Understanding and Interpreting X-ray Emission Data from Ultrashort Pulses

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With the development of X-ray free electron laser (X-FEL) sources there has been a paradigm shift in the way many systems are being studied. From fast fundamental transitions, such as bond formation, to creating completely ionized atoms, the ultrashort (<100fs) intense pulses allow for new electronic states and processes to be studied. In this work we focus on the X-ray emission dependence on pulse intensity, pulse duration and photon energy to understand the fundamental processes that will govern shifts in these spectroscopic data. Here we studied $MnCl_2$ in solution and find the magnitude of the spectral shifts and find the parameter space where relatively "damage free" spectra can be obtained.

Using a liquid jet, $MnCl_2$ in solution was ejected into the vacuum chamber into the interaction region of the X-ray beam. The X-ray spot size used the Coherent X-ray Imaging instrument (CXI) at the Linac Coherent Light Source (LCLS) was ~1-2μm^2. Pulse durations were chosen to be ~20fs and 40fs for these studies. The incident photon energy used to probe the sample was 6.9keV and 8.7keV and a range of pulse intensities were also used. An upstream gas monitor measured the pulse energy and was read out each shot. The number of photons was estimated from the pulse energy and assuming an estimated 60% X-ray transmission efficiency through the X-ray optics to the downstream interaction point.

During two separate beamtimes at LCLS a series of data were collected under various parameters. The data are represented below showing the trends for spectroscopic changes which are quantified by shifts in the first moment of the $Kb_{1,3}$ peak. These shifts are compared given the pulse parameters.

We show the dependence of first moment shifts given the various pulse conditions to support our argument for the dominate effect for these shifts. Additionally we identify other contributors as part of process that causes shifts in these spectra. These results are also given in context to suggested parameters for XES measurements at XFEL sources.

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