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Three-Dimensional Resist Development Simulation – Benchmarks and Integration with Lithography

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We present a rigorous, three-dimensional model for the simulation of resist exposure and development. The development simulation is based on a cellular surface movement algorithm and benchmarked for several prototypical test cases. Exposure simulation is performed by an extension of the two-dimensional differential method to three dimensions. This method relies on a Fourier expansion of the electromagnetic (EM) field in the lateral coordinates. We demonstrate simulation examples for exposure and development over a planar substrate, a dielectric and a reflective step.

1. INTRODUCTION

Photolithography holds the leading position in pattern transfer in today's semiconductor manufacturing. The steady decrease of the minimal feature size reaching the wavelength used for the exposure and effects of non-planar surface scattering push state-of-the-art lithography technologies to their limits. Rigorous three-dimensional simulation tools for illumination, exposure, and resist development assist in better understanding of the optical and physical effects of submicron photolithography and significantly support research and development aiming at higher resolution and better depth of focus over non-planar surfaces.

This paper describes a three-dimensional simulation of resist development coupled with a three-dimensional extension of the differential method for the simulation of resist exposure. Section 2 describes the model setup for development and exposure. In Section 3 we investigate the accuracy and robustness of the development simulation by applying it to typical benchmark examples and show simulation results for a coupled illumination/exposure/development simulation.

2. SIMULATION MODELS

2.1. Resist development

For the simulation of the time evolution of the resist surface we use a cell-based topography simulator [1] which uses morphological operations derived from image processing. The geometry is represented by an array of cubic cells and a material index is assigned to each cell (see Fig. 1).

The surface advancement algorithm applies a structuring element along the exposed surface, which successively removes cells of the underlying cellular geometry by switching the material index of the cell from resist (R) to vacuum (0). For the lithography simulation a sphere is used as structuring element, whose radius is determined by the local development rate multiplied with the chosen time step (see Fig. 2). The local development rate of the cells is either given by a mathematical expression as for the benchmark examples or extracted from the exposure simulation. A sufficiently high number of cells has to be chosen to resolve the strong variations of the rate originating from standing waves or notching effects during photoresist exposure.

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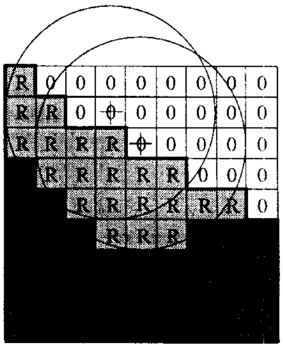

Figure 1. Cellular geometry representation.

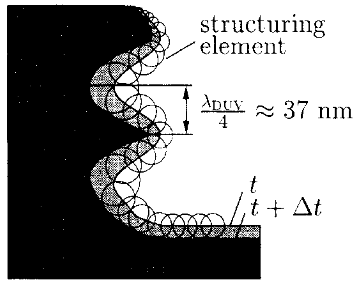

Figure 2. Structuring element surface propagation algorithm.

2.2. Exposure simulation

The exposure state of the photoresist is described by the photoactive compound (PAC) $M(\mathbf{x};t)$. We use Dill's "ABC"-model to relate the bleaching of the resist and the change in the resist's refractive index $n(\mathbf{x};t)$ to the exposure intensity $I(\mathbf{x};t)$

$$\frac{\partial M(\mathbf{x};t)}{\partial t} = -C\, I(\mathbf{x};t)\, M(\mathbf{x};t)$$
$$n(\mathbf{x};t) = n_0 + j\frac{\lambda}{4\pi}\Big(A\, M(\mathbf{x};t) + B\Big). \tag{1}$$

For the exposure simulation we use a three-dimensional extension of the differential method [2]. Assuming a time-harmonic field distribution within a time step $t_k \le t < t_{k+1}$, the EM field obeys the Maxwell equations in the form

$$\begin{aligned} \operatorname{curl} \mathbf{H}_k(\mathbf{x}) &= -j\omega_0\varepsilon_0\, \varepsilon_k(\mathbf{x})\, \mathbf{E}_k(\mathbf{x}) \\ \operatorname{curl} \mathbf{E}_k(\mathbf{x}) &= j\omega_0\mu_0\, \mathbf{H}_k(\mathbf{x}). \end{aligned} \tag{2}$$

Due to the spatially periodic nature of the incident light and the assumption of a laterally periodic simulation domain the EM field inside the simulation domain can be expressed by a Fourier expansion

$$\begin{aligned} \mathbf{E}_k(\mathbf{x}) &= \sum_{n,m} \mathbf{E}^k_{nm}(z) e^{j2\pi(nx/a+my/b)} \\ \mathbf{H}_k(\mathbf{x}) &= \sum_{n,m} \mathbf{H}^k_{nm}(z) e^{j2\pi(nx/a+my/b)}. \end{aligned} \tag{3}$$

