X-Ray Scattering Analysis

SLAC NATIONAL ACCELERATOR LABORATORY

Grace Owolabi, Adi Natan[2+]

[1]Department of Electrical Engineering and Computer Engineering, Howard University, Washington, DC 20059,USA.

[2]Linac Coherent Light Source, SLAC National Accelerator Laboratory, 2575 Sand Hill Road, Menlo Park, CA 94025, USA.

[+]Contact: natan@slac.stanford.edu

Introduction

In the study of the structure of matter at LCLS, X-rays have been very useful in revealing the structure of a wide range of materials. An X-ray interacts with an atom either by being scattered or being absorbed. In analyzing the scatter data from an ultra-fast X-ray interaction with diatomic molecules, we can read information that can hep us determine the structure. Using Legendre decomposition, we broke the data down to the isotropic and anisotropic diffraction patterns and densities.

The goal of the project is to analyze higher order anisotropic patterns/densities and analyze the molecular rotation information .
The Keywords: X-ray Scattering, X-ray isotropic diffraction, X-ray anisotropic diffraction

Model of X-ray Scattering

Modeling the X-ray scattering of a diatomic Molecule i.e. Oxygen.

X-rays are scattered by electrons of atoms. As the wavelength of the X-rays of the order of the atom diameter, most of the scattering is in the forward direction.
The X-ray scattering power will depend on the number of electrons in an atom (the heavier the atom, the more it will scatter) and will decrease with increasing scattering angle.

Assuming only elastic scattering: $|k1| = |k2|$
The scattering vector $\vec{q} = \vec{k_1} - \vec{k_2}$
$|q| = 2|k|\sin(\theta)$ (units: 1/Angstrom) (Reference: Fig 1)
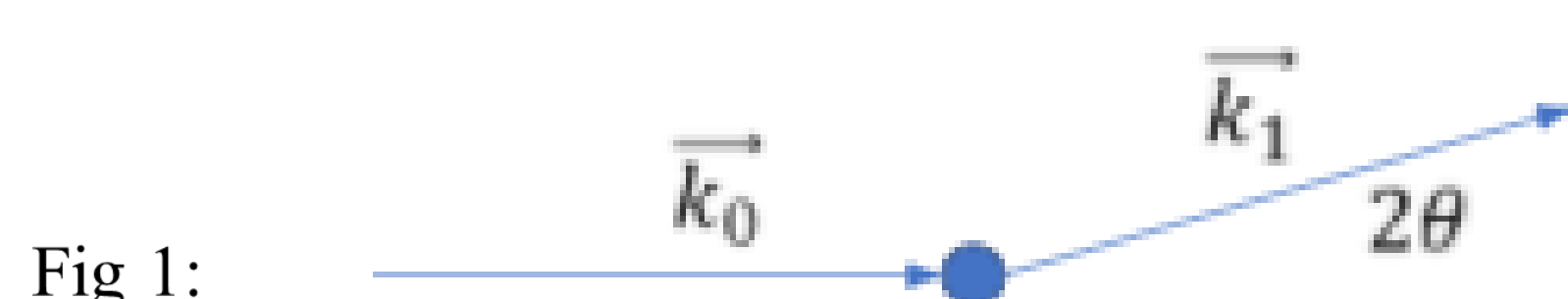
Fig 1:

The atomic form factor (total scattering of an atom) =
$F(\vec{q}) = \int \rho(\vec{r})e^{i\vec{q}\cdot\vec{r}}d\vec{r}$

Calculating atomic form factor using Cromann's 9 coefficients:
$f(\vec{q}) = \sum_{i=1}^{4} a_i\exp(-b_i (^q/_{4\pi})^2) + c$

Calculating Form factor for a molecule(2 or more atoms):
$F_{mol}(\vec{q}) = \sum_j f_j(\vec{q})e^{i\vec{q}\cdot\vec{r_j}}$
We cannot measure F_{mol} so we measure Intensity = $|F_{mol}|^2$

