

Optimizing the Performance of Keyhole Diffraction Microscopy
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Non-destructive inspection of integrated circuits requires a microscope that features high resolution (< 20 nm) and high penetration (> 0.07 mm of silicon substrate), thus suggesting the use of x-ray microscopy. The advent of intense coherent sources of hard (< 1 nm wavelength) x-rays has led to the study of x-ray diffraction microscopy¹ in which the image is reconstructed from the far-field diffraction pattern. Atomic resolution is possible with this lensless approach. Because this pattern records only intensity information, additional information, e.g. the phase distribution, is needed for image reconstruction. In our approach² this information is provided by illuminating the sample with a collimated beam of well-defined shape and thus is a form of “keyhole diffraction microscopy”.

Previously from computer simulations and scaled optical experiments, we found that illumination with asymmetric shapes (such as a triangle) sharply bounded gave the best reconstruction. In this paper, we further study the theoretical limitations on keyhole diffraction microscopy, including phase retrieval algorithms, illumination patterns, and samples’ properties (geometry, periodicity, etc.), to optimize the performance of this technique.

Different reconstruction algorithms³ were compared on the same diffraction data from scaled optical experiment (632 nm He-Ne laser, refer to [2]). The error reduction (ER) algorithm itself was slow and only gave a fair result (Fig. 1(b)) even after 7500 iterations. The hybrid input-out (HIO) algorithm gave a better result (Fig. 1(c)) after merely 460 iterations. The best result came from 80 iterations using HIO followed by 420 iterations using ER (Fig. 1(d)).

Dynamic support⁴ was used to improve the convergence of computation (Fig. 2). The “support” is defined as a boundary to separate the sample and its surrounding featureless area. Tighter support, which better follows the outline of the sample, leads to better reconstruction. Here the support was automatically updated by thresholding the intensity of the reconstruction during computation, so that it quickly shrunk to wrap around the object, resulting in faster convergence and better reconstruction quality (Fig. 2(b)) comparing with the fixed support (Fig. 2(c)).

We further demonstrate this technique with a soft x-ray experiment (Fig. 3) and a hard x-ray experiment (Fig. 4). The soft x-ray experiment was conducted at Stanford Synchrotron Radiation Laboratory (SSRL) BL13-3 with 900 eV (1.38 nm) soft x-rays. Samples were fabricated by focused ion beam (FIB) milling through 600 nm thick gold film on 200 nm thick SiN membrane. HIO algorithm with dynamic support was used for image reconstruction. The reconstruction was able to resolve sub-20nm features. The hard x-ray experiment was performed at Spring-8 synchrotron facility in Japan, with 7 KeV (0.177nm) x-rays. Deeply buried structures on thick substrate were successfully reconstructed without the knowledge of the sample. Linewidth variations were shown in the reconstruction.

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¹ J. Miao, *et al*, High Resolution 3D X-ray Diffraction Microscopy, *Phys. Rev. Lett.*, **89**, 088303 (2002)

² B. Dai, *et al*, *J. Vac. Sci. Technol. B* 28, issue 6, (2010)

³ J. Fienup, Phase retrieval algorithms: a comparison, *Appl. Opt.*, **21** (15), 2758-2769 (1982)

⁴ S. Marchesini, *et al*, “X-ray image reconstruction from a diffraction pattern alone”, *Phys. Rev. B* **68**, 140101 (2003).