Additionally, the inhomogeneous permittivity $\varepsilon(\mathbf{x})$ and its reciprocal $\chi(\mathbf{x}) = 1/\varepsilon(\mathbf{x})$ can be expanded in Fourier series

$$\begin{aligned} \varepsilon_k(\mathbf{x}) &= \sum_{n,m} \varepsilon^k_{nm}(z) e^{j2\pi(nx/a+my/b)} \\ \chi_k(\mathbf{x}) &= \sum_{n,m} \chi^k_{nm}(z) e^{j2\pi(nx/a+my/b)}. \end{aligned} \tag{4}$$

Insertion of (3) and (4) into (2) transforms the partial differential equations into an infinite dimensional set of coupled ordinary differential equations (ODE) for the Fourier coefficients of the lateral field components.

Above the simulation domain we have to consider incident and reflected waves, whereas below only outgoing waves occur. The incident light is known from the aerial image simulation [3], whereas the unknown reflected and outgoing fields are eliminated by applying radiation BC's. The finally obtained boundary value problem is solved by a numerically efficient implementation of the shooting method [3]. The thus calculated EM field coefficients are transformed back to the spatial domain and the solution of the EM field $I(\mathbf{x};t)$ within one time step t_k is obtained. In case of strongly bleaching resists this process is repeated until the total exposure dose is reached. Next we use Kim's "R"-model to relate the final PAC distribution of the exposure simulation to a spatially inhomogeneous development rate.

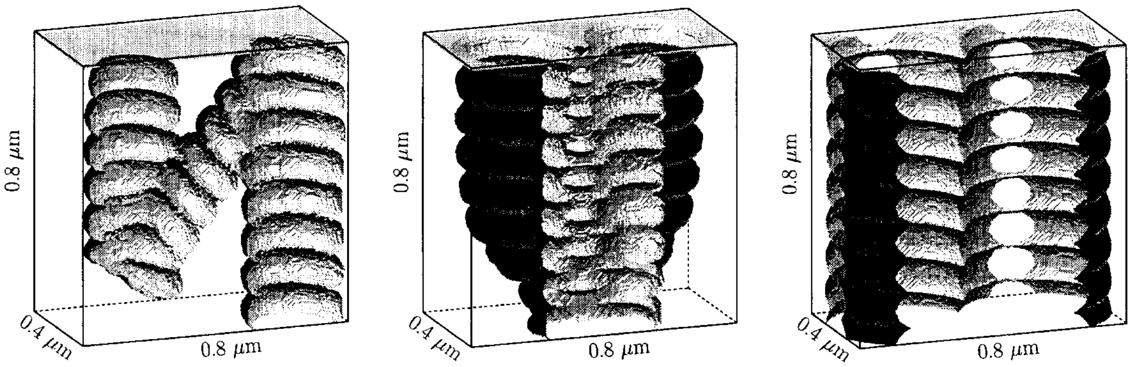

Figure 3. Benchmark examples: reflective notching (left) and contact with phase shifted outriggers (middle and rigth).

3. SIMULATION RESULTS

3.1. Development benchmarks

For checking the accuracy and stability of the resist development simulation benchmark examples as proposed in [4] have been simulated. For the benchmark examples the local development rate r is given as mathematical expression of the position of the single cells $r = F(x, y, z)$.

The first example is a test representing incident reflection from a defect in the wafer. The plane of reflection is 22.5°, thus forming a reflected Gaussian beam with standing waves at an angle of 45°. As can be seen in Fig. 3 (left) there is no dependence of the etch rate on the placement of the cubes since all high intensity regions evolve equally. Moreover the simulator is able to account for the formation of an inclined tunnel underneath the resist surface, which even in the cellular representation conforms very closely to the expected cylindrical shape. The inclined tunnel also exhibits the regular evolution of the standing waves.

The second example represents a contact cut with phase shifted outriggers. The figures in the middle and on the right hand side of Fig. 3 show two different time steps of the surface propagation for this case. Note the tips in the final structure on the right, formed when two outriggers intersect. In both test cases the regularity of the standing waves in the cellular representation is very good.

For the two benchmarks a grid with 160×160×160 cells was used. 36 and 42 time steps were used for the development time of 300 s. The simulation times are in the range of 10 to 15 minutes on a DEC 600/333 workstation.

3.2. Exposure/development simulation

To demonstrate the general capabilities of our approach we have simulated 248 nm DUV contact hole printing over different substrates with various aperture systems.

