Investigating the Interaction between Quartz and Water using Molecular Dynamics Simulations with LAMMPS Software

Willian Fábio Radel[1], Marcelo Lopes Pereira Júnior[2]

[1]Universidade de Brasília (*Instituto de Física*), [2]Universidade de Brasília (*Faculty of Technology Department of Electrical Engineering*)

e-mail: willradel@gmail.com

Quartz is a widely abundant mineral found in various types of rocks and present in all terrestrial regions [1]. It is known for its high thermal and chemical stability, as well as its hardness, making it a valuable material for a range of applications. Its interaction with water is also relevant due to its abundance in the Earth's crust. Molecular dynamics is a branch of physics that studies the movements and interactions of molecules through modeling, simulation, and analysis. The LAMMPS software is a powerful tool for simulating atomic and molecular systems on a large scale using numerical integrators and a variety of interatomic potential models, such as Lennard-Jones potential, Morse potential, REAXFF, and the AIREBO potential. To investigate how fracture patterns affect wettability [2], thisstudy uses molecular dynamics simulations with LAMMPS. The system has periodic boundary conditions and is equilibrated with the NPT ensemble before strain is applied for100 ps to eliminate residual stresses. The system is also thermally equilibrated at ambienttemperature using the NVT ensemble for 100 ps. Strain is then applied with and withoutwater to evaluate mechanical properties, and other simulations are performed to assess thewettability. Overall, this study provides insights into the properties of quartz and its interaction with water, as well as the behavior of molecular systems using LAMMPS and theAIREBO and REAXFF potentials. The findings have implications for a range of fields, including materials science, geology, and physics.

Acknowledgements:
FAPDF, CNPq, CAPES, and UnB.

References:
[1] Klein, Cornelis. “mineral”. Encyclopedia Britannica, 3 Feb. 2023, https://www.britannica.com/science/mineral-chemical-compound. Accessed 16 April 2023.
[2] Luz, A. B. D., Sampaio, J. A., França, S. C. A. (2010). Tratamento de minérios. CETEM/MCT.