

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

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With minimal feature sizes of today's semiconductor manufacturing technology reaching the physical limit of the wavelength used for the exposure, rigorous three-dimensional simulation of off-axis illumination, exposure and development becomes indispensable for accurate investigation of all possibilities for improving resolution and depth of focus over non planar surfaces. We present a rigorous, three-dimensional model for the simulation of exposure and development. The development simulation is derived from a cell-based topography simulation approach and benchmarked for several prototypical test cases. Exposure simulation is done by extending the two-dimensional differential method to three dimensions. Thereby the electromagnetic (EM) field is Fourier expanded in the lateral coordinates. We demonstrate simulation examples for exposure and development over a planar substrate, a dielectric and a reflective step.

The development of the photoresist is modeled as a surface-controlled etching reaction. For the benchmark examples three-dimensional mathematical formulations correlate the local development rate with the geometric position within the resist layer. For the coupling with lithography simulation we choose Kim's 'R'-model to relate the chemical state after the exposure simulation to a spatially inhomogeneous development rate. For the simulation of the time evolution of the development front we use a cell-based topography simulator [1] which uses morphological operations derived from image processing. The surface advancement algorithm applies a structuring element along the exposed surface, which successively removes photoresist cells of the underlying cellular geometry (see Fig. 1). The radius of the sphere used as structuring element within the scope of lithography simulation is determined by the local development rate multiplied with the chosen time step. A sufficiently high number of cells has to be chosen to resolve the strong variations of the development rate originating from standing waves or notching effects during photoresist exposure.

For checking the accuracy and stability of the resist development simulation benchmark examples as proposed in [2] have been performed. The first example (see Fig. 2 left) 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 the simulator is able to account for the formation of an inclined tunnel underneath the resist, which even in the cellular representation conforms closely to the cylindrical shape. The second example represents a contact cut with phase shifted outriggers. The figures in the middle and on the right hand side of Fig. 2 show two different time steps of the surface propagation for this case. In both test cases the regularity of the standing waves in the cellular representation is very good. This is especially remarkable for the inclined cylinder of the first example. For the two benchmarks a cell grid with $160 \times 160 \times 160$ 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 min on a DEC 600/333 workstation.

The exposure simulation uses a three-dimensional extension of the differential method. The electromagnetic field on the lateral x- and y-coordinates is expressed by Fourier expansions [3]. Insertion of the expansion into the Maxwell equations transforms the partial differential equations into an ordinary differential equation (ODE) system. The ODE system is solved using the appropriate boundary conditions and the resulting EM field coefficients are transformed back to the spatial domain. Fig. 3 shows the application of this method to the exposure using a simulation domain of $1.0 \mu\text{m} \times 1.0 \mu\text{m} \times 0.7 \mu\text{m}$. A quadratic 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 ($n_{\text{a-Si}} = 1.69 + j2.76$). 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, circular, and annular) have been performed to analyze the contact opening diameter depending on the exposure parameters. The selected examples for coherent illumination reveal the decreasing contact opening over the non-planar geometries and the capability of the presented integrated three-dimensional exposure and development simulation to perform rigorous investigation of effects arising in state-of-the-art lithography techniques.

- [1] E. Strasser and S. Selberherr, "Algorithms and Models for Cellular Based Topography Simulation," *IEEE Trans. Computer-Aided Design*, vol. 14, no. 9, pp. 1104-1114, 1995.
- [2] J. Helmsen and A. Neureuther, "3D Lithography Cases for Exploring Technology Solutions and Benchmarking Simulators," in *Proc. SPIE Optical/Laser Microlithography VI*, vol. 1927, pp. 382-394, 1993.
- [3] H. Kirchauer and S. Selberherr, "Rigorous Three-Dimensional Photoresist Exposure and Development Simulation over Nonplanar Topography," *IEEE Trans. Computer-Aided Design of Integrated Circuits and Systems*, vol. 16, no. 12, pp. 1431-1438, 1997.

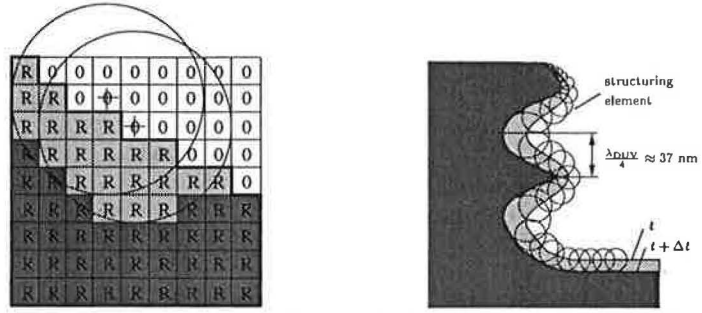


Figure 1: Scheme of cellular geometry representation and structuring element surface propagation algorithm.

