Investigation of Dispersion Effects in Proximity Field Nanopatterning Lithography Using the Finite Difference Time Domain Method

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1. Introduction

Photonic crystals, or photonic band gap materials, are artificially designed, three-dimensional periodic structures possessing the remarkable ability to control light propagation. When designed properly, light at a range of frequencies is prohibited from propagating inside the photonic crystal. As a result, light outside the structure is reflected, whereas light inside the structure is trapped. Applications of photonic crystals have been explored, resulting in many devices such as waveguides and highly efficient light sources [1]. Many of these devices require reliable manufacturing of submicron sized features, rendering mass production prohibitively difficult and expensive with existing lithographic tools.

Proximity Field Nanopatterning (PnP) is a lithography technique which has the potential to serve as an easy and inexpensive alternative method of producing photonic crystals and photonic crystal-based devices [2]. PnP uses a two-dimensional elastomeric phase mask to produce three-dimensional interference patterns. These patterns are imprinted on a slab of light sensitive polymer, known as a photoresist, which undergoes certain changes upon exposure to light photons. In particular, solubility of photoresist material in certain liquids, commonly known as developers, is modified. By soaking exposed photoresist slabs in a developer liquid, PnP produces three-dimensional structures. All of the described procedure requires inexpensive, unsophisticated equipment, yet it can consistently produce structures with submicron features on an area of several square millimeters in size. Unlike other lithography methods, PnP does not require clean, shockproof or vacuum environments or extensive alignment procedures to achieve this feat.

Dissections of structures obtained from PnP experiments performed by our group indicate washout and incomplete pattern formation beyond 5-10 micrometers into the photoresist. Dispersion is one possible cause among several others. Research in this paper concentrates on effects of dispersion on PnP structures produced by masks with periodic arrangements of posts, investigated using the Finite Difference Time Domain (FDTD) method. The next section gives the simulation details. In the third section we show how dispersion modifies the PnP interference patterns generated by two different mask designs. The effects become noticeable around 5-6 micrometers into the resist and become more pronounced as one moves deeper.

2. Simulation Details

The Finite Difference Time Domain (FDTD) method is used in this work due to its advantages in PnP modeling. Compared to the widely used, Rigorous Coupled Wave Analysis (RCWA) method, FDTD calculates the PnP light field directly without resorting to approximations through sums of diffraction orders. FDTD can be used for PnP simulations with both periodic and nonperiodic mask patterns, whereas RCWA is only suitable for structures with inherent periodicity.

Figure 1 depicts the general setup of FDTD simulations performed throughout this work. An OpenMP parallelized simulation program [3] was utilized on an SGI Altix system to simulate PnP experiments using two different periodic mask designs. The first mask has a square lattice (550 nm periodicity) of cylindrical posts (400 nm diameter, 420 nm height), whereas the second mask has a hexagonal lattice (600 nm periodicity) of cylindrical posts (450 nm diameter, 420 nm height). Both masks are made of Polydimethylsiloxane (PDMS) (\(\varepsilon = 2.0449\)). The photoresist used is a 15 micrometers thick slab of SU-8 (\(\varepsilon = 3.03665476\)). A Total Field/Scattered Field plane wave
source is used to inject circularly polarized, single-frequency plane waves directly into the mask backplane. The FDTD grid is terminated by periodic boundary conditions in four transverse directions and by Uniaxial Perfectly Matched Layer (UPML) absorbing boundaries [4] in the remaining two directions. The grid is composed of 60x60x641 cells of 27.5x27.5x27.5 nm cubes when the first mask is used and 148x128x1044 cells of 16x16x16 nm cubes for simulations with the second mask.

Figure 1 Cross-sectional (vertical) view of FDTD based Proximity Field Nanopatterning (PnP) simulation.

3. Results and Discussion

Simulations for 13 wavelengths between 359 and 371 nm have been performed separately for both mask designs. Steady state results have been obtained by Fourier transforming the FDTD generated electric field magnitudes through the last 1000 time steps (Figure 2). An experimentally calibrated intensity threshold was used to render expected photoresist structures at the end of PnP process (Figure 3). Pixel-by-pixel differences between the black/white images generated at 12 frequencies (359-371 nm) and the center frequency (365 nm) were calculated. The difference images were added up to reveal dispersion effects to the 365 nm patterns (Figures 4-5). In the figures, white pixels show additions while black pixels indicate removals from the interference patterns generated at 365 nm. Figure 6 shows a vertical cross-section generated by the hexagonal mask design. Dispersion effects expected for the structure depicted in Figure 6 are rendered in Figure 7. While Figures 4, 5 and 7 illustrate modifications of various sizes and shapes, dispersion caused modifications are more pronounced throughout the bottom half of the photoresist below the 8 micrometer mark in all three figures.

Figure 2 Vertical cross-section depicting electric field magnitudes for mask with square arrangement of posts illuminated by 365 nm light. Lengths are given in nanometers.

Figure 3 Application of threshold to Figure 2 produces an image of photoresist structures retained after development process.
Figure 4 Expected changes caused by dispersion to Figure 3 patterns (mask with square arrangement of posts). White pixels depict growth areas while black pixels indicate eradication zones. Gray pixels exist in unchanged areas.

Figure 5 Dispersion effects for a different vertical cross section frame (mask with square arrangement of posts).

Figure 6 Vertical cross-section depicting expected structure for the mask with hexagonal arrangement of posts illuminated at 365 nm.

Figure 7 Dispersion effects for different vertical cross section frame (mask with hexagonal arrangement of posts in Figure 6).

In this work we have demonstrated a method to estimate dispersion effects on PnP generated patterns by combining black/white structural images for a number of monochromatic sources. We have shown expected dispersion effects on structures generated by two different mask designs. The location and extent of the dispersion effects vary, however they become more pronounced at 5-6 micrometers or deeper into the photoresist.

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5. References