The Figures below (fig 2 and fig 3) show the plot of the modeled form factor of an oxygen atom and intensity of an oxygen molecule.
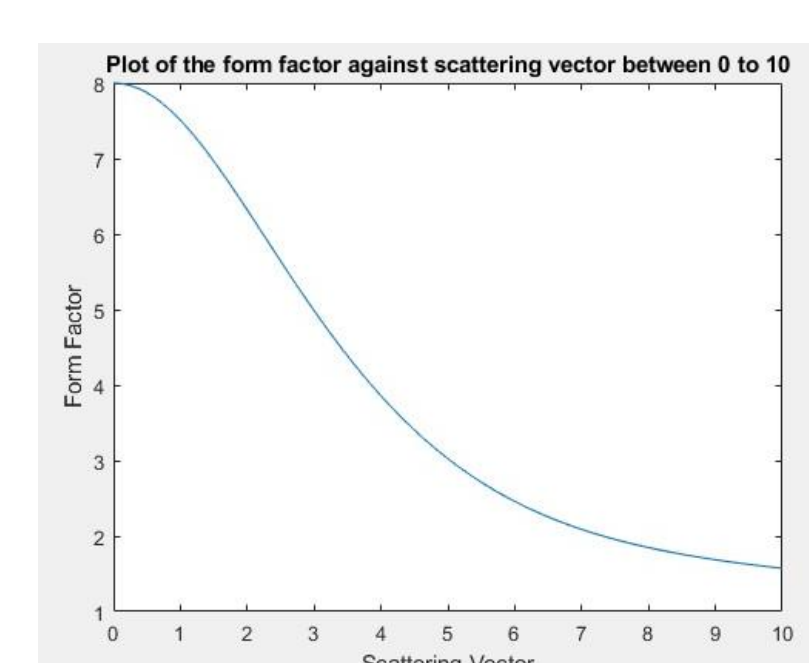

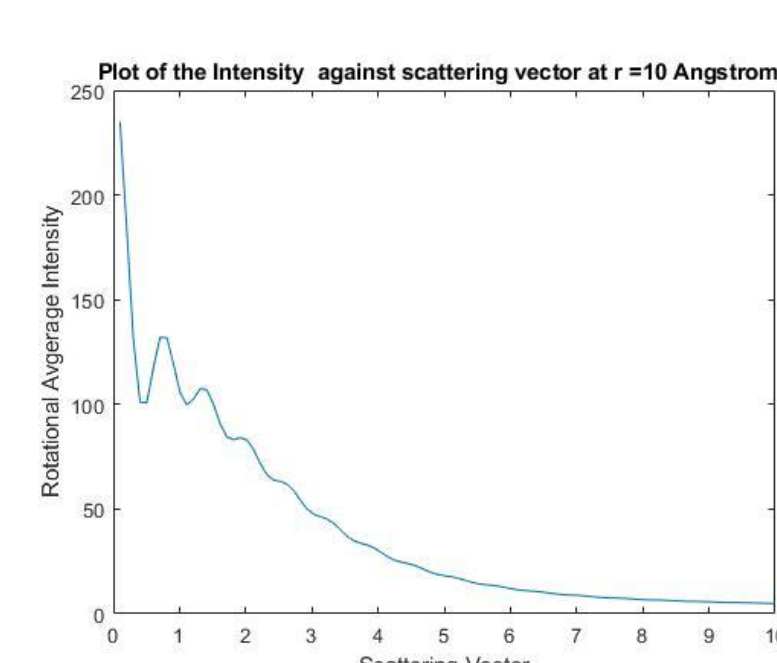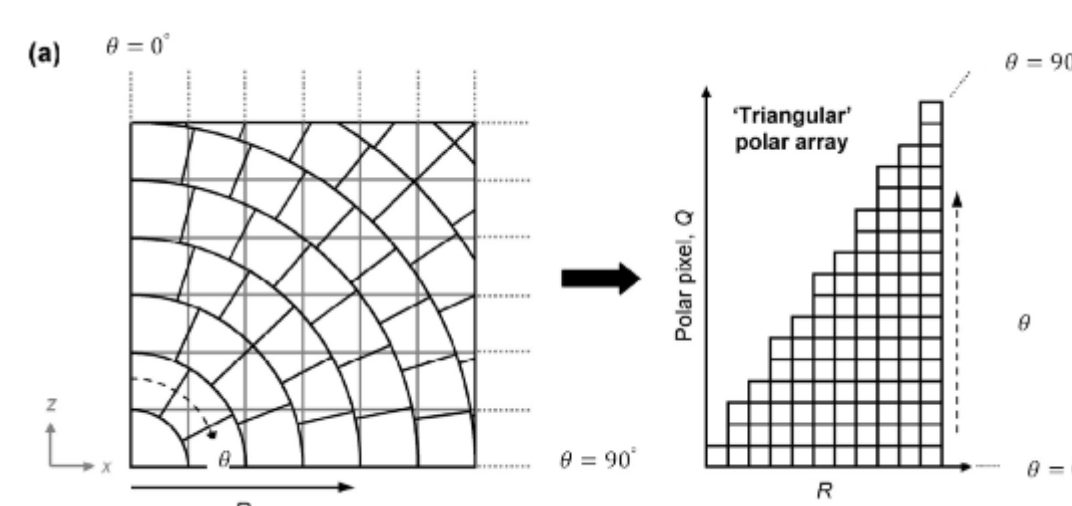Fig 2: Form Factor vs Scattering Vector for oxygen atom

