

Quantitative XRD analysis of {110} twin density in biotic aragonites

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{110} twin densities in biotic aragonite have been estimated quantitatively from the peak widths of specific reflections in powder X-ray diffraction (XRD) patterns, as well as direct confirmation of the twins using transmission electron microscopy (TEM). Influence of the twin density on the peak widths in the XRD pattern was simulated using DIFFaX program, regarding (110) twin as interstratification of two types of aragonite unit layers with mirrored relationship. The simulation suggested that the twin density can be estimated from the difference of the peak widths between 111 and 021, or between 221 and 211 reflections.

Biotic aragonite in the crossed-lamellar microstructure (three species) and nacreous microstructure (four species) of molluscan shells, fish otoliths (two species), and a coral were investigated. The XRD analyses indicated that aragonite crystals in the crossed-lamellar microstructure of the three species contain high density of the twins, which is consistent with the TEM examination. On the other hand, aragonite in the nacre of the four species showed almost no difference of the peak widths between the paired reflections, indicating low twin densities. The results for the fish otoliths were varied between the species. Such variation of the twin density in biotic aragonites may reflect different schemes of crystal growth in biomineralization.

Keywords: {110} twin, aragonite, biomineralization, DIFFaX, TEM, X-ray diffraction