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STORM VERSION 2.0

by

Ebo Croffie

Memorandum No. UCB/ERL M99/60

3 December 1999

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1.0 Introduction

1.1 Overview

STORM (Simulation Tools for Resist Models) is a program for simulating Top Surface Imaging (TSI), bilayer resist (BLR) and chemically amplified resist processes. The principal components of STORM are SPLAT for exposure simulation, BAKE for Postexposure bake (PEB) simulation, SILY2D for silylation simulation and O2ETCH for oxygen reactive ion etching image transfer simulation. The computer programs for O2ETCH, SILY2D and BAKE solve a set of chemical kinetics nonlinear partial differential equations using the finite element method for space discretization and a backward difference formula time advancement scheme for time discretization. In addition to the chemical kinetics equations, SILY2D also solves the virtual power equation to determine the mechanical stress fields and polymer deformation. O2ETCH also utilizes Monte Carlo methods to simulate the ion bombardment during the etching process. The simulation domain may be a cross section or a top view of a photoresist. This release includes the Contour, X-Window^{TM} plotting program to visualize the simulation results.

The algorithm for BAKE is capable of simulating problems such as postexposure bake, line end shortening and resist film top loss. The algorithm for SILY2D is capable of simulating problems such as stress induced reaction retardation effects on polymer swelling during silylation.

This version of STORM comes without GUI; the user must execute the program by modifying the appropriate input parameter files. The included software tools may be run as separate stand

alone programs. Communication between programs is primarily through files. This form of information transfer allows intermediate steps to be saved and retrieved for later use.

STORM is designed for use on engineering workstations running under the Unix^{TM} operating systems. The plotting program require the X window system. Memory requirements depends on the number of nodes approximating the simulation domain. Practical simulations require between 1 and 200 megabytes of physical memory. Run times depends on machine and problem size. For example, BAKE and SILY2D run under 1 minute on 600MHz DEC Alpha and under 10 minutes on a 200MHz Sun Ultra Sparc machine (441 nodes).

1.2 What's new in STORM ver2.0

This release of STORM utilizes a generalized model for postexposure bake (PEB) including free volume enhanced diffusion, resist shrinkage and acid quenching effects during PEB. The models for silylation have also been generalized to include positive and negative tone silylation schemes, as well as diffusion enhanced and non-diffusion enhanced silylation schemes. A new simulator for oxygen reactive ion etching of surface imaged resists is included for top surface imaging simulations.

1.3 Source Code Information and Acknowledgments

This release of STORM comes without the source code. However, the following information on the source code is given for ease of document modification for future releases. BAKE and SILY2D code of STORM ver2.0 are written in the C++ programming language. The code uses the libraries below. We acknowledge the following people for making these libraries available in the public domain:

Triangle	Jonathan R. Shewchuk
SuperLU	Sherry Li
MV++	R. Pozo
Meschach	David E. Stewart

The class description files are:

bake.h	Postexposure bake simulator class definition
etch.h	O_2 RIE simulator class definition
sily.h	Silylation simulator class definition
node.h	Domain grid point class definition
ele.h	Domain element class definition
myblas.h	Auxiliary BLAS header file

The corresponding class implementation files are:

bake.cc	
etch.cc	
sily.cc	
node.cc	
ele.cc	
myblas.cc	
main.cc	Class user file

STORM uses the following files:

splat.out	PEB initial condition file
bake.par	PEB parameters file
etch.par	Etching parameters file
sily.par	Silylation parameters file
viewsplat.m	MATLAB script for viewing SPLAT results
viewbake.m	MATLAB script for viewing BAKE results
viewsily.m	MATLAB script for viewing SILY2D results
viewetch.m	MATLAB script for viewing O2ETCH result
sim_region to simulate	PERL script for choosing appropriate region
get_region to simulate	PERL script for choosing appropriate region

1.4 About this manual

Section 1.0	**Introduction** A general overview of STORM is provided.
Section 2.0	**Installation** This section discusses how the simulation program STORM is compiled and installed.
Section 3.0	**Running STORM and its components** A brief introduction to commands and input file keywords is presented in this section.
Section 4.0	**Lithography Simulation Tutorial** Tutorial examples to let the user become familiar with the commands and procedures of running STORM are given
.Section 5.0	**Physical Models in STORM** This section describes the physical models implemented in the various programs contained SPLAT, BAKE, and SILY2D.

The conventions used throughout this users' guide are as follows:

- Words which are in ALL CAPITAL LETTERS represent programs or shell scripts.
- Words in **bold** letters represent commands to be typed exactly as it appears on the users' guide.
- Words in *italics* represent input or output filenames for command line arguments
- Words inside [square brackets] are options to commands.
- Words in the `Courier font` represent characters in a file or output from programs.
- The string "ws%" represents the unix prompt on a workstation.
- The string ">>" represents the MATLAB prompt.

2.0 Installation

2.1 Resource Requirements

The computing environment of the user should:

- be capable of compiling and running C and FORTRAN programs.
- have at least 10 mega bytes of disk space available to hold the data files
- have MATLAB ver 4.0 or higher software. (The user could write his/her own script files for another program or even write their own analysis programs.)

2.2 Organization

Since this version of STORM comes without the source code, the distribution files are separated into different platforms:

1. DEC-OSF
2. DEC-ULTRIX
3. DEC-UNIX
4. HP-UX
5. SGIRIX
6. Solaris
7. Solaris-x86
8. SunOS

2.3 Installation

This software package consists of the main program STORM as well as other supporting routines to be run on the user's workstation.

