START-TO-END SIMULATIONS FOR MODERN LIGHT SOURCES

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The talk will present an overview of the progress in high-accuracy simulations of the processes of emission and propagation of synchrotron radiation, made over the last decades, and will discuss numerous applications of such simulations, from electron beam diagnostics to complete simulation of experiments exploiting high brightness and coherence of modern synchrotron light sources. A special attention will be dedicated to description of methods, their implementation, and application examples of such Start-To-End (S2E) simulations for modern synchrotron light source facilities.

The presentation will focus on implementation of the S2E simulations in the "Synchrotron Radiation Workshop" (SRW) code, that uses physical optics methods for high-accuracy calculations of the emission and propagation of partially-coherent synchrotron radiation, from electron beam, through X-ray beamline optics, to experimental sample, and in many cases (like in coherent X-ray scattering and imaging experiments) through the sample and further on to a detector. The presentation will cover the direct partially-coherent calculations that are available in SRW code since more than a decade, and recent updates improving efficiency of these simulations, in particular the new memory- and CPU-efficient coherent mode decomposition methods implemented in the code.

Several simulation examples will be presented for new soft and hard X-ray beamlines, that are currently in the process of design at the National Synchrotron Light Source II (NSLS-II). Among special features of the new soft X-ray beamlines is the use of large-aperture final focusing optics (zone plates in the case of the Soft X-ray Nanoprobe beamline and K-B mirrors in the case of the Angle-Resolved Photoemission Spectroscopy and Resonant Inelastic X-ray Scattering beamlines) targeting nearly diffraction-limited resolution and requiring physical-optics calculations that are valid beyond the traditionally-used paraxial approximation. The peculiarity of the Coherent Diffraction Imaging hard X-ray beamline is high flexibility in providing variable radiation spot size (in 1 – 10 μm range) at sample at variable degree of coherence and highest-possible flux for a given degree of coherence.

The simulation examples will also include assessment of optical performances of the existing beamlines of NSLS-II, when operating with today's ~0.8 nm horizontal emittance electron beam and at different options of the eventual NSLS-II upgrade, including the high-brightness (16 pm emittance) one. The results of these simulations help to determine the optimal upgrade option for the storage ring and identify critical components of the beamlines that need to be changed to allow these beamlines to fully benefit from the storage ring upgrade.

The talk will also cover updates in S2E simulations of coherent X-ray scattering experiments performed at the Coherent Soft and Hard X-ray beamlines of NSLS-II. Planned extensions of the S2E simulations will be discussed, including the use of Molecular Dynamics calculation results for defining 3D models of samples, applications of the forward-simulations for testing feasibility of experiments with given types of samples and determining best beamline settings for them, as well as eventual applications of the forward-simulations for improving stability of beamline components and for solving complicated inverse problems of sample reconstruction.