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Resonant X-ray Ptychographic Tomography of P3HS Solar Cells

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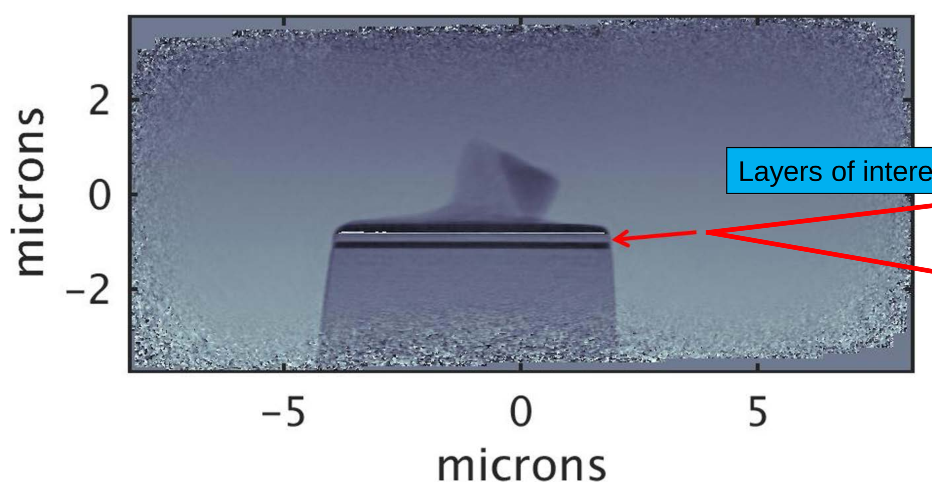
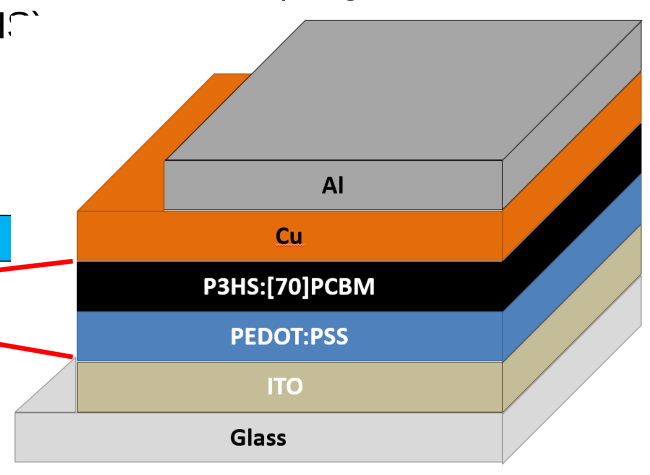
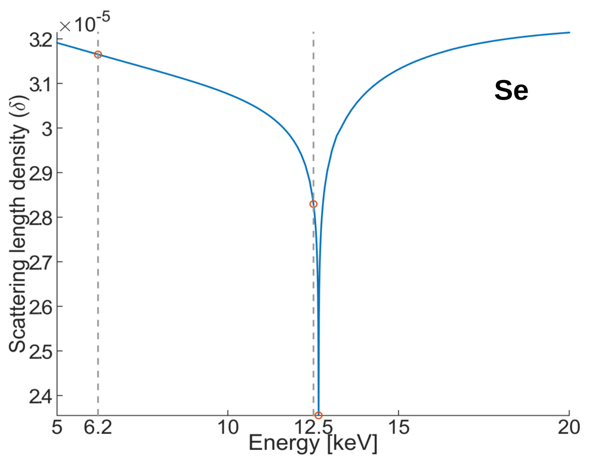
Overview and motivation

Organic solar cells are a promising technology as a cost efficient alternative to silicon solar cells. Imaging of the internal structure is crucial for fundamental understanding of the internal processes and future developments. Of particular interest is the P3HT:PCBM layer which has proven challenging to image due to small differences in the refractive index of the two constituent materials. In this work we present preliminary results on attempting to increase the contrast in the layer by replacing S in P3HT with Se (P3H…

