Freshwater pearls as near single crystals for vaterite structure resolution

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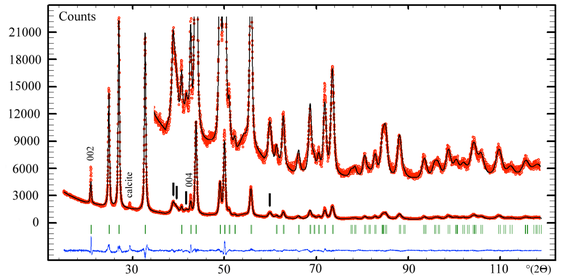
Introduction

There has been lots of controversies about vaterite structure [1-4]. Extra peaks occurring out of the hexagonal structure and best described by Kamhi [1] still resist any indexing. One of the major difficulty in resolving the vaterite structure lies in the absence of single crystals.



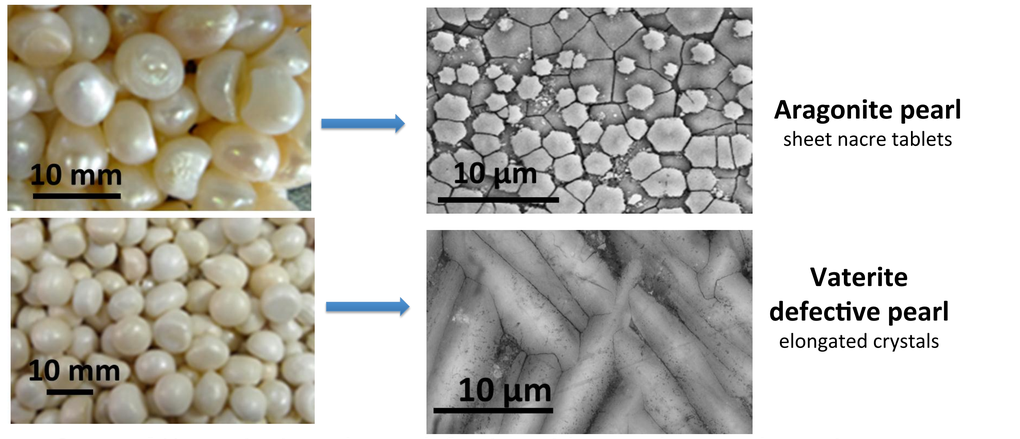
Le Bail fit of a vaterite powder (Kamhi's $P6_3/mmc$ model). Arrows: extra peaks

Hyriopsis cumingi (freshwater mussel), China

We use *Hyriopsis cumingii* pearls to help proving that vaterite is definitely crystallizing within the original $P6_3/mmc$ space group (both synthetic and biogenic vaterite exhibit the same extra peaks)

Vateritic defective pearl

H. cumingi pearls

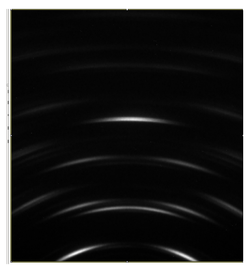


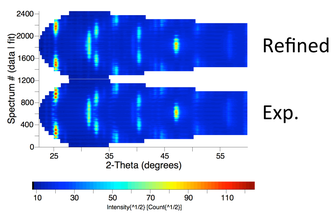
Aragonite pearl
sheet nacre tablets

Vaterite defective pearl
elongated crystals

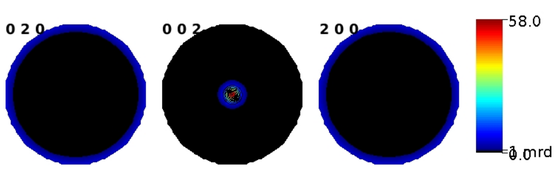
Some of *H. cumingi* pearls are defective with growth toward vaterite

Texture of aragonite pearls



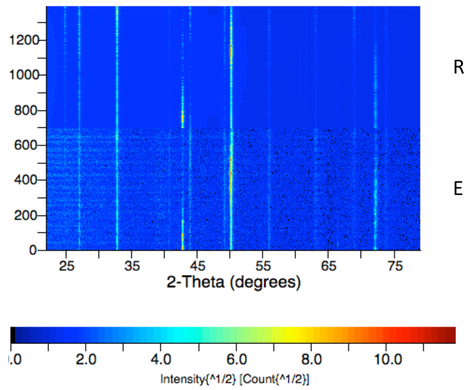


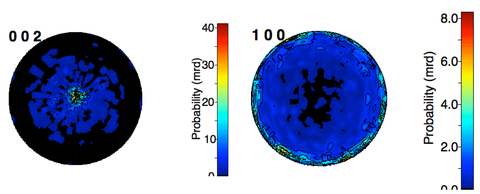
Using CCD + Mo-µsource experiments, Combined Analysis shows strong aragonite texture with c-axes perpendicular to the nacre tablets



a = 4.9785(2) Å; b = 7.9801(3) Å; c = 5.7258(2) Å

Texture of vateritic pearls



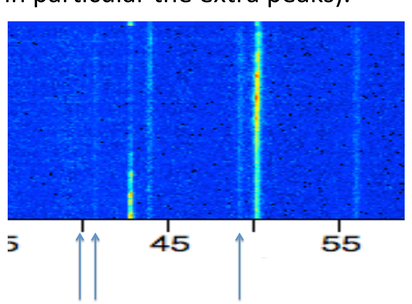


Using an INEL CPS120 detector + point Cu-tube, Combined Analysis evidences strong vaterite texture with c-axes aligned with the long crystal axes

a = 4.11428(3) Å; c = 8.43450(5) Å

	x	y	z
Ca	0	0	0
C	0.290(1)	0.579(3)	1/4
O1	0.120(6)	0.240(1)	1/4
O2	0.38(2)	0.760(1)	0.120(1)

Combined Analysis also allows structure refinement of vaterite.
But some small peaks do not show intensity variations (do not obei the main phase texture, in particular the extra peaks).



Conclusions

In *Hyriopsis cumingi*:

- Vaterite defects grow from aragonite (a,b) planes:

c(aragonite) // c(vaterite)

- Vaterite is strongly textured while extra lines are not !

Kamhi's model takes account of all textured vaterite peaks

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References: [1] Kamhi, S. R. (**1963**) Acta Cryst. **16**, 770; [2] Le Bail et al. (2011) Powder Diffraction 26, 16; [3] Wang, J. and Becker, U. (**2009**) Am. Mineral. **94**, 380; [4] Kabalah-Amitai et al. Science 340, 454