Contribution ID: **281** Type: **Poster Presentation**

Ab initio density functional theory of Fe5Ni4S8 (P4_2/nmc) (311) and (111) surfaces : Computational study

The properties of the surfaces of materials play a crucial role in determining the behaviour and functionality of materials as the bulk properties, since they control the interaction between the substance and the external environment. They dictate how the material interacts with other substances, such as gases, liquids, or other solids. Many chemical reactions, especially heterogeneous catalysis, occur predominantly at the surface of materials. Pentlandite [(Fe,Ni)9S8] is the principal BMS host of the majority of PGEs and also primary source of Nickel. Pentlandite (Pn) is recovered by milling and flotation. The difficulty in recovering pentlandite is mostly associated with oxidation and the brittle nature of pentlandite. Understanding the surface chemistry of Pn minerals is very crucial as it will improve the recovery of this precious mineral and its hosts. This understanding helps in optimizing processes such as flotation, leaching, and milling, which are commonly used in mineral processing. In the present study we used density functional theory (DFT) technique to study and compare stability of Fe5Ni4S8 (P4_2/nmc) (111) and (311) surfaces. The XRD of Fe5Ni4S8 (P42/nmc), shown in Figure 5.2a, revealed that the (311) plane exhibited the highest intensity, followed by the (111) plane. Structural optimization for possible terminations of both (111) and (311) surfaces was performed. Additionally, the calculated surface energy for (311) was less than that of (111) suggesting (311) was the most stable surface and thus the Pn mineral is likely to cleave through (311) during crushing of these mineral.

Apply for student award at which level:

PhD

Consent on use of personal information: Abstract Submission

Yes, I ACCEPT

Primary author: Mr MOLALA, Barnard (University of Limpopo)

Co-authors: NGOEPE, Phuti Esrom (University of LImpopo); MKHONTO, Peace (University of Limpopo); MEHLAPE, Mofuti (University of Limpopo)

Presenter: Mr MOLALA, Barnard (University of Limpopo)

Session Classification: Poster Session

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