Fig 3: Intensity vs Scattering Vector for Oxygen molecule

Data Analysis

Analysis of data from an actual x-ray scattering experiment

Coordinates Conversion

The first step of the analyzing the data is to convert the cartesian image of the data to a triangular polar image. The Cartesian image is centered then partitioned into 4 and each quadrant is converted to a triangular array of the polar form. The four quadrants are then folded resulting in an images which is a quarter of the initial size and still contains all relevant information. This method greatly reduces computation time for the next step, which is the Legendre Decomposition.
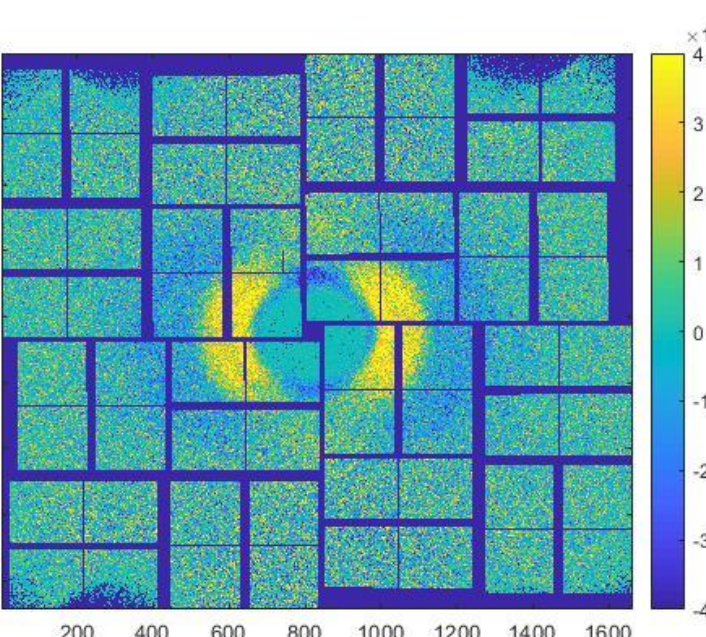

