

Time-resolved X-ray diffraction experiments including those performed at XFEL sources require modification of data analysis procedures as sample destruction in the X-ray and/or laser beam typically requires multi-crystal data collection. Modifications introduced include a scaling technique for relative scaling within multi-crystal data sets, use of the RATIO technique in which measured I_{ON}/I_{OFF} ratios are used in combination with conventional data [1], and the use of refinement methods [2] and R-factors [3] specific for dynamic-structure crystallography. The procedures have been applied to several sets of Laue data collected at beamline 14-ID at the Advanced Photon Source [4]. The extended bandwidth of the pink Laue technique allows use of one or a few X-ray pulses per data frame, thus minimizing crystal damage by laser exposure and optimizing the attainable time-resolution.

Results for the α -modification of $Rh_2(\mu\text{-PNP})_2(\text{PNP})_2(\text{BPh}_4)_2$ (PNP = $\text{CH}_3\text{N}(\text{P}(\text{OCH}_3)_2)_2$, Ph = phenyl) (**1**) show a shortening of the Rh-Rh distance of 0.136(8) Å and significant displacements of the ligands on excitation. This may be compared with those on an earlier monochromatic study of the $[\text{Rh}_2(1,8\text{-diisocyno-p-menthane})_4]^{2+}$ ion in which a Rh-Rh shortening of 0.85(5) Å was observed [5]. The polychromatic results on (**1**) are clearly the more accurate ones. They are not well reproduced by isolated molecule calculations, but can be accounted for quantitatively by taking into account the confining effect of the crystal environment with the QM/MM (Quantum Mechanics/Molecular Mechanics) method [6], thus underlining the differences between isolated molecules and molecules in crystals. Additional data have been collected on a number of phosphorescent Cu(I)-phenanthroline chromophores which are candidates for use in photovoltaic cells.

The modified Laue method is capable of producing excited state structures at atomic resolution of a quality compatible with or better than those of monochromatic synchrotron experiments. The modifications described are relevant for monochromatic data sets collected at X-ray Free Electron Laser sources.

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Dynamic Investigation of photoinduced phase transition in prussian blue analogs by picosecond time-resolved XAFS

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Prussian blue analogs have recently attracted great interest due to their various characteristics in the photoinduced phase transition (PIPT) as a photo-induced magnetization as well as photo-induced structural change.[1], [2] The investigation of the dynamics of PIPT allows us to obtain information how the photo-excitation in the single site expands into a macroscopic phase transition. Picosecond time-resolved XAFS experiments were performed on the NW14A at the Photon Factory Advanced Ring (PF-AR).[3], [4] The time-resolved XAFS spectra were collected by the pump-probe technique with a femtosecond laser system. In EXAFS and XANES regions, transient features attributed to the PIPT were obtained at 100 ps resolution. The detailed results will be presented.

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X-ray diffraction methods as a complementary tool for analyses of historical objects

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This presentation summarizes the research done by our team using different X-ray diffraction (XRD) methods to characterize historical objects such as paintings, ceramics, metals and stones. Also pigments and salts are typified since XRD is essential for analyzing materials with similar elemental composition but differing mineralogy. Our goals are to apply XRD methods as non-destructive, routine laboratory analyses combined with complementary techniques to fully characterize historical items, and thus, to draw artistic/archaeological conclusions and supply information to enable conservation/restoration interventions.

X-ray thermodiffraction (XRTD) is a powerful tool to track time-resolved, *in situ* mineralogical and phase transitions of varied materials such as pigments and hydrated salts. Using XRTD we studied the azurite decarbonation process [1] and sulfate-rich salt dehydration. New routines for 2D mapping allow us to better interpret reaction trends and kinetic rates [2].

Micro-XRD is a non-destructive technique that enables direct analysis of small (<1mm) artwork samples. Via micro-XRD we characterized pigments used in Islamic palaces from Granada (e.g. the Alhambra), bricks, potteries, enamels, bronze artifacts, patinas and stones, as well as newly formed minerals (salts and high T silicates) [3]. We used a single-crystal diffractometer and the software XRD2Dscan [4] to transform Debye-Scherrer rings into conventional powder diffractograms. The microtextural data of crystalline phases obtained from the Debye-Scherrer rings were used to determine crystal sizes of mineral grains and quantify grain sizes of phases present in the same layer. This novel micro-XRD application used on painting samples sheds light on the nature, manufacture and weathering of pigments [5].

Grazing incidence XRD (GIXRD) is a potent method for surface characterization of thin films and monolayers such as metal and alloys, providing information on corrosion processes. Few papers are published on the application of GIXRD to artworks, and most focus