

determination, photochemistry coordination compounds

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Picosecond crystallography of homogeneous [2+2] photodimerisation reactions

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In the following we will present ultrafast crystallographic studies on the photo-induced single-crystal-to-single-crystal dimerisation of α -styrylpyrylium(TFMS) ($C_{23}H_{29}O_3F_3S$). α -styrylpyrylium(TFMS) is well known as an optical switcher with the ability to be used as a storage device. The mechanism underlying the storage process is a ultrafast [2+2] photodimerisation reaction, which is reversible (higher temperature) or irreversible (lower temperature) implying temporal stability. In this contribution we show the possibility to switch the material between the ground state (monomer phase) and the photoactivated state (dimer phase) in an ultrafast manner with time-scales below 50 ps. The static x-ray diffraction studies have been performed down to electron density resolutions. For the time-resolved studies of the structural dynamics in the solid, picosecond time-resolved crystallography has been employed. Additionally, we discuss the influence of the exciting photon energy on the structural photoswitching of α -styrylpyrylium(TFMS) and its influence on the dimerisation mechanism.

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Modeling of single molecule imaging by X-ray free electron laser

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We study the possibility of imaging a small cluster of atoms by short x-ray free electron laser pulses. Since this type of sources are under construction no experimental data is available, which could reliably tell the conditions of successful imaging. Therefore modeling of the experiment and evaluation process is crucial. On the experimental part one of the most important questions is how fast the sample deteriorates in the beam. We have developed a special molecular dynamics model for the description of the Coulomb explosion of the clusters. Using this model we can follow the time evolution of all particles (including atoms, ions, electrons) of the sample. Beside the modeling of samples with different compositions, we also studied the effect of a thin sacrificial temper layer about the sample. We found that with a proper choice of the temper layer the deterioration of the sample can be significantly slowed down. This may help

the realization of the planned experiment. Based on the results of molecular dynamics modeling we can calculate the 2D continuous elastic scattering pattern of the sample for a given shot. However, the most often used density modification type algorithms needs 3D data in the reciprocal space. Therefore the full dataset have to be built from scattering patterns of several independent exploding clusters taken at various unknown sample orientations. The first and most critical step in the evaluation process is the classification of the many million 2D patterns into a few thousands of bins. In every bin the sample orientation is the same, so that one can add the intensities of these patterns to improve the statistics to a level where reconstruction is possible. We show the results of our numerical study of the classification process.

Keywords: free electron laser, single molecule imaging, X-ray diffraction

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Geometry and resolution of area detectors for X-ray powder diffraction

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Application of area detectors for powder x-ray diffraction has dramatically increased in recent years due to many advantages, including high speed and better sampling statistics with small samples or textured samples. In high-throughput x-ray diffraction screening, such as pharmaceutical research and discovery, two-dimensional x-ray diffraction is the preferred choice for many users. The Bragg-Brentano (BB) geometry has long been the classic configuration for collecting phase identification data from bulk powder or polycrystalline samples. With the increased usage of area detector, many users have noticed some discrepancies between the diffraction patterns collected with a BB system and an area detector system. In the BB geometry, the 2θ resolution is controlled by the divergence slit, receiving slit and scanning steps of the point detector. With an area detector, the 2θ resolution is mainly determined by the spatial resolution of the detector and the sample-to-detector distance. In order to have the optimum combination of 2θ range and resolution with an area detector, several frames covering different 2θ ranges may have to be collected and merged. The 2θ resolution may vary with 2θ range, sample shape and detector geometry. The relative peak intensity from a textured sample may be different from the results measured with BB geometry. It is imperative to study the nature of these discrepancies so that the diffraction patterns collected with area detectors can be used for phase ID with proper understanding and correction. This presentation compares the conventional Bragg-Brentano diffractometer with diffractometers using area detectors in terms of geometry convention, detector resolution, data collection and processing strategies.

Keywords: area detectors, X-ray powder diffraction, instrumentation

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Effect of pressure and temperature on the crystallization behavior of As Te glasses with selenium

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