Three-Dimensional Photolithography Simulation

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An overall three-dimensional photolithography simulator is presented, which has been developed for workstation based application. The simulator consists of three modules according to the fundamental processes of photolithography, namely imaging, exposure/bleaching and development. General illumination forms are taken into account, and the nonlinear bleaching reaction of the photoresist is considered. Electromagnetic light-scattering due to a nonplanar topography is treated by solving repeatedly the Maxwell equations within the inhomogeneous photoresist. The development process is simulated with a cellular based surface advancement algorithm.

1. Introduction

Among all technologies photolithography holds the leading position in pattern transfer in today's semiconductor industry. The reduction of the lithographic feature sizes towards or even beyond the used wavelength and the increasing nonplanarity of the devices place considerable demands onto the lithography process. The large cost and time necessary for experiments make simulation an important and especially cost-effective tool for further improvements. However, a rigorous description of the fundamental physical effects governing sub-micrometer-photolithography places considerable demands onto the modeling, whereby a three-dimensional simulation becomes necessary.

We present an overall three-dimensional photolithography simulator consisting of three modules. Each module accounts for one of the fundamental processes of photolithography: imaging, exposure/bleaching, and development.

2. Imaging Simulation

The imaging module describes the illumination of the photo-mask. The light propagation through the optical system and the light transmission through the photo-mask has to be simulated. The output of the imaging module is the aerial image which is the light intensity incident on top of the wafer.

Our aerial image module is based on a vector-valued extension of the scalar theory of Fourier optics [1]. The photo-mask is assumed to be laterally periodic and infinitesimal thin with ideal transitions of the transmission characteristic. The piece-wise constant transmission function is real-valued (zero or one) for binary masks, in case of phase-shift masks it is complex-valued with module less than one. For the simulation of general illumination forms like annular and quadrupole the aperture is discretized into mutually independent coherent point sources. The resulting image on top of the wafer due to one coherent point source can be expressed by a superposition of discrete diffraction orders. Due to the assumed periodicity of the photo-mask this superposition corresponds to a Fourier expansion, whereby the diffraction orders are homogeneous plane waves with amplitudes given by the vector-valued diffraction theory [1].

3. Exposure/Bleaching Simulation

The exposure/bleaching module simulates the chemical reaction of the photosensitive resist. The light propagation within the optically nonlinear resist as well as electromagnetic (EM) scattering effects due to a nonplanar topography have to be modeled. The result of the exposure/bleaching module is the latent bulk image.

According to Dill's 'ABC'-model [2] the exposure state of the photoresist is described by the concentration of the photoactive compound (PAC). The PAC concentration constitutes the bulk image. As it is transferred into the resist by light absorption the EM field inside the photoresist has to be determined. Because the bleaching rate is negligible as compared to the frequency of the EM field, we apply a quasi-static approximation, i.e., we assume a steady-state field distribution within a time step and solve repeatedly a time-harmonic version of the Maxwell equations with a linear but spatially inhomogeneous permittivity.

Our solution of the Maxwell equations [3], [4] corresponds to the three-dimensional extension of the differential method. This method was originally developed for the simulation of diffraction gratings [5] and was later adapted for two-dimensional photolithography simulation [1]. The strategy behind the differential method is briefly described as follows: First, the dependency of the EM field on the lateral coordinates is expressed by Fourier series. Insertion of these expansions into the Maxwell equations transforms the partial differential equations into a system of ordinary differential equations. Above and below the simulation domain analytical expressions can be found for the incident, reflected, and transmitted light. Matching these expansions with the Fourier series valid inside the photoresist yields decoupled boundary conditions for the top and the bottom of the simulation domain. Hence, we have to solve a two-point boundary value problem [6]. This is accomplished with a newly developed algorithm [4], [5], that is based on the memory saving "shooting method" [6]. Once the ordinary differential equation system is solved, the obtained field coefficients are transformed back to the spatial domain to calculate the absorbed EM field intensity as necessary for the Dill model.

