Poster Presentation

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Freshwater pearls as near single crystals for vaterite structure resolution

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There has been lots of controversies about vaterite structure in the past decades. Extra peaks occurring out of the hexagonal structure and best described by Kamhi [1] still resist any indexing. Lower space group symmetries, superspace groups, microtwinning, and first-principle calculations [2], all failed in taking account of these minor peaks, surprisingly always present in all synthetic and biogenic vaterite formations. Recently, secondary interspersed domains observed in high-resolution TEM images indicated their incoherence and rather incompatible character with the vaterite matrix [3]. One of the major difficulty in resolving the vaterite structure lies in the absence of single crystals. Powder diffraction patterns are always composed of hexagonal and extra, but small, peaks, and temptation to index the pattern as a single phase is large, particularly since x-ray fluorescence invariably probes for CaCO3. We used Hyriopsis cumingii freshwater mussel pearls to help proving that vaterite is definitely crystallizing within the original hexagonal space group. Some of these pearls suffer defective growth toward vaterite. In such cases the hexagonal peaks clearly exhibit a strong texture while the extra peaks look more random. This is an invaluable evidence of the existence of clearly separated phases, though the minor phase (or phases) still resist indexing. The hexagonal structure refinement, thanks to the strong vaterite texture, is obtained with larger resolution than before.

[1] *S.R. Kamhi, Acta Cryst., 1963, 16, 770,* ***[2]*** *Le Bail et al., Powder Diffraction, 2011, 26, 16,* ***[3]*** *L. Kabalah-Amitai et al., Science, 2013, 340, 454*

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