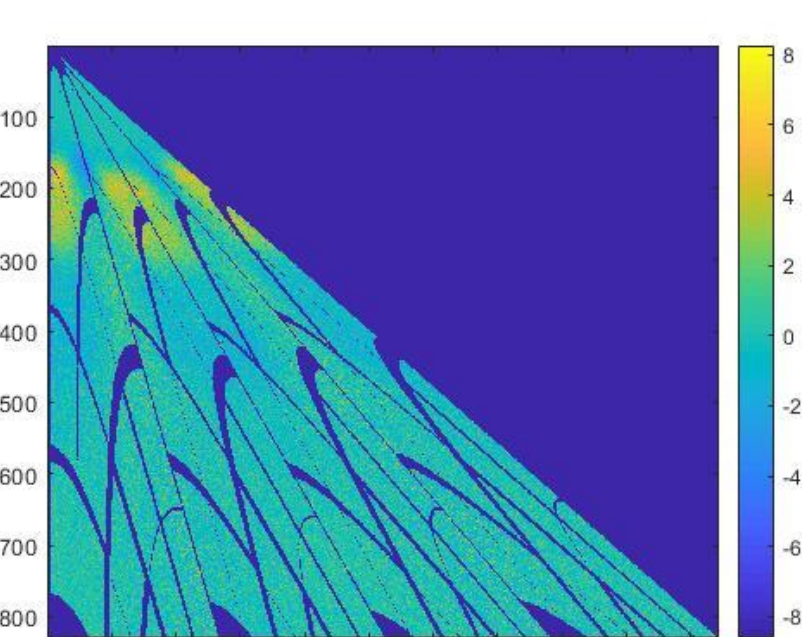Fig 4: Image representation of the data at t = 30fs

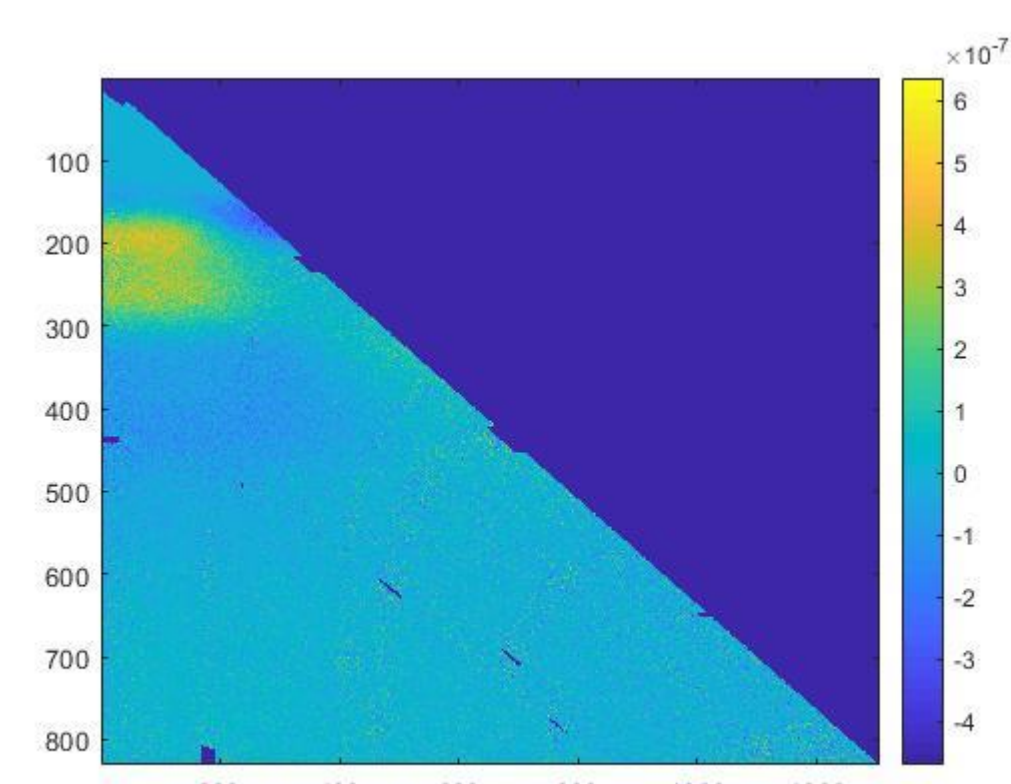Fig 5: Tripolar representation of the 4 quadrants of the image