4. Development Simulation

The development of the photoresist is modeled as a surface-controlled etching reaction [2]. We use Kim's 'R'-model [7] to relate the bulk image to a spatially inhomogeneous etch or development rate. This development rate is stored on a tensorproductgrid, because the differential method requires a laterally uniform spaced grid to apply the numerically highly efficient Fast Fourier Transform (FFT). For the simulation of the time-evolution of the development front the recently proposed cellular-based topography simulator of [8] has been extended to read the development rate from the tensorproductgrid [4]. The basic idea behind this surface advancement algorithm is to apply a structuring element along the exposed surface which removes successively resist cells of the underlying cellular geometry representation. Within the scope of lithography simulation the shape of the structuring element depends on the precalculated development rate multiplied by the chosen time step.

5. Simulation Results

To demonstrate the capability of our approach we simulated contact hole printing over a planar and a stepped topography. In Fig. 1 we show the aerial image obtained by the vector-valued approach used for our imaging module. Conventional I-line illumination with a numerical aperture of NA = 0.5 and a partial coherence factor of S = 0.7 was used. Nine coherent point sources were needed to account for the partial coherence.

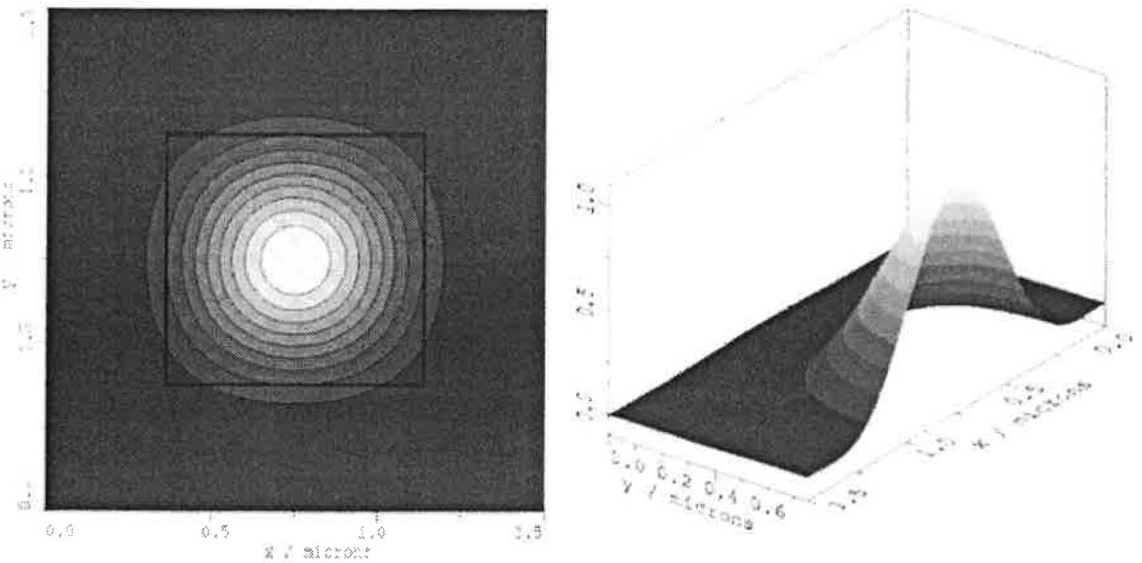

Fig. 1: Aerial image of a 0.75 mm x 0.75 mm wide contact hole.

In Fig. 2 contour plots of the PAC are shown in the upper two figures and the developed photoresist profiles in the lower two figures. The exposure-dose was 120 mJ/cm^2 and the development time was 50 sec. The simulation parameters were for the Dill-model no = 1.65, A = 0.55 μm^{-1}, B = 0.045 μm^{-1}, C = 0.013 cm^2/mJ and for the Kim-model R1 = 0.25 μm/sec, R2 = 0.0005 μm/sec, R3 = 7.4 (cf. Table IV in [7]).