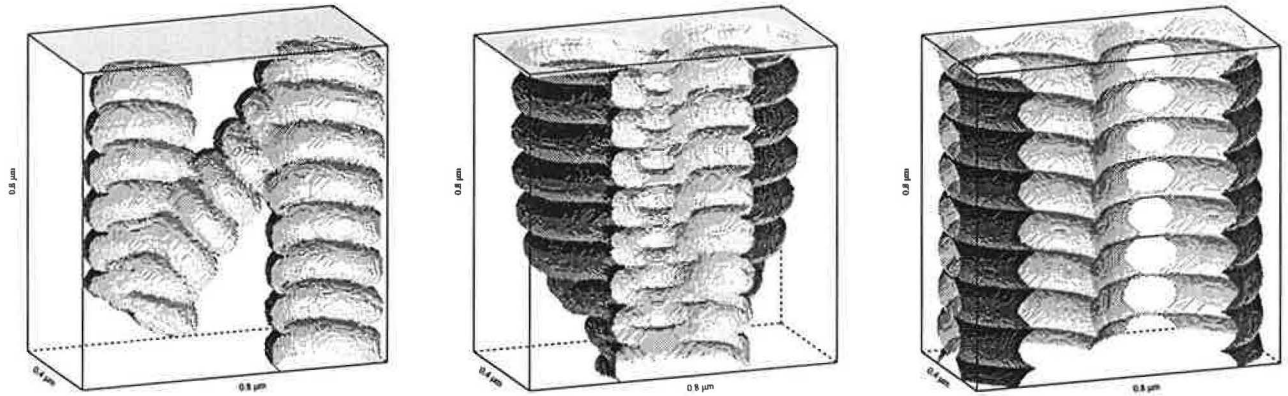


Figure 2: Benchmark examples: reflective notching and contact with phase shifted outriggers.

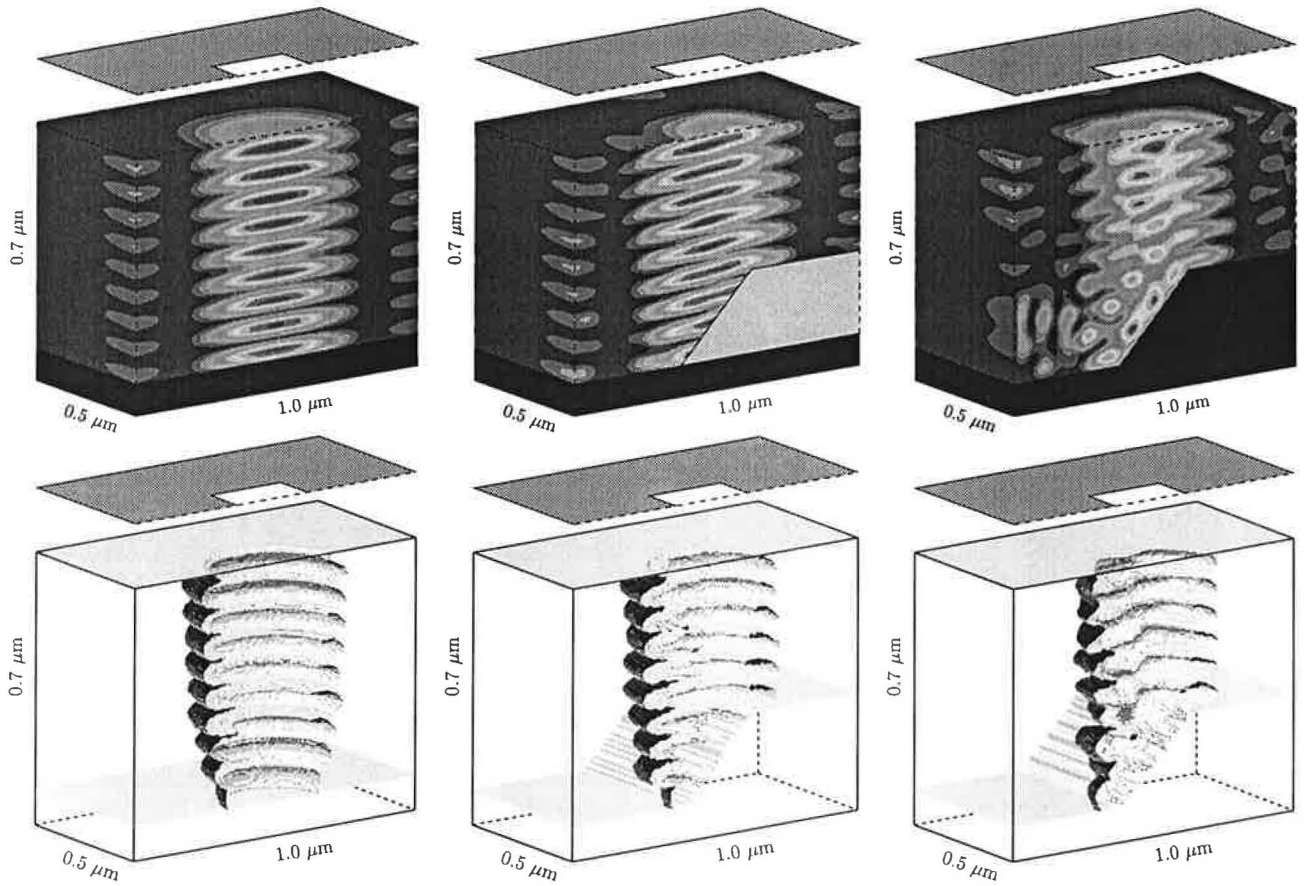


Figure 3: Exposure and development simulation over a planar substrate, a dielectric and a reflective step.