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# Effect of Co on structural, stability and ductility of Fe5Ni4S8 (P4_2/nmc): Cluster expansion method

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Pentlandite ((Fe,Ni)9S8) is a primary source of nickel and is largely found in the Merensky reef which host the largest amounts of base metal sulphides (BMSs) and is also known to host platinum group elements (PGEs). Palladium and rhodium are the PGEs contained mostly in pentlandite, cobalt (Co) is also one of the metal found in association with pentlandite. The milling of pentlandite prior to flotation has presented challenges which are associated with its brittle nature. In the present study the cluster expansion (CE) method was used to predict the stable (Fe,Ni)9S8 pentlandite structure. The Fe5Ni4S8 pentlandite compound was found as the most stable structure, which possessed a space group of P4_2/nmc. Furthermore, Fe5Ni4S8 was doped with Co using cluster expansion and found that the (CoFe4Ni4S8, Fe4CoNi4S8 and Fe5Co2Ni2S8 i.e Co doped at Fe(O), Fe(T) and Ni(T)) composition were the most stable. The calculated Bulk to Shear modulus ratio (Pugh's ratio) of CoFe4Ni4S8, Fe4CoNi4S8 and Fe5Co2Ni2S8 system were greater than 1.75, which showed that Co increased the ductility of Fe5Ni4S8 (P4_2/nmc). Additionally, the symmetry of Fe5Ni4S8 (P4_2/nmc) remained tetragonal after Co doping.
Moreover, the heats of formation for Co doped systems was greater than of un-doped Fe5Ni4S8 (P4_2/nmc), suggesting that Co increased the thermodynamic stability of pentlandite.

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

Yes

## Level for award;(Hons, MSc, PhD, N/A)?

PhD

**Primary author:** MOLALA, Kgwajana Barnard (University of Limpopo)

**Co-author:** Dr MEHLAPE, Mofuti Abram (University of Limpopo)

**Presenters:** Dr MKHONTO, Peace Prince (University of Limpopo); Prof. NGOEPE, Phuti E. (University of Limpopo)

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