X-ray waveguides at ROBL: New developments and applications

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A great number of optical devices and experimental techniques has taken a tremendous benefit in recent years from the development of optical fibers and related structures. In particular, the field of optical near-field microscopy combined with fiber optics and spot sizes of under 1000 nm has led to a variety of new and important results concerning the structure and physical properties of various materials in the nm-range. Unfortunately, the resolution is still limited for light in the visible range and an extension to smaller wavelengths is therefore an interesting and important venture. One could envision hard x-rays with wavelengths of ~ 0.1 nm and specially designed optical components. X-rays can be focussed either coherently by Fresnel zone plates and Bragg Fresnel lenses, or incoherently by bent crystal optics and coated fiber optics (generally speaking by highly reflective materials, e.g. supermirrors etc.). Typical beam spots in the micrometer range can be achieved for x-rays by these approaches. However, a beam with a still significantly smaller cross section could open up a whole new range of applications in scattering, microscopy and spectroscopy with real space resolution on the sub nm scale, e.g. elemental analysis of nanoparticles by x-ray fluorescence analysis or high resolution tomography, currently referred to as x-ray microscopy.

As a new approach, multilayered systems can be used for one-dimensional beam concentration, where a precise control of layer thickness, index of refraction (density), and interface roughness by modern deposition techniques (spin-coating, MBE, rf sputtering) allows for the construction of efficient waveguide structures, which operate under grazing incidence and guide the beam by a resonant beam coupling mechanism within a layer of a few nm thickness until it exits at the side of the layered structure (see Fig 1).

Fig. 1: Sketch of a hard x-ray waveguide consisting of a low density guiding layer (e.g. Carbon) sandwiched in between layers of higher density (e.g. Ni).

Fig. 2: Logarithmic contourplot of the calculated transverse electric field intensity inside a x-ray waveguide structure, demonstrating the field-enhancement for excited modes.
The theoretical model was obtained by applying basic optical principles and results from waveguides for visible light to the general optical treatment of hard x-rays, where the index of refraction is less than 1 and typical wavelengths are 0.1 nm. Following this approach, we have discussed the guiding mechanism in planar waveguides and resonant beam couplers. By calculating the internal electric field (Fig. 2) and the corresponding farfield distribution of exiting modes as a function of various parameters we showed that these structures can be considered as waveguides themselves with defined properties of the angular acceptance, coupling length and efficiency.

We have applied the principle of resonant beam coupling to structural studies of organic or biomolecular thin film samples. In this approach the samples are directly incorporated in the waveguide (Fig. 3). The resonantly enhanced diffraction signal can then be measured by tuning the incidence angle to a resonant mode of the waveguide. We have applied this scheme to a highly oriented stack of ten 1,2-dimyristoyl-sn-glycero-3-phosphatidylcholine (DMPC) bilayers, which was shown to be structural isomorphous to a control sample without metal cap layer. In the future, the novel kind of organic/inorganic hybrid structure may offer several new experimental options. For example, the metal cap layer may serve as a solid state electrode, which would allow interesting experiments on biomolecular films in well controlled AC or DC electrical fields. To this end, details of the sample preparation will be published elsewhere.

The scattering signal measured by grazing incidence diffraction could significantly be enhanced by making use of the resonantly enhanced field-distributions corresponding to the TE₀/ TE₁-modes. The measured diffraction peaks would otherwise be unobservable under the given experimental conditions. As a corollary, even smaller signals (of more disordered systems) become observable at highly brilliant third generation undulator beamlines using the technique presented here. Simulations indicate that signal-to-noise ratios can be improved by up to two orders of magnitude. In the future, high spacial resolution can be gained by the combined analysis of measurements carried out under the excitation of different modes, leading to a depth profile of the scattering signal, stemming e.g. from molecular ordering, lattice constants, or phase state.
Waveguide-enhanced scattering from various macromolecular and supramolecular structures, ranging from synthetic polymers to two-dimensional protein crystals, can thus be envisioned. In addition to sample structure, dynamics may be probed by photon correlation spectroscopy, with the RBC acting as a coherence filter for the incoming radiation. In another experiment, the waveguiding effect could be observed in a single moded waveguide structure with a 100 nm thin guiding layer resulting in an exiting divergent beam with a FWHM beam size smaller than 10 nm (Fig. 4).

Furthermore we have successfully demonstrated the principle of multiple guiding layer x-ray waveguide structures (Fig. 5) and have shown that they can be understood by a straightforward generalization of the single waveguide case. The results can most simply be understood as a diffraction pattern of a grating structure for hard x-rays with a tailored periodicity in the range $100 \text{ Å} < d < 2000 \text{ Å}$, controlled by the design and growth of the structure (Fig. 6). Importantly the device differs from a hypothetical transmission grating in that the field intensity impinging on the grating is enhanced up to two orders of magnitude by the waveguide resonance. Furthermore, one should be able to tailor specific shapes of the exiting coherent x-ray beam after careful parameter studies in the simulation of the electric field intensity (right) and measurement of the farfield pattern (left) from a single mode x-ray waveguide with a 100 Å guiding layer.

**Fig. 4:** Calculation of the electric field intensity (right) and measurement of the farfield pattern (left) from a single mode x-ray waveguide with a 100 Å guiding layer.

**Fig. 5:** Sketch of a waveguide containing multiple guiding layers.
field and the corresponding farfield, possibly leading to new focussing devices. Such optical components could be of particular interest for thermal and cold neutrons, where one could use structures with more than a hundred resonance layers without significant limits by absorption. Guiding layer structures for hard x-rays e.g. with two guiding layers could lead to novel applications in x-ray interferometry, as the far field distribution is crucially sensitive to phase changes in one of the interference beams. In this way information on the local, nanoscale electronic density can be projected onto macroscopic area detectors. Furthermore dynamic properties could also be probed in a two-beam or multi-beam interference setup, as the exiting beam is fully coherent and therefore amenable to photon correlation spectroscopy.

Fig. 6: Measured farfield interference pattern of a waveguide containing multiple guiding layers.

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