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.

Hyriopsis cumingi (freshwater mussel), China

We use Hyriopsis cumingii pearls to help proving that vaterite is definitely crystallizing within the original P63/mmc space group (both synthetic and biogenic vaterite exhibit the same extra peaks)

Texture of vateritic pearls

<table>
<thead>
<tr>
<th></th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ca</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>C</td>
<td>0.290(1)</td>
<td>0.579(3)</td>
<td>1/4</td>
</tr>
<tr>
<td>O1</td>
<td>0.120(6)</td>
<td>0.240(1)</td>
<td>1/4</td>
</tr>
<tr>
<td>O2</td>
<td>0.38(2)</td>
<td>0.760(1)</td>
<td>0.120(1)</td>
</tr>
</tbody>
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Combined Analysis also allows structure refinement of vaterite. But some small peaks do not show intensity variations (do not obey 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