Computational Studies of Pentlandite Mineral: Structural and Dynamical Properties Probed by Molecular Dynamics

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Introduction

- Sulphide minerals are minerals containing sulphide (M_9S_8) (M=metal) and economically important as metal ores (e.g. zinc, copper, lead, nickel and cobalt, rhodium, gold, iridium.
- The significance of mineral sulphides with pentlandite structure is their provision of nickel [1], and precious metals: ruthenium, rhodium, palladium, osmium iridium and platinum, gold and silver.
- Pentlandite minerals play an important role in the production of cleaner fuels with low or ultra-low sulphur content that require a continuous improvement of catalytic materials used in the refinement industry [2].
- In order to extract the precious metals from the ores effectively it is necessary to study and understand structural and physical properties, of sulphide minerals in detail.

Structures and Applications

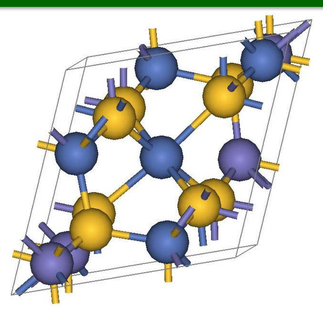
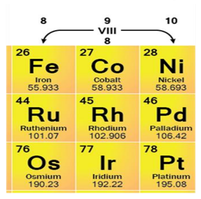


Figure 1: Primitive Unit Cell of $Fe_4Ni_5S_8$ Space Group, *Fm3m.* Yellow spheres represent Sulphur, blue spheres represent iron and purple spheres represent nickel.



Group 9 (VIII) of the periodic table

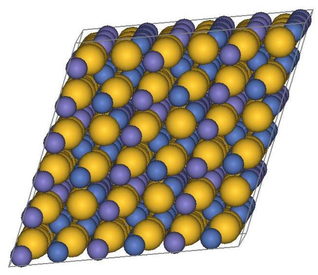
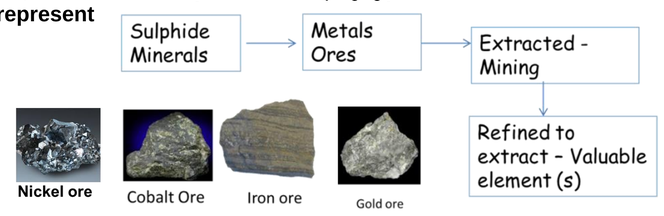


Figure 2: The initial configuration of 3x3x3 supercell of $Fe_4Ni_5S_8$ pentlandite.



Flowchart showing how metal ores are extracted through mining and refined to obtain valuable elements.

Methodology

- The study is based on atomistic simulation of pentlandite structure ($Fe_4Ni_5S_8$).
- The atomistic simulation method uses interatomic potential functions to describe the total energy of a system in terms of atomic coordinates.
- The static energy minimization code, General Utility Lattice Program (GULP) [3] was used to derive interatomic potentials [4], and to calculate the properties of pentlandite structure through molecular dynamics (MD).
- The MD simulation were run for 500 ps and equilibrated for 100 ps.
- Temperature is controlled by the canonical ensemble (NVT) constant number of particles (N), volume (V) , temperature (T)

RESULTS AND DISCUSSIONS

Table 1: The structure and elastic properties calculated by the interatomic potentials used in the study compared with the density functional theory (DFT) properties [4]. The potential models reproduces the structure and elastic constants reasonably

	Potential Model	DFT
Parameter (Á)		
a	7.015	7.012
b	6.856	7.039
c	6.976	7.024
Vol (Á)^3	238.236	237.358
Density of Cell (g/cm^3)	5.390	5.410
Bond lengths		
Fe-S	2.11	2.22
Fe-F e	3.45	3.50
S-S	3.27	3.22

	Potential Model	DFT
C_{ij}	GPa	GPa
C_{11}	205.50	207.18
C_{12}	100.72	102.38
C_{44}	49.40	47.07
Bulk Modulus	131.35	137.31

