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Modulation Excitation Spectroscopy applied to Crystallography

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This presentation will focus on our recent methodological developments. Periodic external stimulations such as concentration light flux, pressure and temperature were introduced. Periodic perturbations are already used frequently in spectroscopic investigations because they enhance the sensitivity and introduce selectivity into experiments. This technique has been called Modulation Excitation Spectroscopy (MES). We transferred this methodology to diffraction and named it Modulation-Enhanced Diffraction (MED). First we present the theory that is developed to explain the kinematic diffraction response of a crystal when it is subjected to a periodically varying external perturbation. We show that if a part the local electron density varies linearly with an external stimulus, the diffracted signal is not only a function of the stimulation frequency Ω, but also of its double 2Ω. These frequency components can provide selective access to partial diffraction contributions that are normally summed up in the interference pattern. MED simulations and experiments will be presented where a phasing process applied to partial diffraction terms allow to recover directly the substructure actively responding to the stimulus. MED can be applied when crystals are changing physically (i.e. electron density/site occupies) but also when varying the x-ray energy and thus the resonant contributions. When comparing MED with existing phasing tools it indicates that there is future potential.

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