Fig 6: Mean of the four quadrants: reducing the size of the original data to a quarter of it.
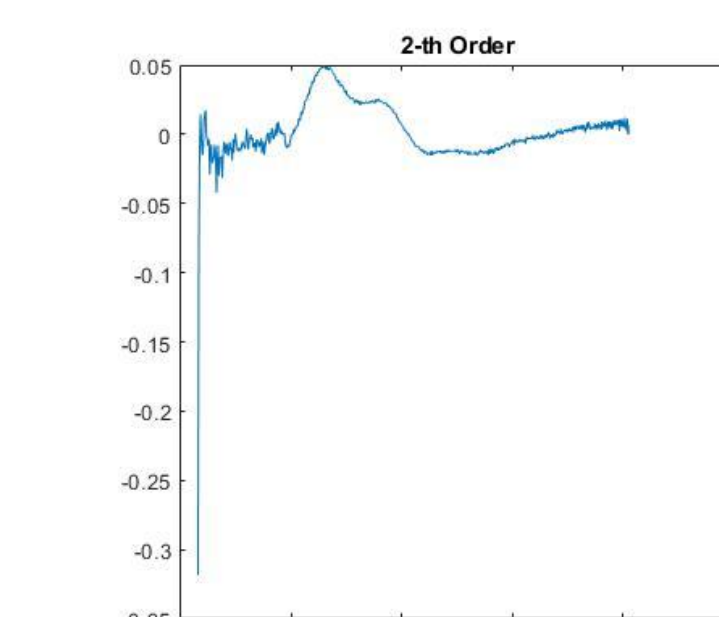
Legendre Decomposition

The folded image was filtered by Legendre decomposition procedure to produces anisotropy plots that can give more details on the result of the experiment.