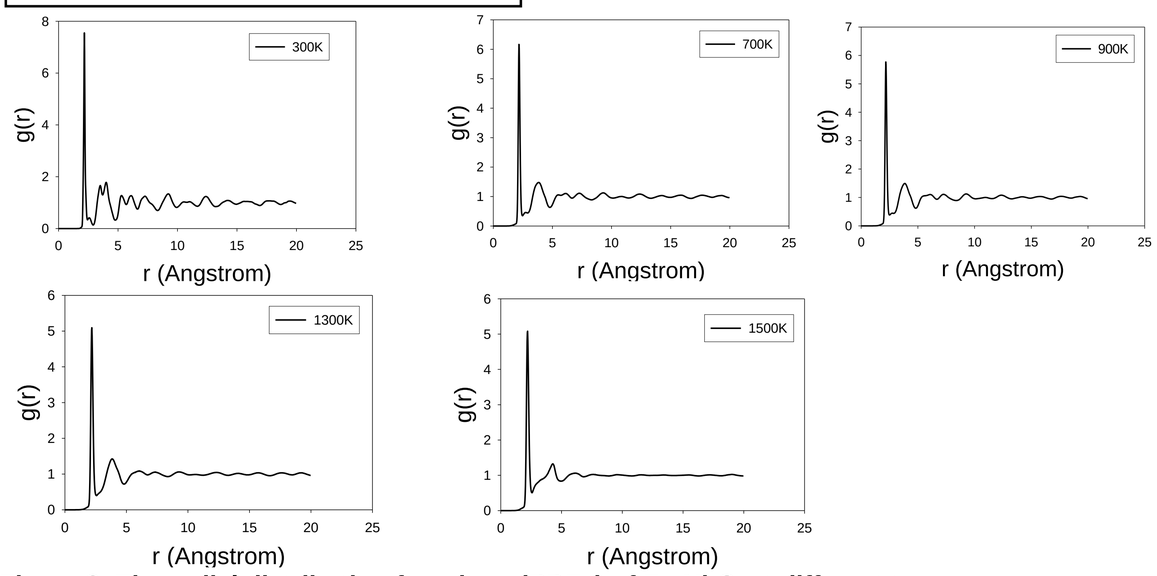


Figure 3: The radial distribution functions (RDFs) of $Fe_4Ni_5S_8$ at different temperatures

- The simulated structures and radial distribution functions of $Fe_4Ni_5S_8$ at the temperatures between 300 K and 1500 K.
- At the temperatures between 300 K and 900 K we have a well-ordered structure and RDFs have many peaks, however between 1300 K and 1500 K the arrangement of atoms is fading and the peaks are broad. This implies the melting of the structure between 1300 K and 1500 K.
- Experimentally the melting temperature of $Fe_4Ni_5S_8$ was observed at ~1255 K [5].

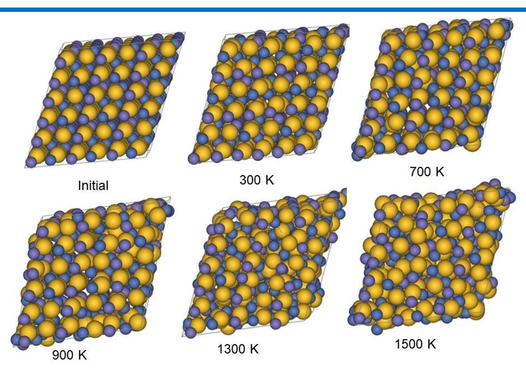


Figure 4: Structural changes of $Fe_4Ni_5S_8$ structure after MD simulations at different temperatures

- From 300K to 900K the shape of the structure is still maintained, showing crystallinity.
- From 1300K to 1500K the structure loses shape , showing phase change at 1300K. This temperature is closer to the experimental melting point value of ~1255K [5].
- Our potential model is able to produce the melting point of our structure.

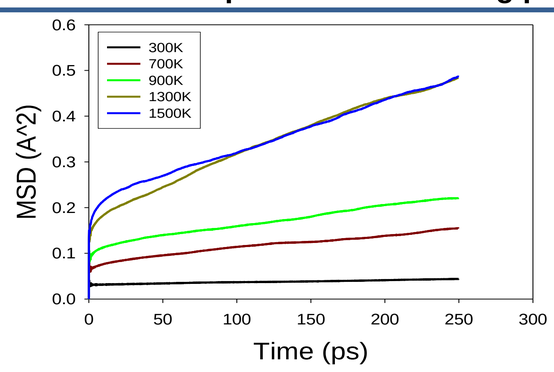


Figure 5: The variation of MSD of $Fe_4Ni_5S_8$ with time at different temperatures.

- The mean-squared displacement (MSD) for bulk pentlandite structure calculated for our model also predicts the high mobility of pentlandite structure. The graphs shows the total MSD for $Fe_4Ni_5S_8$ at different temperatures.

CONCLUSION

Molecular dynamics simulations were performed with the aim of investigating the dynamic and structural properties of pentlandite structure. The melting of the structure was observed through the radial distribution function (RDFs). At low temperatures (300 K – 900 K) the RDFs have many and sharp peaks, however, at higher temperatures (1300 K – 1500 K) the RDFs curve are relatively smooth and does not exhibit any defined peaks, indicative of structural change from solid to liquid phase. Furthermore, through the mean-squared displacement (MSD), the results show that MSD increases with temperature and atoms are able to move more at high temperature. MSD increases with time in all investigated temperatures and there is a linear relationship between MSD and simulation time.

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