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Research Paper

Comparison of NaOL Adsorption on the Hematite 001 Surface with Water Molecules Adsorption on the Hydrophilic Hematite Surface Using Molecular Dynamics Simulation

Hashemi Sh.[1], Noaparast M.[2*], Mabudi A.[3]

1- Ph.D Student, Dept. of Mining Engineering, Faculty of Engineering, University of Tehran, Tehran, Iran
2- Professor, Dept. of Mining Engineering, Faculty of Engineering, University of Tehran, Tehran, Iran
3- Assistant Professor, Dept. of Mining Engineering, Sahand University of Technology, Tabriz, Iran

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Abstract: This article reports on a molecular dynamics simulation-based research that investigates the adsorption of sodium oleate (NaOl) on the of the highly hydrophilic 001 hematite surface in froth flotation and its effect on the mineral's wettability properties. The molecular dynamics simulation was conducted using LAMMPS. The wettability properties were evaluated by comparing the thermodynamic characteristics of two surfaces, one net and the other coated by the collector. Surface energy, center of mass location of water molecules, water density in contact layers and adjacent to the surface, and fluid permeability coefficient were used as indicators of wettability. The simulation results showed that the 001 surface of hematite is highly hydrophilic due to strong electrostatic interactions and feasible hydrogen bond formation sites. However, with the adsorption of the collector, the surface became hydrophobic due to a sharp decrease in surface tension, reduction of intermolecular interactions, and loss of hydrogen bond formation sites. The results confirm that the selective absorption of the collector on the hematite surface enables its floatability.

Keywords: Adsorption, Molecular dynamics simulation, Hematite, Sodium oleate, Wettability.

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*Corresponding Author Email: *noparast@ut.ac.ir*

INTRODUCTION

The flotation mechanism of oxide and silicate minerals depends mainly on their electrical properties, solubility, surface charge, collector chain length, and metal-collector salt stability [1-6]. Hematite (iron oxide) enrichment is a crucial process as it is one of the primary sources of iron ore and steel production [7]. Flotation and magnetic separation are commonly used for hematite enrichment or removal [8]. Unlike Sulphides, hematite is highly hydrophilic due to the presence of oxygen in its chemical composition, which forms hydrogen bonds. Therefore, flotation is not possible without the presence of collectors [8,9]. Molecular dynamics simulation (MDS) is a method that analyses the microscopic properties of a system, such as the mass and interactions of atoms or molecular structure, to predict its macroscopic properties [9]. This simulation method is advantageous because it can study many conditions and states of the system from a molecular perspective [10].

METHODS

In this research, the mechanism of sodium oleate (NaOl) adsorption on the 001 surface of hematite in the flotation environment and its effect on the wettability of this mineral were investigated using MDS. The simulation was carried out in the LAMMPS open source code environment. Wettability was investigated by comparing the thermodynamic characteristics of the hematite surface with and without the collector, including surface energy, center of mass of water molecule location, water density in contact layers and adjacent to the surface, and fluid permeability coefficient.

FINDINGS AND ARGUMENT

The results showed that, without the addition of a collector, strong electrostatic interactions between water molecules and the mineral surface caused the absorption of water molecules, resulting in system equilibrium being achieved in a very short time (approximately 0.5 nanoseconds) and a diffusion coefficient. However, on hematite surfaces coated with a collector, the time increased to 4 nanoseconds due to the sharp decrease in surface tension and the reduction of intermolecular interactions between the hematite surface and water molecules, resulting in hydrophobicity of the surface (see Figure 1). The results of the water density distribution profile at different distances from the hematite surface indicated changes in the wetting regime of the surface due to the absorption of the collector. Additionally, the difference in water density in different fluid layers near the solid surface confirmed the hydrophobicity of the hematite surface covered by the collector. Furthermore, the collector led to a decrease in the number of hydrogen bonds, confirming the important role of hydrogen bond formation in the hydrophilic behavior of this mineral.

The variation in wettability regime and hydrophobicity of the hematite surface after collector absorption was mainly due to the loss of absorption sites and possible locations for hydrogen bond formation. The center mass of water molecules diagram on the hematite surface along the z-axis was in good agreement with other results and confirmed that the center of gravity of water molecules moved away from the hematite surface (indicating hydrophobicity of the hematite surface).

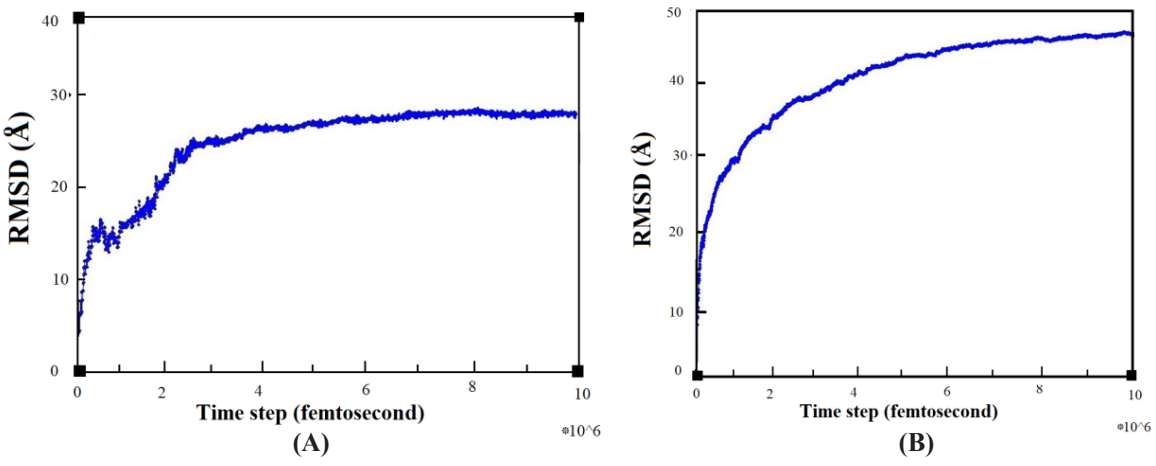

Figure 1. A: Carbon RMSD in sodium oleate composition and **B:** hydrogen RMSD in water molecule

CONCLUSIONS

The simulation findings generally showed good agreement with the laboratory results [11,12], revealing that the selective absorption of sodium oleate collector on the hematite surface leads to a hydrophobic surface that enables hematite floatability.

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