Scanning X-ray Imaging Techniques for Characterization of Energy Materials

The large and ever-growing energy needs call for an urgent shift for sustainable energy sources. Associated to the current production of energy is the emission of noxious gases that among other undesirable effects contribute for an increase of the greenhouse effect and consequently to global warming. From the currently available energy sources, solar energy is the one with the biggest potential to fulfil our current and future energetic needs. To date, the main factors impeding upscaling and mass production of solar cell devices are associated to their high production costs or low efficiencies, for which fossil fuels are still economically competitive.

The performance of solar cells, especially those from second- and third-generation, is largely determined by their micro- and nano-scale. To improve their conversion efficiency, scientists must first be able to measure and characterize the nanostructure of the devices produced by current synthesis methods, so that these may be improved or tuned to fulfil a specific need. Emerging X-ray imaging techniques, such as coherent diffractive imaging methods, have the potential to reach extremely high resolutions and are well suited for this task. Currently the available spatial resolution delivered by such methods is limited by the X-ray beam properties and by the performance of the numerical algorithms used for image reconstruction. Furthermore, the combination of different X-ray imaging methods allows for complementary information about the sample from which the local electronic and chemical compositions can be derived.

This thesis is devoted to the improvement of current X-ray scanning imaging methods. Our main contributions lie in the development of numerical algorithms for image data analysis of X-ray fluorescence and X-ray ptychography. More specifically the thesis includes the theoretical background of the main types of X-ray-matter interaction, a brief description of some X-ray scanning imaging techniques, the description of the developed algorithms and the report of recent experimental measurements for the characterization of third-generation kesterite solar cells.
Automated angular and translational tomographic alignment and application to phase-contrast imaging

X-ray computerized tomography (CT) is a 3D imaging technique that makes use of x-ray illumination and image reconstruction techniques to reproduce the internal cross-sections of a sample. Tomographic projection data usually require an initial relative alignment or knowledge of the exact object position and orientation with respect to the detector. As tomographic imaging reaches increasingly better resolution, thermal drifts, mechanical instabilities, and equipment limitations are becoming the main dominant factors contributing to sample positioning uncertainties that will further introduce reconstruction artifacts and limit the attained resolution in the final tomographic reconstruction. Alignment algorithms that require manual interaction impede data analysis with ever-increasing data acquisition rates, supplied by more brilliant sources. We present in this paper an iterative reconstruction algorithm for wrapped phase projection data and an alignment algorithm that automatically takes 5 degrees of freedom, including the possible linear and angular motion errors, into consideration. The presented concepts are applied to simulated and real measured phase-contrast data, exhibiting a possible improvement in the reconstruction resolution. A MATLAB implementation is made publicly available and will allow robust analysis of large volumes of phase-contrast tomography data.
Resonant X-ray Ptychographic Tomography of P3HS Solar Cells

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