Contribution ID: **204** Type: **Poster Presentation**

Electronic structures of oxygen adsorption on {110} nickel-rich pentlandite (Fe₄Ni₅S₈) mineral surface

Wednesday, 9 July 2014 17:10 (1h 50m)

Abstract content
   (Max 300 words)
Formatting &
Special chars

Pentlandite (Co,Fe,Ni)₉S₈ is the most abundant iron-nickel sulphide ore containing mineral and has a wide range of applications in industries. The mineral is of commercial importance and can be extracted using floatation processes; one of the processes is oxidation. The oxidation plays a significant role in forming air bubbles that float the pentlandite mineral. Despite reports that oxidation tend to depress the sulphide minerals, it has good preferential oxidation of iron. The present study investigated the clean and oxidised nickel-rich {110} pentlandite surface using ab-initio density functional theory (DFT). The Bader analysis have been evaluated for clean and oxidized surfaces and suggests that both Fe and Ni have 2+ and 3+ oxidation state, respectively. Furthermore, when oxygen is adsorbed at the (fcc hallow site, on Fe-top site) and on Ni-top site, it was found that the {110} pentlandite surface oxidises as (Fe-O-Fe) and Ni-O-O, respectively. Oxidation had also shown preferential oxidation of iron and we noted a charge transfer from the metals to the oxygen molecule. We also observed that the oxygen (O1) coordinated to the Fe accepts electrons to σ_s and Π_p bonding orbitals, while the oxygen (O2) coordinated to O1 only occupies the Π_p *antibonding for the fcc hallow site and Fe-top site adsorption. The Ni-top site adsorption is observed to occupy similar to the just mentioned case however, we noted that the Π_p* antibonding orbital is occupied on O1 atom. This study gives an understanding of oxidation of pentlandite naturally and during flotation.

Apply to be
 considered for a student
   award (Yes / No)?

yes

Level for award
 (Hons, MSc,
   PhD)?

MSc

Main supervisor (name and email)
and his / her institution

Prof P.E. Ngoepe, phuti.ngoepe@ul.ac.za
, University of Limpopo

**Would you like to
 submit a short paper
 for the Conference
 Proceedings (Yes / No)?**

yes

Primary author: Mr MKHONTO, Peace Prince (University of Limpopo)

Co-authors: Prof. CHAUKE, Hasani R. (University of Limpopo); Prof. NGOEPE, Phuti E. (University of Limpopo)

Presenter: Mr MKHONTO, Peace Prince (University of Limpopo)

Session Classification: Poster2

Track Classification: Track A - Division for Physics of Condensed Matter and Materials