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Dynamic method for measurement of piezoelectric coefficients

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The determination of piezoelectric constants d_{ijk} is classically done by measurement of the electric charge generated by application of static or dynamic mechanical stress on differently oriented samples of a piezoelectric crystal [1] - a method that frequently suffered from inhomogeneity all over the crystal of the applied stress - or, alternatively, by interferometric or capacitive measurement of strain of the crystal induced by applied voltage, using the converse piezoelectric effect ("linear electrostriction", e.g.[2]); this latter method, however, requires high effort of suitable sample preparation. In this contribution we present a device for measurement of piezoelectric constants using the direct piezoelectric effect, that allows to overcome the above mentioned difficulties and inconvenience. The crystal sample (a slab for longitudinal, a parallel-epipedon for transverse measurements) with parallelity of faces of $\pm 1 \mu\text{m}$ is arranged in a sandwich-like stacking between two auxiliary quartz crystal slabs. A dynamic, low-frequency (0.1 - 10 Hz) uniaxial stress, the homogeneity and magnitude of which is controlled and measured by the quartz crystals, is applied by a ceramic piezo actuator. Lock-In technique aids the detection of the periodically generated charges. The homogeneity of applied stress has as well been examined by laterally resolved measurement of piezooptic constants [3]. The achieved accuracy of determination of all independent coefficients of the piezoelectric tensors [d_{ijk}] of $\text{Li}_2\text{SO}_4(\text{H}_2\text{O})$ (point group 2) and of $\text{Na}_3\text{Li}(\text{MoO}_4)_2(6\text{H}_2\text{O})$ (point group 3m) proves the suitability and efficiency of the set-up for routine investigations of piezoelectric constants.

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Polarized Resonant Scattering in Macromolecular Crystallography

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Methods that are based on the resonant scattering properties of selected atomic species have been used successfully for phase determination in both, small-molecule and macromolecular X-ray crystallography [1]. The anisotropy of resonant (anomalous) scattering (AAS) is sufficient to cause substantial changes in diffraction intensity with polarisation direction [2]. In macromolecular samples, the variation of anomalous scattering factors with orientation can be very substantial [3], similar in magnitude to those obtained in a Multiple-wavelength Anomalous Diffraction (MAD) experiment by changing the wavelength of the incident radiation. Treating the anomalous scattering factors as scalars (isotropic scattering) therefore gives rise to systematic errors in MAD phase estimates.

On the other hand, we can consider AAS as an effect that can give rise to supplementary phase information, rather than considering it merely as an additional complication: phase information can be extracted by considering the symmetry-breaking effects of polarized resonant scattering. While these effects have been extensively studied in the context of forbidden reflections [4,5], the non-equivalence of symmetry-related non-forbidden reflections is particularly important for applications in macromolecular crystallography.

In this communication, we will review the various effects of AAS and their incidence in macromolecular crystallography. Further, we will discuss the possible experimental strategies for exploiting these effects for phase determination.

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