Faculty and PostDoc, Science and Engineering

DFT-MD dissolution of oilfield pyrite scale using borax

Borax aids pyrite scale dissolution leading to scale removal in **oil** and **gas** pipelines.

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BACKGROUND

Iron sulfide form scales such as pyrite in pipes which lead to loss of production in the oil and gas industry. Computational tools such as DFT-MD (Density Functional Theory-Molecular Dynamics) may be used to understand and model chemical compounds that would be effective in removing these scales.

METHODS

Pyrite-Borax Model
- **QUANTUM ATK's Virtual Nano Lab**

DFT-MD calculation
- **VASP**

MD Trajectory analysis
- **RDF**

RESULTS

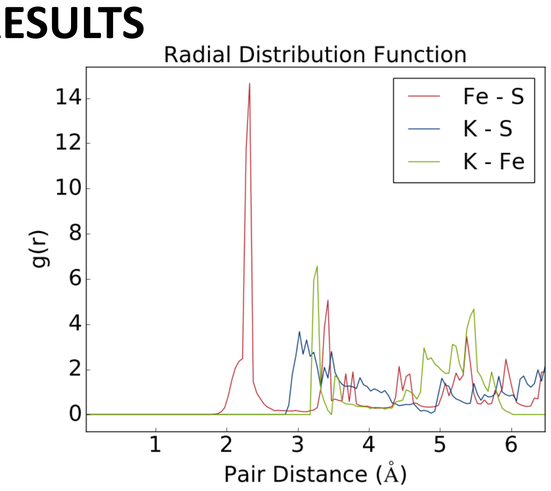

Fig 1. The RDF of the pyrite-borax system for Fe-S, K-S, and K-Fe bonds

- The potassium ion (K^+) form bonds with the sulfur (S) atoms in the top layer of the pyrite rather than iron (Fe) as shown in the radial distribution function (RDF), and geometrical structures.
- K^+ present in borax is the predominant factor that accounts for pyrite dissolution.
- The absence of chelating agent may lead to the formation of Fe-S bonds therefore, restoring the system to its initial state.

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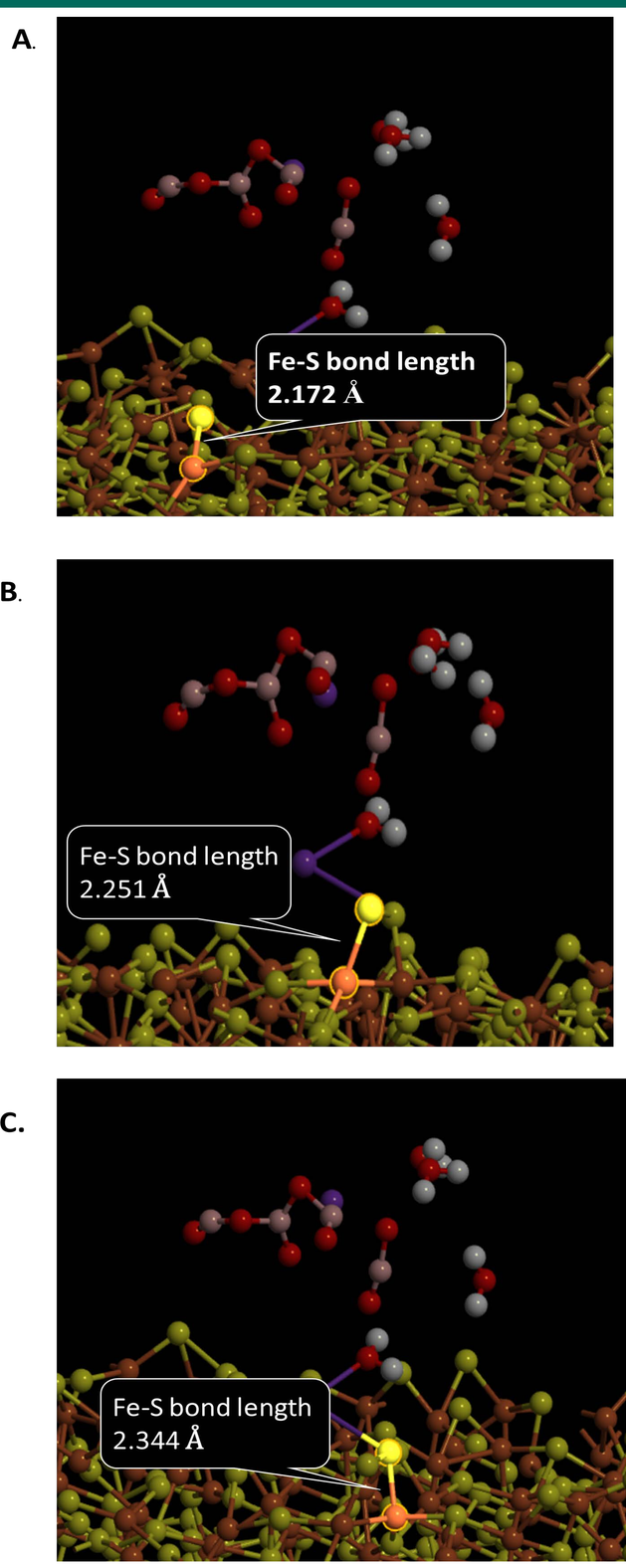
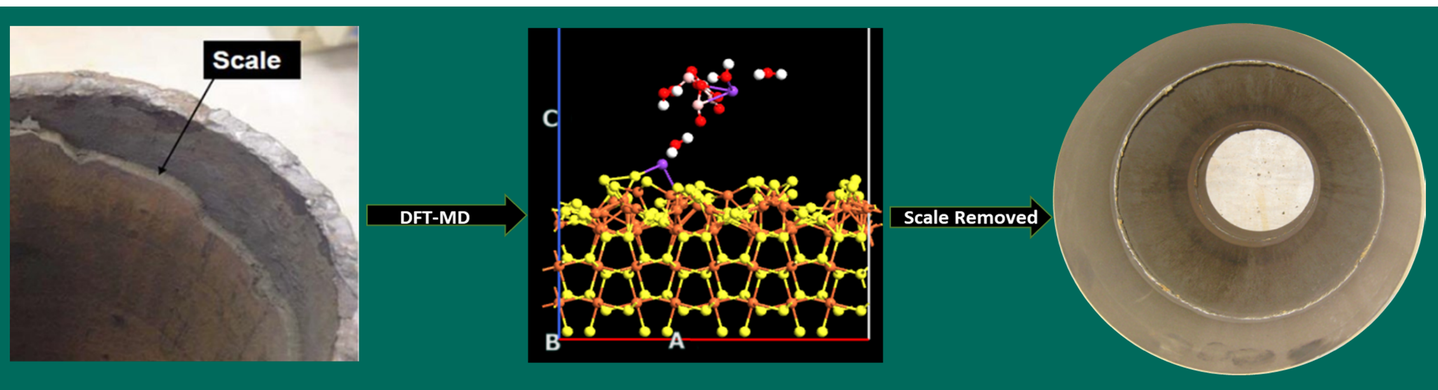


Fig 2. Difference in bond lengths of Fe-S bonds depicting that Sulfur atoms are leaving the surface



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SCAN ME

Sulfur (S) Iron (Fe) Hydrogen (H) Potassium (K) Boron (B)