WORKSHOP ON
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Possibility for one-shot tomography using a high-gain free-electron laser

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Background

Although x-ray holography has a long history, it is only in recent years that the technologies needed for it to be successful have begun to be available. The advent of undulators and x-ray lasers and the prospect of even more advanced pulsed sources such as high-gain free-electron lasers [Winick 1993] have led to an increase in the level of interest and activity in x-ray holography at several centers around the world. This is based in part on the high interest in three-dimensional imaging experiments and the realization that diffraction-tomography experiments in the x-ray region can only be done via a holographic type of recording because that is the only known way to record the x-ray phases.

Given that true three-dimensional imaging will require a diffraction tomography experiment [Spiller, 1987; Devaney, 1986] and that x-ray holography is the right way to record each view [Howells, 1990], we are faced with the challenge of recording experimentally the many views, probably dozens, that will be required. Moreover, it appears as though such a sequence will not be possible for unfrozen biological material without alteration of the sample during data collection. The traditional response to the damage problem in x-ray imaging is to propose a flash experiment. One of the advantages of holographic imaging is compatibility with this type of exposure. However, there is still a problem in acquiring a sequence of flash images because the first one or first few may still change the sample. There are two ways out of the dilemma. One is to argue that there is no dilemma. Given that the data from each view will be combined in forming the final three-dimensional image, we might argue that the total counts needed (and hence the total dose) may not be much greater than for a single high-quality two-dimensional image [Nugent 1993]. The second way is to perform a flash experiment where all the views are taken simultaneously [Trebes 1990]. The latter is the option we want to explore in this presentation.

Possibility for One-shot Flash Tomography

In order to illuminate a sample with a considerable number of beams with different directions at the same time we need a device that can receive a single coherent beam as input and deliver a multiplicity of similarly coherent beams in a variety of directions as output. The setup could be as
shown in Fig. 1 with the "beam splitter" mounted on the upstream side of a thin membrane and the sample on the downstream.

For the beam splitter to work it would have to be thin enough to transmit a major fraction of a soft x-ray beam. This suggests a two-dimensional crystal-like structure. The advantage of this would be that the spots in the reciprocal lattice of a three-dimensional crystal become rods for a two-dimensional one. This means that they would be certain to make a hit with the Ewald sphere and thus would always represent an observable reflection. In other words we would switch from the Bragg equation to the grating equation.

Diffracting structures to realize the beam-splitter concept

Ordinarily, we think of a transmission grating as having a square-wave transmission function with a bar-to-period ratio of about 1:2. This does what we usually want which is to concentrate as much diffracted light as possible into the +1 and −1 orders. However we can produce the opposite effect by making the bar-to-period ratio either close to zero or to one. This means that either the bars would change into narrow walls or the gaps would change into narrow trenches either of which would distribute the diffracted intensity over many orders. We can do the same in two dimensions in which case the walls or trenches would be replaced by an array of either towers or holes. The diffraction pattern is the same (by Babinet's principle) for both towers and holes (the sizes being taken as equal) anywhere outside of the footprint of the incident beam. As an example, an array of 10nm holes on a 50nm grid would give 4% transmission which would be divided among 49 beams on a square grid with the orders \( m, n \) such that \(-3 < m < 3, -3 < n < 3\) having significant relative strength. If such a system were used to disperse 3nm radiation then a set of 48 holograms with numerical aperture of 1/20 (resolution 30nm) and a maximum angle of over 30° between illumination directions, could in principle be recorded. The low efficiency of such a system based on holes in an opaque background can be improved by a factor four by using \( \pi \)-phase-shifting towers on a transparent background or holes on a \( \pi \)-phase-shifting background. Further details of projected efficiencies are given in the presentation.

Proposed scheme to do a complete tomography experiment using one pulse of the high gain free-electron laser

The layout of the proposed experiment is shown in Fig. 1, to which should be added some focusing of the beam and a beam-defining aperture upstream of the sample. To get a rough idea of the amount of light we need consider the following

- coherent energy per pulse of LCLS = 3mJ
- fluence needed to expose PMMA at 30Å = 0.5 J/cm²
• therefore energy needed for a 20x20 μm^2 hologram = 2μJ

Thus without accounting for any losses we would have enough energy to make 1500 holograms. For a useful reconstruction we would need at least 30 views so we would need to maintain an x-ray exploitation efficiency of about 2% which does not seem unreasonable.

Caution

Successful x-ray diffraction tomography experiments will deliver a value for the complex refractive index as a function of position. This quantity is meaningful because the complex refractive index of all well-defined materials is known and tabulated in the Henke tables [Henke 1993]. However if the materials are driven nonlinear by strong fields as one gets from a strong pulsed source then resulting refractive indices which are derived will not be intelligible in the usual sense. The x-ray imaging community has not needed to address this matter up till now and it may turn out that it poses no difficulties at the Stanford LCLS. However the issue should be examined in future studies of applications of the LCLS.

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References


Fig. 1. Principles of a possible method of one-shot flash tomography. A total of six holograms are shown but they are part of a two-dimensional array of 7x7-1=48.