The simulation domain is $1.0\,\mu\text{m} \times 1.0\,\mu\text{m} \times 0.7\,\mu\text{m}$. A quadratically shaped mask with side length of $0.25\,\mu\text{m}$ is centered over a planar silicon substrate with a refractive index of $n_{\text{Si}} = 1.68 + j3.58$, a dielectric oxide step with $n_{\text{SiO}_2} = 1.508$, and a reflective a-silicon step with $n_{\text{a-Si}} = 1.69 + j2.76$. The stepper wavelength is 248 nm and a non-bleaching DUV resist is chosen with $n_{\text{Resist}} = 1.65 + j0.02$. Several simulations with different illumination (coherent, partially coherent with $\sigma = 0.8$, and quadrupole with $\sigma = 0.1$ and $X = Y = 0.7$) for a fixed NA of 0.5 have been performed to analyze the contact opening diameter depending on these exposure parameters.

A comparison of the simulations shown in Fig. 4 for the coherent illumination only exhibits a wider opening in the developed photore-

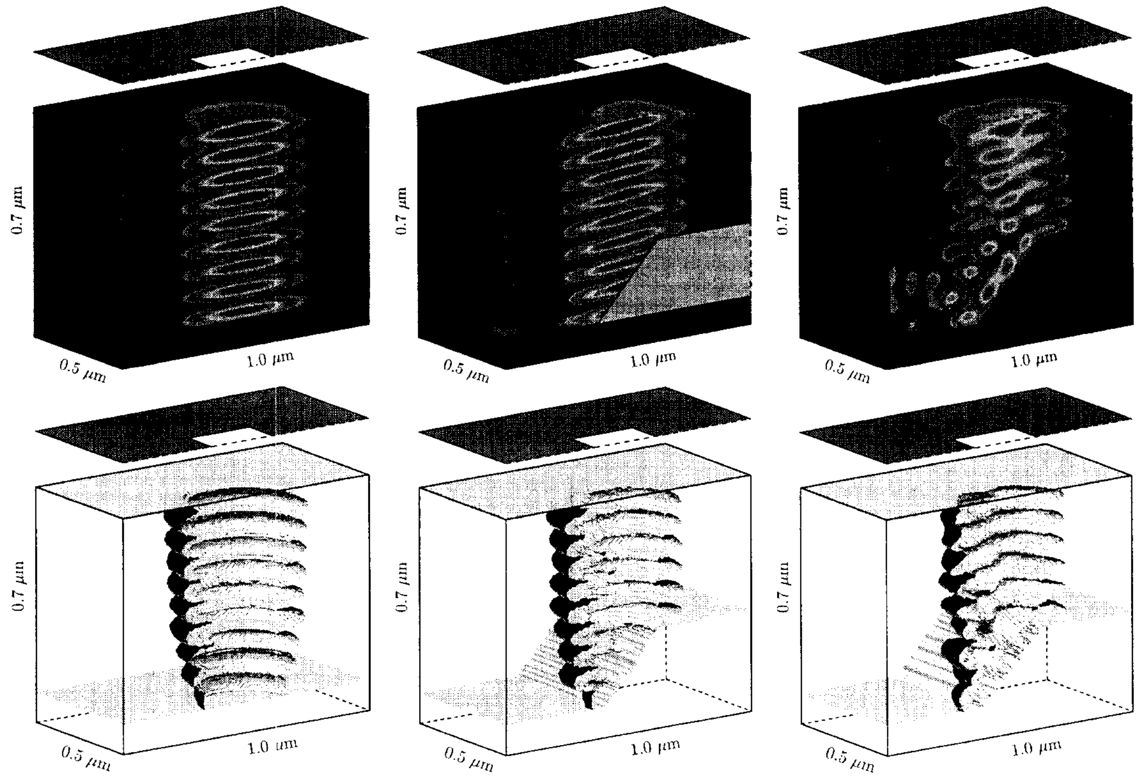

Figure 4. Exposure and development simulation over a planar substrate (left), a dielectric (middle), and a reflective step (right).

sist for the stepped topographies. Hence, the effective diameter of the contact hole depends on the nonplanarity of the wafer topography. This dependence is stronger for the reflective silicon than for the dielectric oxide. The standing waves and thus the resist profiles are also more conformal along the reflective silicon step in comparision with the dielectric step.

The run time for the simulation was about 6 hours requiring about 250 MB of memory.

4. CONCLUSION

An embedded three-dimensional model for resist exposure and development was presented. It was implemented on a common engineering workstation. The approach proved to be very robust and provides a high level of accuracy within reasonable computation times and system resources.

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