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Atomistic simulation of the structure and elastic properties of pentlandite

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Atomistic simulation was carried out to study the effect of pressure on the structure and elastic properties of pentlandite structures of the form M₉S₈ sulphides (M = metal). The lattice parameters, bond lengths and elastic constants as a function of pressure are calculated. Pentlandite is a major precious metals-bearing mineral and plays a very important role in mining. Precious metal ores co-exists with base metals either as solid-solution and intergrowths, hence rendering its detailed understanding important for efficient extraction of these precious metals. This work relates to problems in applied areas such as mineralogy, geophysics and geochemistry, whereby phase transition is modified by impurities, so there is the additional concern of the effect of high pressures. We want to see how pressure changes the lattice parameters, elastic constants and bond lengths. We used computational techniques to investigate the effect of high pressure on the pentlandite structures. It was noted that as the pressure increases, the volume decreases. The elastic properties were found to be positive, which satisfies the conditions for a mechanically stable cubic structure.

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Primary author: Dr MEHLAPE, Mofuti (University Of Limpopo)

Co-authors: Ms TANZWANI, Dakalo (University of Limpopo); Prof. NGOEPE, Phuti (University of Limpopo)

Presenter: Dr MEHLAPE, Mofuti (University Of Limpopo)

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