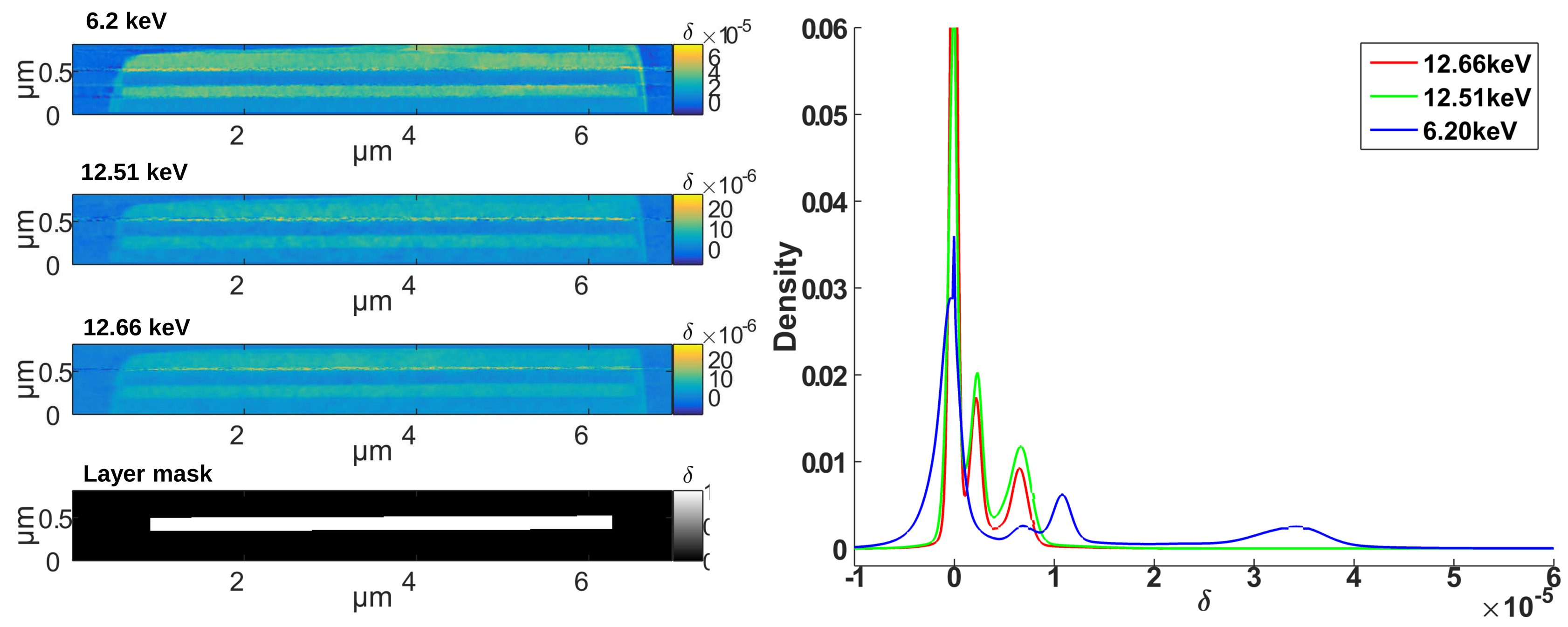




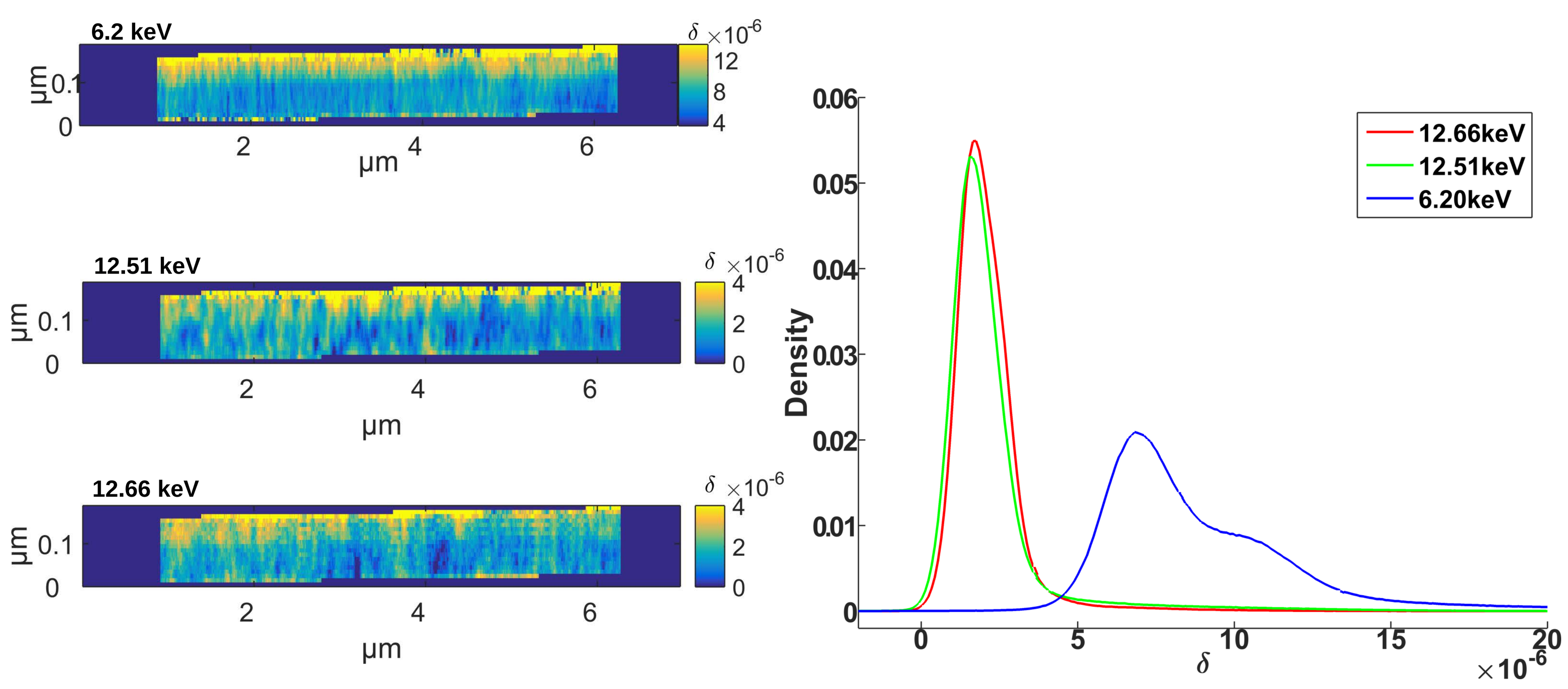
The same sample was imaged at three energies by ptychographic X-ray computed tomography. The energies were chosen as: the optimal energy for the beamline (6.2 keV), just below the Se K edge (12.51 keV) and at the Se K edge (12.66 keV) respectively. All the data was acquired at the cSAXS beamline at the Paul Scherrer Institute, Switzerland.



