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# Computational modelling studies of the sulphide minerals with the pentlandite structure

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Metal sulphide minerals are of great industrial and economic significance, since they are the main source of various base and precious metals such as zinc, copper, lead, nickel, cobalt, platinum and iridium. The sulphide minerals are the most important, most diverse, and richest in terms of physical, chemical, and structural properties [1].

Pentlandite $(Co,Ni,Fe)_9S_8$, serves as a source of nickel and cobalt in continental deposits and also exhibits solid solutions and intergrowths with precious metals [2]. Detailed understanding of structural and electronic properties of such compounds is important for metal extraction.

The stability of the pentlandite compounds were previously studied using computational modelling methods [3]. Furthermore, the experimental high temperature phase transitions of pentlandite structures are available [4]. Computational modelling techniques are a helpful tool for analysing and predicting various fundamental properties of materials. In the current study atomistic simulations, involving empirical interatomic potentials, are employed to determine structure, mechanical properties and ion transport of various pentlandite structures, i.e. $Co_9S_8$, $Rh_9S_8$, $Ir_9S_8$, $Ni_9S_8$ and $(FeNi)_9S_8$ at different temperatures. The first interatomic potentials of $Co_9S_8$ were derived with input data such as structure and elastic properties from experiment and electronic structure calculations, respectively. The accuracy of the derived interatomic potentials was checked by comparing the known experimental and calculated data which include lattice parameters, interatomic distances, and elastic properties. High temperature properties were deduced from molecular dynamics calculations and related phase transformations were reproduced up to high temperatures. The empirical potentials are further intended for studies of surfaces and nanocrystals of pentlandites, which involve large number of atoms and tend to be computationally intensive.

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