Computational Lithography for Electromagnetic Wave Propagation in Photoresist

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Abstract

The details of how photo resist is exposed during lithography processes are extremely important to optimizing fabrication. Features such as sloped sidewalls, undercut, scalloping can be caused by the diffraction, absorption and reflection of light as it passed through the layers of mask, resist and substrate. A current method of simulating this process is with a full Finite Difference Time Domain process, which is computationally intensive and time consuming. In this project I propose and demonstrate a forward/backward spatial propagation simulation without time steps, which will capture the full electromagnetic solution including diffraction and reflections. By combining this with physical Dill Parameters of the resist a complete picture of the exposing process can be efficiently created.

Theory
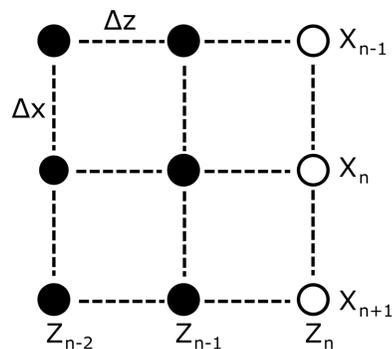
The wave equation is discretized with a finite difference scheme using 9 points, 6 from past steps and 3 from the future step, to solve for the new electric field.

$$A \frac{\partial^2 E}{\partial x^2}\bigg|_{z-1} + B \frac{\partial^2 E}{\partial x^2}\bigg|_{z} + A \frac{\partial^2 E}{\partial x^2}\bigg|_{z+1} \quad A \frac{\partial^2 E}{\partial z^2} = -n^2 k^2 E$$

This process is repeated until the final interface in the system is passed. At this point the field is decomposed into forward and backward moving parts. The backward moving field is propagated back through the system in the same manner, then subtracted from the forward moving field.

Results

Free Space Propagation

Dielectric Pane

Metal Mirror

Numerical Stability

A Von Neumann stability analysis was run on the system to determine the optimal parameters for grid spacing and derivative weighting for maximum numerical stability. The following equation is the "Amplification Factor" which must be 1 or less to ensure random numerical or statistical noise does not become amplified and overwhelm the simulation.

$$G = \frac{\frac{4B}{dX^2} + k^2 n^2 - \sqrt{-(-\frac{16A}{dX^2} + \frac{4}{dZ^2})(-\frac{4C}{dX^2} + \frac{1}{dZ^2}) + (-\frac{4B}{dX^2} - k^2 n^2 - \frac{2}{dZ^2})^2} + \frac{2}{dZ^2}}{-\frac{8C}{dX^2} + \frac{2}{dZ^2}}$$

Unfortunately even at the optimal parameters, the simulation is still very unstable. This had lead to a restriction in the grid spacing, meaning we have not been able to run the simulation at a high enough resolution to obtain useful photolithography results at this time.
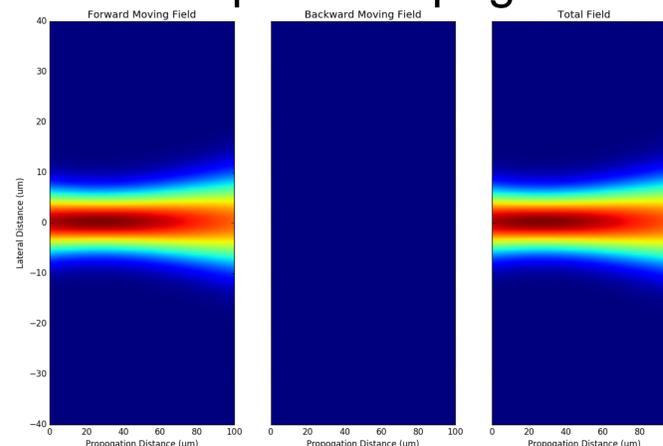
Future Work

The source of the instability of the system appears to be the Runge effect, in which the Taylor expansion of the derivatives under samples the field and causes extreme variations in the results. The immediate goals of this project are to implement higher order derivative approximations, and non-constant grid spacing to suppress these effects and allow the use of higher resolution grids.
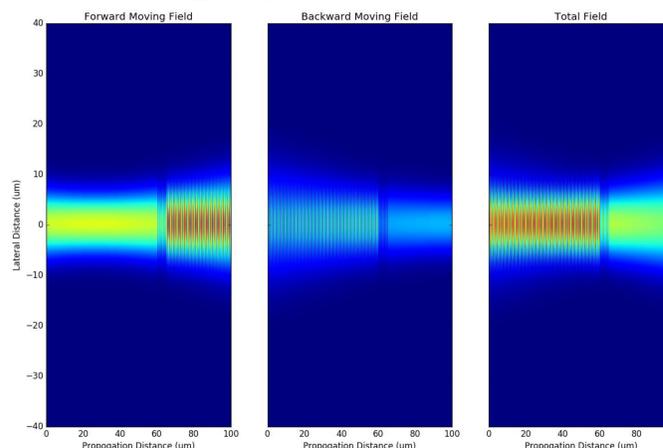
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