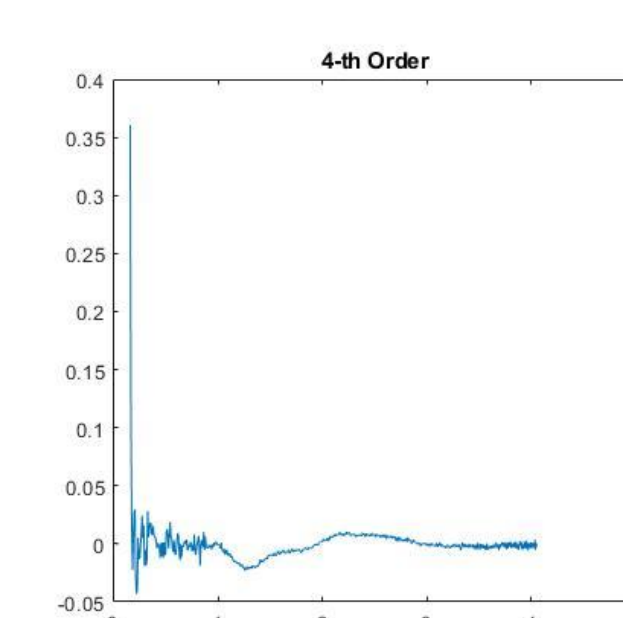
From the figures below we can see that the readings really take place between 1 A^{-1} to 4 A^{-1}
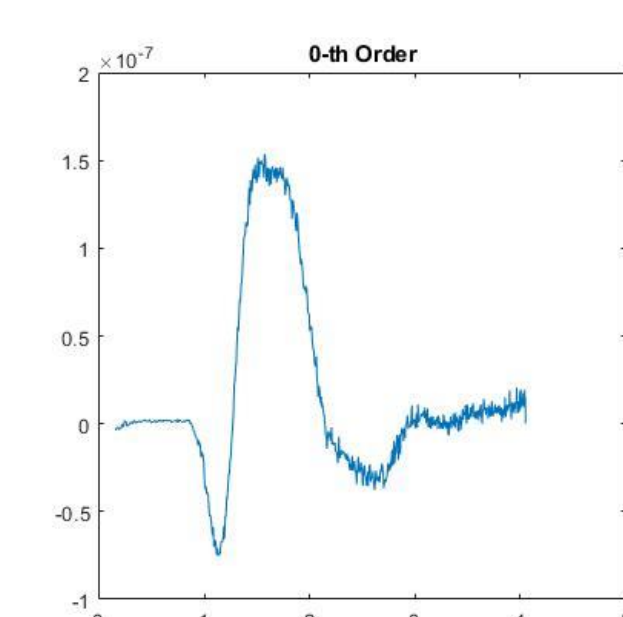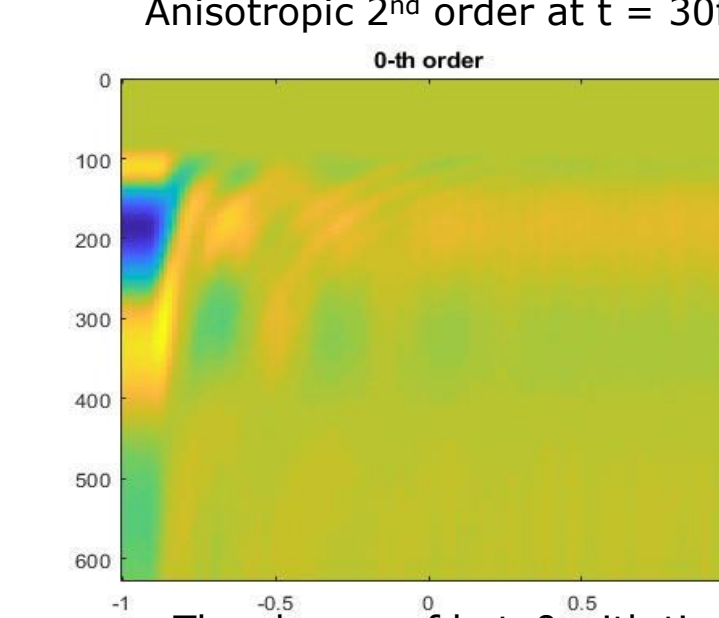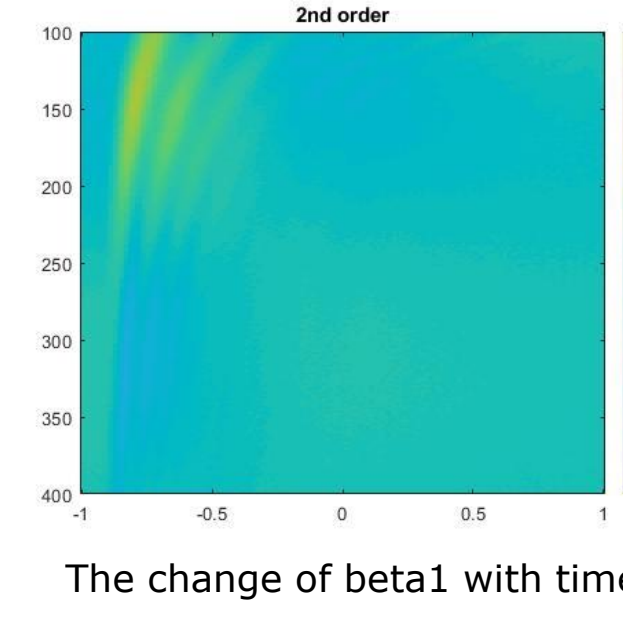