The layer of interest and its neighboring layers



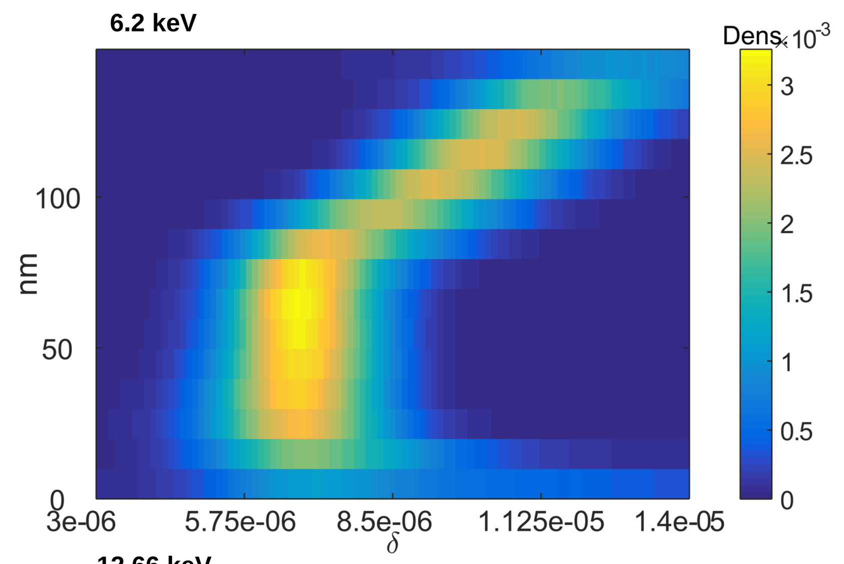
The layer of interest

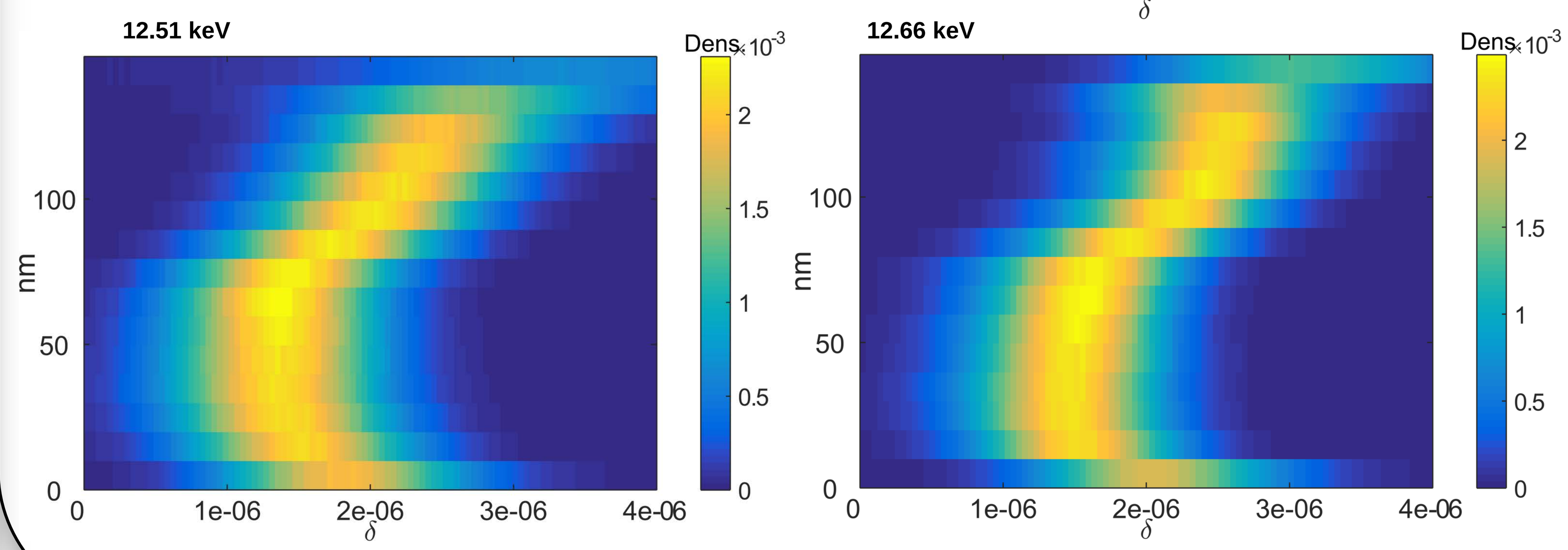


Individual voxel layers in the layer of interest

In the layer of interest a histogram was constructed for each layer of voxels. The images show the probability density of each histogram as a function of δ and the layer location (relative to the bottom of the layer of interest)

Layers were sampled parallel to the bottom layer transition to correct for the minor tilt of the sample relative to the voxel grid.

