[3] Mugnaioli, E., Gorelik, T. E. & Kolb, U. (2009). Ultramicroscopy 109, 758-765

[4] Palatinus, L., Petricek, V., and Correa, C.A. (2015). Acta Crystallographica Section A, 71(2), 1-10.

[5] Jacob, D., Palatinus, L., Cuvillier, P., Leroux, H., Domeneghetti, C., and Camara, F. (2013) American Mineralogist, 98(8-9), 1526-1534.

Keywords: electron crystallography, structure refinement, pyroxene, cooling history

MS14-P18 Structural distortion of biogenic aragonite in Ranella Olerea mollusc shell layers

Salim Ouhenia[1], Daniel Chateigner[2], Stéphanie Gascoin[2]

1. Equipe de cristallographie et de simulation des matériaux, Laboratoire de physique des matériaux et catalyse, Université de Bejaia, Bejaia 06000, Algérie.
2. Laboratoire CRISMAT-ENSICAEN (CNRS UMR 6508), Université de Caen Basse-Normandie, 6 bd M. Juin, 14050 Caen, France.

email: ouhenia@yahoo.fr

Mollusc shells, mainly made of calcite and aragonite crystalline polymorphs of calcium carbonate, are fascinating organic-mineral biocomposites with high mechanical performances, as they attain a fascinating increase in both strength and toughness compared to the geological mineral. The major part of organic materials is intercrystalline, and in a minor way intracrystalline (Pokroy et al., 2006).The organic represents less than 5% in volume, is a biopolymer dispersed in inorganic crystal of calcium carbonate (Barthelat and Espinosa, 2007). This organic part behaves as nanometer growth-control of the inorganic crystals and also plays an important role in stopping crack propagation in nacre (Cortie et al.,2006). This has stimulated chemists and materials scientists to design and synthesize high performance materials with a microstructure similar to that of nacre (Wang et al., 2013). In the present work we made use of Combined Analysis to determine the structure and unit-cell distortions of constituting aragonite crystallites of the shell layers (figure 1) of the gastropod Ranella olearea. This approach was chosen because it allows working on real samples, without grinding operation (Ouhenia et al., 2008). SEM analyses show the presence of three distinct layers; an inner layer composed of Radial Lamellar, an intermediate comarginal crossed lamellar layer and an outer crossed lamellar layer. The refinement of X-ray diffraction diagrams, gives quantitatively the structure of the three layers and their respective aragonite unit-cell distortions. An anisotropic unit-cell distortion is quantified for the three layers which is attributed to the combined effects of inter- and intra-crystalline macromolecules.

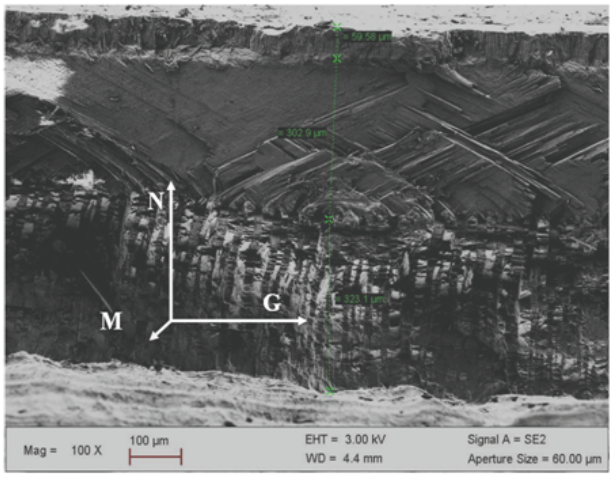

Figure 1. figure 1: Cross-section SEM image of the fractured shell at the location indicated in G, M and N indicate the Growth, Margin and Normal directions, respectively.

Keywords: Ranella Olerea , mollusc shell, combined analysis.

MS15. Structure property relationships

Chairs: Kari Rissanen, Martin Bremholm

MS15-P1 Crystal Math – When numerical algorithms meet black magic

Max Pillong[1], Ekkehard Görlach[1], Gregory A. Landrum[1], Philippe Piechon[1], Jerome G.P. Wicker[2], Richard I. Cooper[2], Trixie Wagner[1]

1. Novartis Institutes for BioMedical Research, Basel, Switzerland
2. Department of Chemistry, University of Oxford, Oxford, United Kingdom

email: max.pillong@novartis.com

Determining the three-dimensional structure of small drug-like molecules is an inevitable process in the design of novel potential drugs in both the industrial as well as the academic domain. The most commonly used method is structure determination by X-ray diffraction, which requires either crystalline powder or a tightly packed single crystal of a compound. When it comes to growing the latter, the optimal conditions differ from case to case and are usually determined by a chemist's experience combined with a practical trial-and-error approach. For our in-house structure elucidation service, we have devised a standard procedure of subsequent crystallization experiments that every compound undergoes. The results from these standardized experiments are stored in an Oracle database accessible via a graphical user interface and have been recorded for the past four years.

In order to further increase our understanding of the conditions and the process of crystallization by solvent evaporation, we conducted several statistical analyses on the abovementioned crystallization database. This includes a first assessment and substitutions of the solvents used in the standard experiments, as well as statistical correlation analysis of compound similarity, solubility and crystallinity, based on molecular fingerprints. Identified correlations in the database were then used to guide rational machine learning approaches.

Machine learning is a collective term for numerous algorithmic approaches that can be used to find regularities and correlations in multi-dimensional data, premised on mathematical models[1]. These models can subsequently be used for classification or predicting properties of previously unknown data points. Applications in pharmaceutical research divisions worldwide include the prediction of a drug's activity, side effects, metabolism and physicochemical properties such as solubility, melting points or transmembrane permeability. However, only few approaches have attempted to amalgamate machine learning techniques with predicting small molecule crystallization[2,3].