001) surface indicated that the reconstructed surface was more stable compared to the un-reconstructed surfaces. The adsorption of O-isopropyl-N-diethyl-thionocarbamate (IPDETC) on the reconstructed Fe5Ni4S8 (001) surface was performed on Fe and Ni sites and showed strong adsorption. This suggested that IPDETC collector may be used in the flotation of pentlandite mineral.
KEYWORDS
Computational modelling, Fe5Ni4S8 pentlandite, Surface reconstruction, Surface energies, IPDETC, Adsorption energies

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Yes

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MSc

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