Coherent Scattering Experiments: Simulation and Measurement

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Exploiting the coherence properties in the hard X-ray regime is an important topic for the emerging ultra-low-emittance synchrotron storage rings. The Coherent Hard X-ray (CHX) beamline [1] at the National Synchrotron Light Source II (NSLS-II) is exploiting the coherent flux to enable best-in-class time-resolved coherent scattering techniques such as X-ray Photon Correlation Spectroscopy (XPCS) or X-ray Speckle Visibility Spectroscopy (XSVS). Since the start of commissioning in 2014, the critical performance parameters for this beamline have been thoroughly characterized and benchmarked against partially-coherent undulator emission and wavefront propagation simulations with the Synchrotron Radiation Workshop (SRW) code [2]. These parameters include the undulator radiation flux, degree of transverse coherence, and focal spot size, as well as the quality of the transported wave front.

After careful optimization of the beamline performance, e.g. by spectral alignment of the undulator source, and taking known imperfections of optical elements like mirror surface and monochromator crystal quality into account [3], wavefront propagation simulations and experimental data show excellent agreement [4].

Based on the commissioning results, a realistic simulation of the whole beamline, including source and optics, has been implemented in the "virtual beamline" module of SRW and in the web browser based interface of the code named Sirepo [5]. This virtual beamline capability is now used to simulate partially coherent small angle scattering patterns of samples relevant to the CHX science case, mimicking 'detector images' of real experiments. The samples are represented by electron density maps, which can be generated from electron microscope images or other methods. A quantitative comparison of simulated and measured datasets, based on standard analysis algorithms for XSVS, will be presented. Simulations and measurements cover the range of photon flux and degree of transverse X-ray beam coherence, which are used for XPCS and XSVS measurements at the CHX beamline. Such source-to-detector simulations of experiments allow for an accurate estimation of feasibility of a given experiment, for an optimization of the beamline setup (e.g. trading photon flux for higher degree of transverse coherence) or estimating impacts of beam instabilities or optical imperfections on experimental data. They can also help to interpret the obtained experimental results by forward simulations of mesoscale models, e.g. simulating the impact of external strain on the nanostructure of a material and using the corresponding mesoscale models as 'samples' to generate scattering pattern via SRW simulations.

References

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