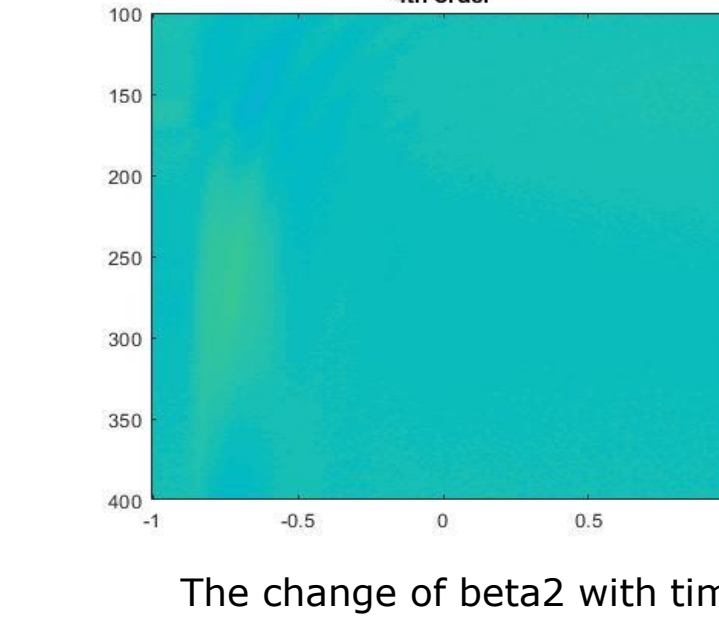Isotropic 0-th order at t = 30fs

Anisotropic 2nd order at t = 30fs

Anisotropic 4th order at t= 30fs
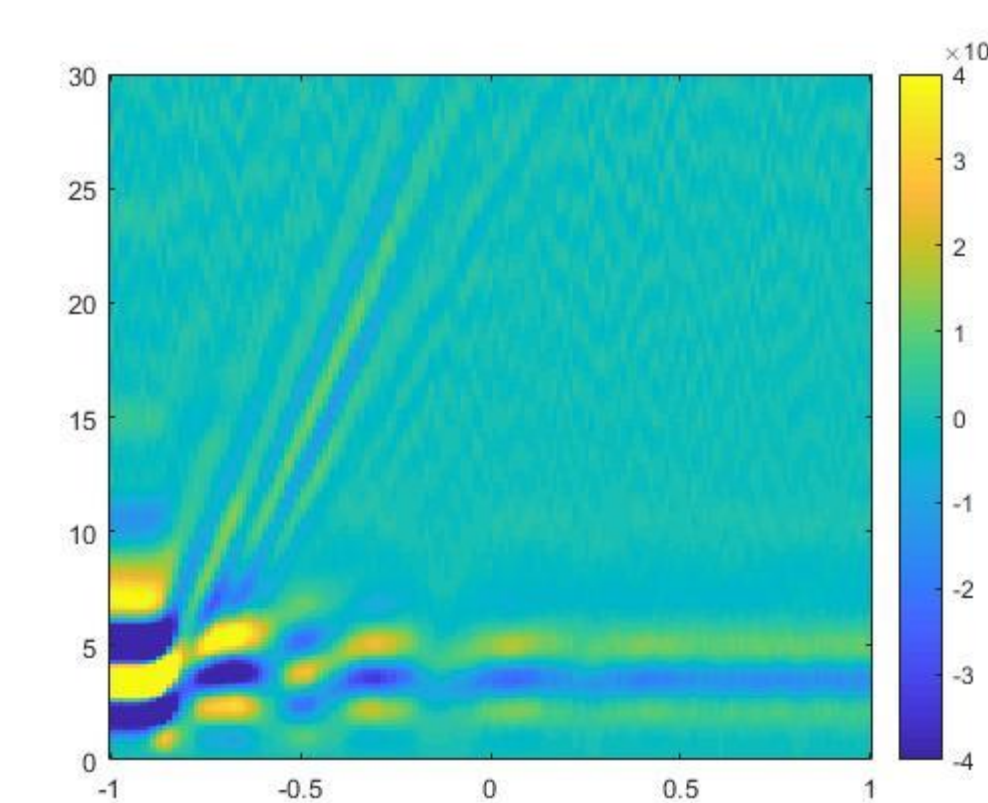
The change of beta0 with time.

The change of beta1 with time.

The change of beta2 with time.

Fourier Analysis

We sine-transformed the isotropic part of the Legendre decomposition(β0) to arrive at the convert the data from scattering vector space(q-space) to real space (the position space).
The sine transform of β0(q,t) results to a pair correction function PC(r,t)

The figure above shows some vibrations and some elements of the dictionary that we can use to map to the distances.

Deconvolution

The Deconvolution of the result is necessary because of the interference from the window function applied to the data during the sine transform. Applying deconvolution will make the dictionary sharper and will remove the vibrations and interferences that are currently present.

Conclusions

This poster showcases the analysis of data measured from an ultra-fast x-ray scattering experiment using cartesian to tripolar co-ordinates conversion, Legendre Decomposition, Fourier sine transform.
This process resulted in the position space equivalent of the scattering vector space data that was initially measured.
The best next step to take is to perform the deconvolution of the sine transform to get a sharper image with little or no interferences.
The next plan is to analyze the higher order anisotropies that contain more information on molecular motion using the spherical Bessel function.

Acknowledgments

Date: 09/10/2020