

Crystallisation of amorphous calcium carbonate

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The importance of amorphous calcium carbonate (ACC) in the crystallisation of calcium carbonate remains a fundamental question in biomineralisation. ACC is generally reported in two different phases [1]: one with a high water content (~50% or greater) that is relatively stable and the other with a low water content that is transient and undergoes a rapid transition to calcite or another CaCO₃ polymorph. The growth of crystalline calcium carbonate remains an intense debate with varying models proposed. ACC is frequently highlighted as a precursor but how and if it directly crystallises is uncertain [2], [3].

We present simulations of calcite and aragonite interfaces with ACC structures of varying water content. Our results demonstrate that the crystalline surfaces are most stable with water rather than hydrated or dehydrated ACC. We use this to explain why crystallisation has been observed to occur on the surface of ACC particles [4] removing the need for dramatic dehydration processes of the ACC.

[1] Addadi, L.; Raz, S.; Weiner, S. (2003) *Advanced Materials* **15**(12), 959–970 [2] Pouget, E.M.; Bomans, P.H.H.; Goos, J.A.C.M.; Frederik, P.M.; de With, G.; Sommerdijk, N.A.J.M. (2009) *Science* **323**(5920), 1455–1458 [3] Hu, Q.; Nielsen, M.H.; Freeman, C.L.; Hamm, L.M.; Tao, J.; Lee, J.R.I.; Han, T.Y.J.; Becker, U.; Harding, J.H.; Dove, P.M.; De Yoreo, J.J. (2012) *Faraday Discussions*, **159**, 509–523 [4] Nielsen, M.H.; Aloni, S.; De Yoreo, (2014) *J.J. Science*, **345** (6201), 1158–1162