

Investigating the role of Mg^{2+} in $CaCO_3$ Crystallization
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Bulk precipitation of $CaCO_3$ has been widely studied over the years, examining the impact of one or two ions. However, in realistic systems the bulk solution is never as pure as the laboratory growth conditions. One realistic system is the growth of $CaCO_3$ in synthetic seawater, a solution containing 11 different inorganic ion species such as high magnesium and sulfate levels. The formation of aragonite from solution based precipitation has been well documented within the literature. It has been known that Mg^{2+} ions within the growth solution influences the formation of aragonite over calcite, despite aragonite being less thermodynamically stable. Multiple theories have been suggested in the literature to explain why this is. One key theory relates to the energy required to dehydrate Mg^{2+} ions, pushing the solution based equilibrium towards the formation of aragonite. The second main theory is the adsorption of the Mg^{2+} ions onto the surface of calcite, increasing the surface free energy of Mg-Calcite making it energetically less favourable than aragonite. Due to the dense unit cell of aragonite, incorporation of Mg^{2+} into aragonite has been thought to be energetically unfavourable. This body of work suggests that due to a synergistic effect between Mg^{2+} and SO_4^{2-} . The Mg^{2+} ions can incorporate into aragonite, albeit at low levels, this prevents the aragonite dissolving and reprecipitating into calcite. This has been observed using high resolution TEM and EBSD. The reasons for this are explored using molecular modelling.