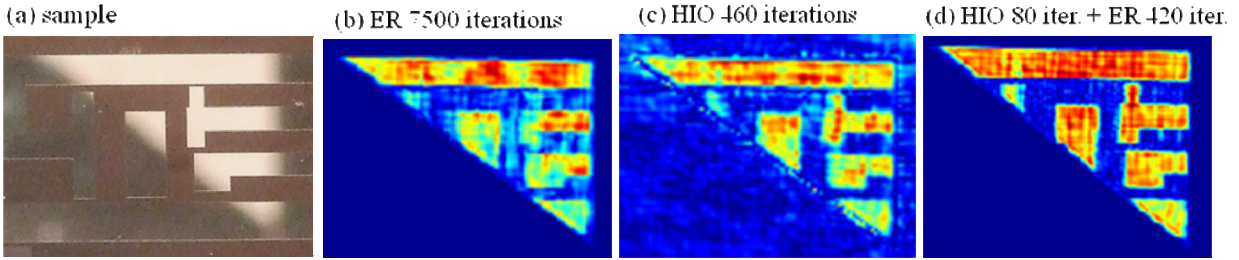


Fig. 1: Comparison between ER, HIO and HIO + ER algorithms. Diffraction data was from optical diffraction experiment (refer to [2]). (a) The sample was 200 nm chromium patterned on a quartz substrate, illuminated by a 2cm x 1.9cm triangle-shaped beam. (b)--(d) were reconstructions with different algorithms.

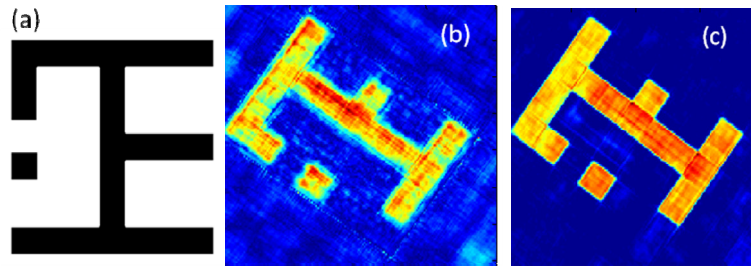


Fig. 2: Comparison between dynamic support and fixed support. Diffraction data was from optical diffraction experiment (refer to [2]). (a) A binary sample. (b) Reconstruction with HIO algorithm and fixed support, after 517 iterations. (c) Reconstruction with dynamic support, after 134 iterations.

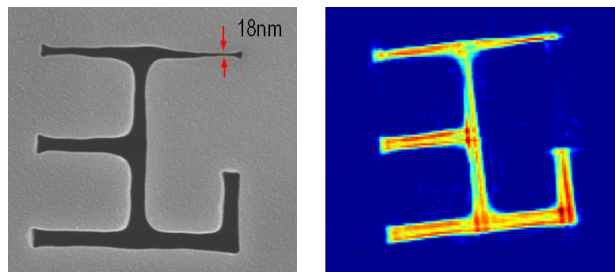


Fig. 3: Soft x-ray experiment. SEM image and reconstruction of a FIB milled sample. Designed linewidth was 170nm but lower dose during milling leads to much narrower linewidth (minimum linewidth = 18nm). Reconstruction was able to resolve the narrowest linewidth. The reconstruction shown here was an average of 50 repeats.

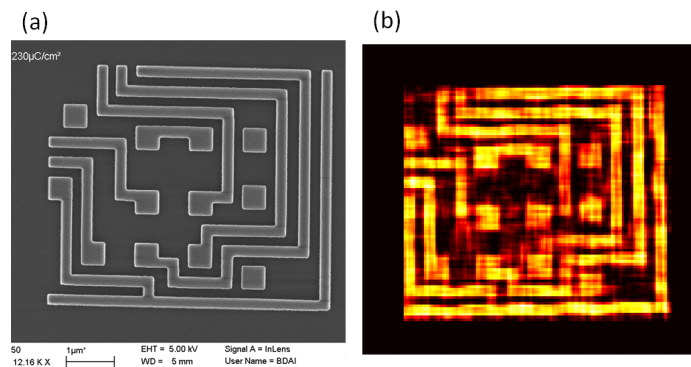


Fig. 4: Hard x-ray experiment. (a) SEM image of an exemplary sample before SiO₂ deposition (PECVD). The sample consisted of a single layer of copper wire with 210 nm linewidth and 90nm thickness, buried beneath 1 µm silicon dioxide, on top of 100 µm thick silicon substrate. (b) A successful reconstruction using HIO algorithm with dynamic support. It was an average of 150 repeats. Note the linewidth variations from the exemplary sample were shown in the reconstruction.