

The Computer Simulation Of Calcite Growth Inhibition: a Monophosphonate Study

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The mechanisms of surface growth inhibition of the mineral calcite by phosphonate threshold poisons has been widely studied experimentally and computationally 1,2,3,4. We have simulated the interaction of monophosphonate growth inhibitor ions with the planar and stepped (211) surfaces of the calcite. The current work builds on a previous study of a diphosphonate/calcite system⁵. The calculations were performed using the MARVINS surface simulation code⁶, employing energy minimization and molecular dynamics techniques. We show that the planar (211) surface has a smaller affinity for the inhibitor ions compared to the stepped (211) in accordance with experiment; and that the predominant mode of interaction of the inhibitor with the surface is via the electrostatic term. Monophosphonate inhibitor ions possessing an enhanced localization of electron density around the phosphonate group and heteroatom groups demonstrate a greater association to the calcite lattice. Replacement processes simulating the irreversible incorporation of monophosphonate ions at terrace and step sites are energetically more favourable than those calculated for diphosphonate ion analogues straddling identical defect sites. However, the

main inhibition mechanism thought to operate over a range of pH values for the monophosphonate/calcite(211) system is via the selective binding of the monophosphonate ions to calcite obtuse step edge sites and kink sites thus decreasing the progression of step movement and therein destroying and/or delaying the formation of potential kink sites and hence future step assembly by pre-docked monophosphonate ions.

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