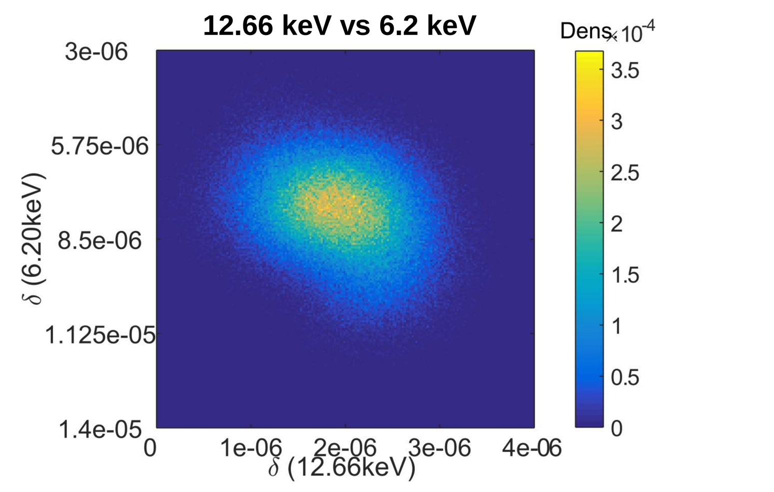


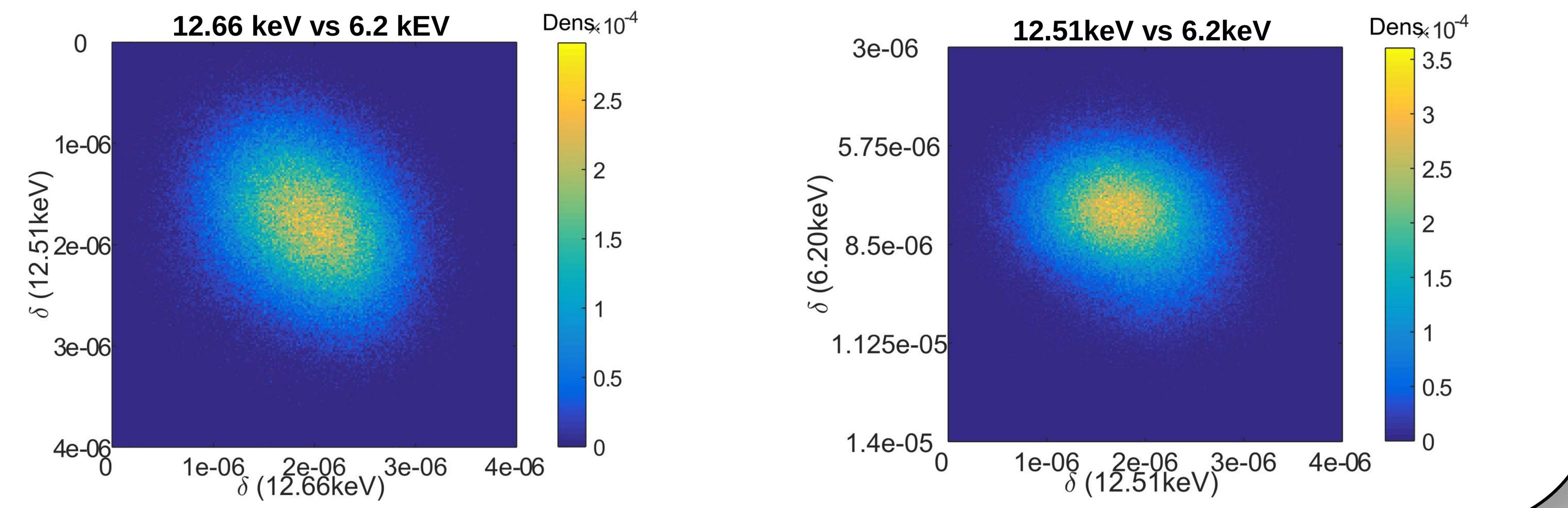


Correlation between tomograms at different energies within a voxel layer in the region of interest

For the voxel layer corresponding to 120 nm above the lower layer transition, correlation between the delta values in each pair of tomograms was tested.

The figures show the probability density of the voxel delta values for pairs of tomograms along with the corresponding correlation factors.





Conclusion

The analysis of the effect of imaging near the Se absorption edge is complicated by two issues: 1) The replacement of S with Se in the P3HT molecule only contributes a small amount to the overall scattering properties of the material. 2) The data shows issues of >2π phase shifts at layer interfaces parallel to the beam resulting in artefacts and increased noise levels near the layers of interest. Combined, these two effects make the Se absoprtion edge challenging to utilize for resolving the internal structure of the P3HS layer for the present data.

These preliminary results are a step towards the overall goal of resolving and studying the internal structure of the absorber layer in polymer solar cells. Future work will revisit the data using new alignment and reconstruction procedures and will also incorporate the absorption in the analysis. Future tomograms will be sought acquired at an orientation where the layers are not parallel to the beam.

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