of P are invariable, the extinction-affected P_m values suffer systematic percentage errors that vary between over 6% for the highest level of interaction and less than 1% for the lowest one. The main advantage of this approach is the gain in accuracy and, hence, physical reality of the data. Another advantage is that it allows for the capability of internal experimental checks without reference to any theoretical estimates. Indeed, the degree of approximation of the $R_{i,i*}$ value to the absolute value of the $i/i*$ ratio qualifies the capability of the XRD apparatus to acquire precise and accurate data.

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Microstructural characterization of polycrystalline materials using a X-ray single-crystal diffractometer equipped with an area detector

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Two-dimensional (2D) diffraction patterns collected with an X-ray area detector (i.e., CDD, Image plate), available in modern X-ray single-crystal diffractometer (i.e., SMART APEX, Bruker, Germany), contain much more information than conventional linear scans (i.e., θ-2θ scan), collected using standard X-ray powder diffractometers equipped with a point detector [1]. For instance, depending on sample microstructural characteristics (grain size, crystallinity, preferential orientation, stress, etc.), Debye-Scherrer rings displayed in the 2D pattern might be continuous, spotty or display specific variation in the intensities along them. These features facilitate to differentiate among mineral phases that might be present in a sample and posibilite to extract useful information regarding their microstructural characteristics (grain size, preferred orientation of mineral grains). To facilitate the analysis of these patterns, we have developed a software tool (XRD2Dscan).

This software allows users to take full advantage of diffractometers equiped with an area detector but that can not readily process the information of diffraction patterns from polycrystalline materials. It has many capabilities for generating different types of scans (2Theta scan, Chi scan, d-spacing versus Chi angle, pole figures) which allows users to extract the maximum information from 2D patterns and use their single-crystal diffractometer as an advanced materials research equipment [2]. It also has a database with main crystalline phases for fast mineral identication. The benefits of using area detectors as applied to polycrystalline sample characterization will be illustrated through several examples. Specifically, we will show how crystal sizes can be calculated from the intensity profile of spotty diffraction rings produced by a polycrystalline sample (i.e., quartz, SiC and α-Al_2O_3).

This technique is complementary to X-ray line-broadening analyses (e.g. Scherrer method) and size range that can be determined is from 3 to 100 microns. On the other hand, we will show how to determine pole figures describing the 3D orientation of crystals in a textured polycrystalline material. In particular, we apply this methodology to study the crystallographic properties (epitaxy, twinning) of different biomaterials such as mollusk shells which are constituted by superimposed layers of calcium carbonate (calcite or aragonite) crystals arranged in highly organized and complex shell microstructures.

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To Deuterate or not? That is the question

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Accepted wisdom when performing diffraction experiments with neutrons is, wherever possible, to deuterate the sample as collecting data from the hydrogenous analogue is complicated by the large incoherent scattering background contribution from hydrogen. Recent work has shown that high-flux, medium-resolution continuous wavelength (CW) instruments can overcome this background problem. [1-5] Here, I present the case for not deuterating small-molecule inorganics and organics as, with proper optimisation procedures for the instrument set-up, data collection strategy and correction techniques, it is possible to investigate a wide range of systems.

Specific focus will be given to the ongoing project to re-determine σ_H incoherent as a function of incident neutron wavelength. The lack of an in-depth study to accurately quantify its variation with wavelength is surprising as it is the largest contributing factor to the absorption coefficient that is used in both single-crystal and powder neutron diffraction experiments to calculate the optimal absorption correction and sample size for hydrogen containing compounds.

The practical effect is that the attenuation of the neutron beam (both incident and scattered) by the sample changes as a function of neutron wavelength and path length through the sample, with striking implications for quantitative analysis of time-of-flight (t-o-f) neutron data. The aim is to collect the necessary information to implement an empirical correction routine for CW and t-o-f data as a function of wavelength in the thermal neutron range. This correction would allow a significant number of users to perform routine data collections on hydrogenous materials without the need for deuteration (and the often observed changes in properties upon deuteration) impacting directly research in technologically important fields such as proton conductors, fuel cells and pharmaceuticals.

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Determining single-crystal elastic constants from neutron powder diffraction

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