Nanoscale processes for calcium carbonate formation: Insights from computer simulation

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Calcium carbonate is an abundant biomineral and also relevant to technological processes, along with other metal carbonates, from carbon sequestration to scale formation. Therefore, understanding the crystallization of this mineral is of great importance. Despite this, the formation mechanisms for $CaCO_3$ remain controversial [1,2,3] and are still yet to be fully characterized at the nanoscale.

In this study, aspects of both the initial pre-nucleation regime and post-nucleation growth of calcite will be examined using computer simulation. Based on enhanced sampling molecular dynamics, it will be shown that it is now possible to map the free energy landscape for growth pathways at surface features such as step edges [4] and kinks, despite challenges due to the rate-limiting slow exchange of water in such regions [5]. This nanoscale understanding of growth and dissolution processes suggests that modification of standard models is required, while providing a physical explanation for recent kinetic models [6]. The role of defects and metal-impurity incorporation will also be discussed.

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