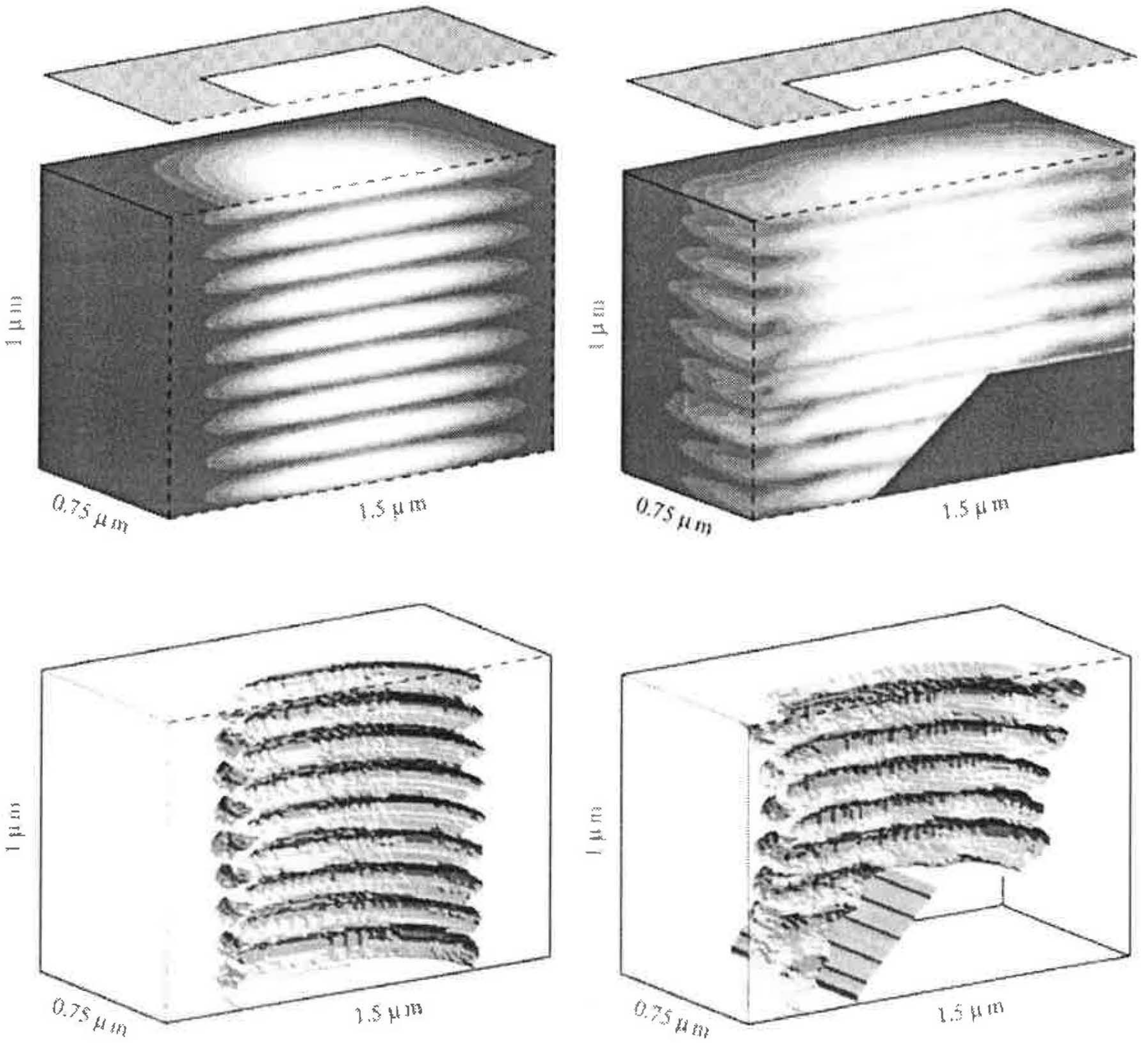

Fig. 2: Bulk image and developed resist profile over a planar and a stepped substrate.

The oval contours are caused from standing waves within the photoresist, which result from substrate reflections. Due to the lateral variation in optical thickness the regular shaped bulk image and resist profile of the planar topography is distorted in case of the stepped topography. Furthermore, the opening for the stepped substrate is wider than for the planar substrate. Hence, the effective diameter of the contact hole depends on the nonplanarity of the wafer topography.

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