PATHWAYS OF MATRIX SELF-ASSEMBLY AND SUBSEQUENT MINERALIZATION



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Abstract

To understand the underlying physical controls governing matrix assembly and mineralization, we have investigated these processes using *in situ* AFM and TEM with dynamic force spectroscopy and molecular dynamics.

Our results reveal the key role played by conformational transformations in controlling the pathways and kinetics of matrix assembly. Moreover, the pathway to the final ordered state often passes through transient, less-ordered conformational states. Thus, the concept of a folding funnel with kinetic traps used to describe protein folding is also applicable to matrix self-assembly.

Analysis of matrix mineralization shows that nucleation is promoted through a reduction in the interfacial energy. However, nucleation via an amorphous precursor is observed at supersaturations that are too low to be explained by classical theory. The existence of pre-nucleation clusters is shown to provide a low-barrier pathway to crystallization that circumvents the large barriers to nucleation. Finally, to understand cluster-and particle-mediated crystallization processes, we have performed *in situ* high-resolution TEM. We show that when primary nuclei approach with a near-perfect lattice match, they undergo a sudden "jump to contact" over < 1nm. Measured translational and rotational accelerations show that strong, highly direction-specific interactions drive crystal growth via oriented attachment. Taken together, these results provide insights into the mechanisms controlling biological crystallization, from formation of the initial matrix to the maturation of final crystalline structures.

Bio

Jim De Yoreo research has spanned a wide range of materials-related disciplines. Most recently, his research has focused on in situ investigation and manipulation of interactions, assembly and crystallization in biomolecular and biomineral systems. He is a Fellow of the American Physical Society and a recipient of the Laudise Prize of the International Organization for Crystal Growth, and an R&D 100 Award. He is Associate Editor in Chief for *Frontiers of Materials Science* and an Associate Editor for the *Journal of Crystal Growth*. He has served on committees for the National Academy of Sciences, the Department of Energy and Congress.

