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Identifying differences in long-range structural disorder in solids using mid-infrared spectroscopy

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Structural disorder in calcium carbonate materials is a topic of intense current interest in the fields of biomineralization, archaeological science, and geochemistry. In these fields, Fourier transform infrared (FTIR) spectroscopy is a standard material characterization tool because it can clearly distinguish between amorphous calcium carbonate and calcite. Earlier theoretical work based on density functional theory (DFT) showed that calcite's in-plane bending mode in FTIR is very sensitive to changes in local (intra-unit-cell) disorder, which accounts for the near vanishing amplitude of this peak for amorphous calcium carbonate [1]. In a subsequent study of polycrystalline calcites, DFT investigations showed that local disorder was also qualitatively consistent with changes in the in-plane bending modes for these materials [2]. Here, we examine this assumption by presenting our study of the structural differences among several different sources of crystalline calcite, all of which show differences in the widths of their FTIR in-plane bending mode peaks. We used X-ray diffraction (XRD) to assess disruptions to long-range periodicity including lattice strain, microstrain fluctuations, and crystalline domain size (crystallinity). These quantities were then correlated with mid-FTIR (carbonate vibrational mode) peak positions, widths and relative intensities. Unlike the earlier studies [2], our results show that the in-plane bending mode can be strongly affected by the long-range disorder (based on XRD data) even when the local environments (based on Extended X-ray Absorption Fine Structure data) are identical. This apparent discrepancy between calculated and experimental models of structural disorder is, in fact, strong evidence for the near continuum of local and long-range structural differences that calcium carbonate materials can accommodate. Thus, we conclude that mid-FTIR spectra can be a powerful diagnostic for identifying differences in long-range structural disorder in carbonate-containing materials.

References:

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[2] K. M. Poduska, L. Regev, E. Boaretto, L. Addadi, S. Weiner, L. Kronik and S. Curtarolo, Adv. Mater., 2011, 23, 550–554.

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