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Atomistic simulation studies of binary M9S8 (M=Ir, Rh) and ternary (RuPd)9S8 Pentlandite-like systems

Pentlandite (Pn) is an iron nickel sulphite with chemical formula of (Fe,Ni)9S8 and is contained mainly in Merensky Reef (˜30%) of Bushveld complex. Pn systems are known to host precious metals in solid solutions or as intergrowths. However, the concentration of the precious metals hosted in the pentlandite structure and the effect of temperature and pressure on Pn-PGEs has not been established. Therefore, the formation of the PGEs in the Pentlandite structure must be explored and could establish new forms of Pentlandite. Pentlandite structures have been studied mostly experimentally but computational studies have been scares. Chauke et al. conducted study on stability of Cobalt pentlandite (Co9S8) and Iron Nickel Pentlandite ((Fe,Ni)9S8) using first principle density functional theory. Moreover, Mehlape investigated various forms of cobalt Pentlandite mineral, (Co9S8) at different temperatures, using classical atomistic simulation methods and found that the melting temperature of Co9S8 was 1300K. In this study, we derived atomic potentials for binary M9S8 (M=Ir, Rh) and ternary Ru5Pd4S8 and Ru5Pd4S8 Pentlandite-like systems, which produced the elastic constants that are in good agreement with ab-inito density functional theory (DFT) results and further conducted the classical atomistic simulation on binary M9S8 (M=Ir, Rh) and ternary Ru5Pd4S8 and Ru5Pd4S8 and found that the melting temperature for binary M9S8 (M=Ir, Rh) and ternary (RuPd)9S8 Pn-like systems 1800K and 1500K respectively.

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

Yes

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

PhD

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