Crystal organization and calcite/aragonite twin formation in biocarbonate structural materials

Erika Griesshaber[1], Jeraldine Lastam[1,2], Xiaofei Yin[1], I. Sánchez-Almazo[3], M. Heß[4], H. Gänsler[4], A. Checa[6], W. W. Schmahl[1]

[1]Department für Geo- und Umweltwissenschaften, Ludwig-Maximilians-Universität München, 80333 Munich, Germany, [2]Forschungszentrum Jülich, Institut für Energie und Klimaforschung, IEK-2, 52425, Jülich, Germany, [3]Centro de Instrumentación Científica, Universidad de Granada, 18071 Granada, Spain, [4]Biozentrum LMU München, 82152 Planegg-Martinsried, Germany, [5]Departamento de Estratigrafía y Paleontología, Universidad de Granada, Granada, Spain

Foraminifera are the most abundant organisms in marine environments and are one of the main carbon producers in the oceans[1,2]. Foraminifera are unicellular organisms that protect their soft tissue with a carbonate shell. The calcite of the shells of some benthic species shows {001} twinning[3].

We investigated the twinning characteristics of shell calcite and aragonite and patterns of biocarbonate crystal assemblies of benthic and planktonic species of rotaliid foraminifera with electron backscattered diffraction (EBSD) and sub-micrometer to nanometer scale imaging of the microstructure with FE-SEM and STEM of chemically etched and fixed shell surfaces (Fig. 1).

We describe in this contribution (i) the very extensive {001} twinning of shell calcite/aragonite, (ii) demonstrate for the twinned crystals a new biocarbonate microstructure and (iii) address twin development from crystal nucleation within an organic template to outermost shell surfaces[4]. We demonstrate that (iv) all rotaliid foraminifera specimens, investigated with EBSD so far, are twinned, however, (v) to different degrees and (vi) show that shell morphology, in particular shell/chamber sphericity, is linked to the strength of calcite twinning. Species that developed perfect/near-perfect spherical shell/chamber morphologies have their shell calcite almost fully twinned, while the calcite of shells with elongated chamber morphologies is little or even not twinned[5].

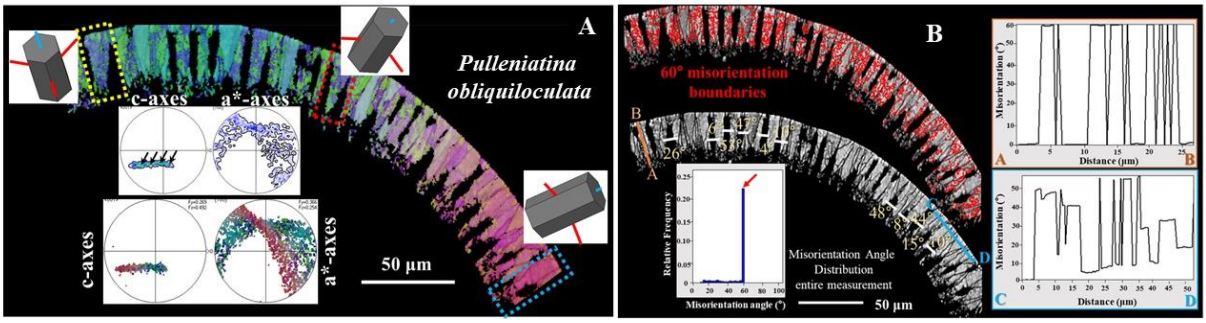

Fig. 1. Pattern of crystal orientation measured with EBSD on a cross-section through the shell of the foraminifera species *Pulleniatina obliquiloculata* (A). The strongly twinned calcite that forms the crystal units/biocrystals of the shell (B), is given with 60° misorientation grain boundaries, the misorientation-distance profile A to B and the huge peak at 60° in the misorientation angle distribution diagram. Neighboring crystal units are not connected through a twin relationship, misorientation profile C to D in (B), but are misoriented to each other by various degrees (B)[3,4].

[1] Erez J., 2003: Reviews in Mineralogy and Geochemistry 54, 115-149; **[2]** de Nooijer L. J. et al., 2014: Earth Science Reviews 135, 48-58; **[3]** Yin X. et al., 2021: Journal of Structural Biology 213, 2, 107707; **[4]** Lastam J. et al., 2021: to be submitted to Journal of Structural Biology.