1. SILY2D (Program for silylation simulation.)
2. BAKE (Programs for Postexposure bake simulation.)
3. SPLAT (Program written in Fortran for calculating aerial images.)
4. O2ETCH (Program for O_2 etching simulations.)
5. DRAWMASK (Program to view mask)
6. DRAWPLOT (Program to plot 1D intensity profile from SPLAT output)
7. CONTOUR (Program to view 2D intensity contours from SPLAT output)

To install STORM, move storm2.0.tar.gz to a directory (say $HOME/bin) where STORM should reside. Uncompress the STORM by typing the following command:

```
ws% gunzip storm2.0.tar.gz
```

If done correctly, the .gz suffix that was previously attached to the file should vanish.

Untar the storm2.0.tar file by typing:

```
ws% tar -xvf storm2.0.tar
ws% cd STORM
```

You should now see the two shell scripts and following directories:

```
O2etch
Bake
Plotters
Sily2D
Splat
```

You are now ready to start compiling SPLAT and Plotter files. Make sure you are in the appropriate directory and type:

ws% **csh** *make (or gmake)*

If compilation is unsuccessful, you should see an error message telling you when and where compilation was terminated. In this case, please see Section 2.4 which gives you suggestions that may help the program compile properly.

After compilation, you may want to remove the object files to recover some disk space.

2.4 Installation Problems

The main reasons for an unsuccessful installation are:

1. Lack of disk space

   Either provide sufficient space or adjust the "build.all" script to build only one module at a time and then delete the installed tar files after the build.
2. Incorrect permission settings

   Make sure you have sufficient permission for the destination directories. Check the status display to see that the destination directories are as desired. If you are installing to a system directory (such as /usr/local/bin), you may have to "su root."

   ##The installation script automatically sets the permission level to 0755 for executables and 0644 for libraries. If you need to set different permission levels, you will have to modify each Makefile manually. There are no provisions for customized permission levels at this point. #
3. Missing header or library files

   This occurs normally because of missing or incorrect X libraries. Check to make sure that your X release is complete and current. If the installation still fails, then contact us.

4. Compilation errors
   Make sure standard compilers (like cc and not gcc, ANSI C, or CC) are used.

3.0 Running STORM and individual components

STORM consists of many essential tools which can be combined together to simulate a process. In order to run SPLAT, for example, the *splat-inputfile* must be specified. Likewise, to run BAKE, SILY2D and O2ETCH, the *bake-inputfile*, *sily-inputfile* and *etch-file* must be given (see below for details on the file formats). MATLAB plots can be generated from the output files. A full simulation using the four modules is performed by running the following:

ws% **splat** < *splat-inputfile*

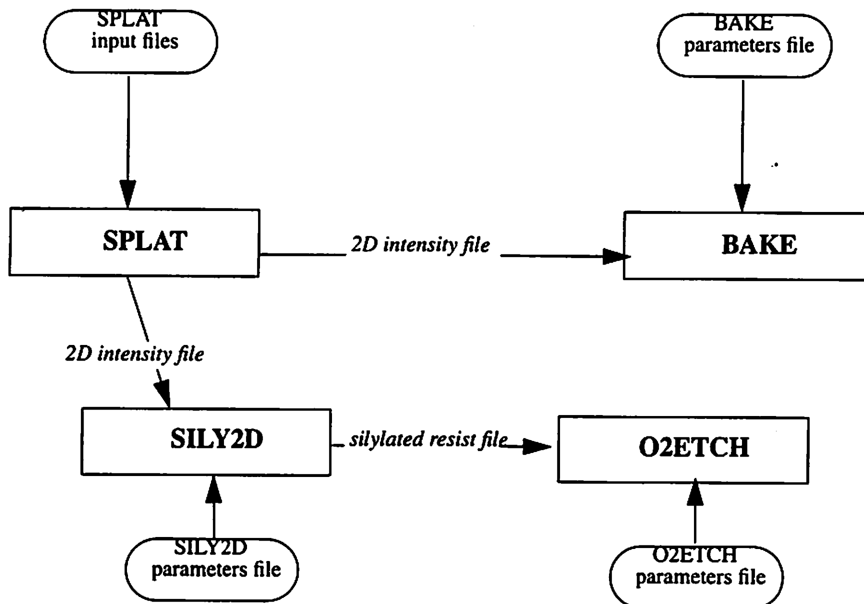
SPLAT outputs a 2D intensity file of the exposed resist needed for BAKE simulation. BAKE can then be run by typing:

ws% **bake**

Silylation can be simulated by typing:

% **sily**

The following STORM process flow diagram will serve to explain the dependency of the various modules in a concise manner.



3.1 Running SPLAT

For detailed information on SPLAT, consult the SPLAT User's Manual. The basic information is presented here as an introduction to running SPLAT as a stand alone program.

SPLAT accepts a file of statement numbers, with each statement number followed by a list of arguments. A command lines beginning with the pound sign (#) is ignored, and a line beginning with an ampersand (&) is considered as a continuation of the previous line.

The projection system is specified by defining the illumination wavelength, numerical aperture, defocus, partial coherence and the five primary lens aberrations: spherical aberration, coma, astigmatism, curvature, and distortion.

The mask is specified as a set of rectangles or triangles, each with a given transmittance and phase. Then the image is simulated for a specified region.

The parser does not recognize key words, and simply skips over them. Thus, the following is a basic valid SPLAT command file:

Example thin film SPLAT input file (*splat.tsi*)

```
#file generation TSI resist
stmt 1: print = 3
stmt 2: lambda = 0.248 um
stmt 3: na = 0.6
stmt 4: defocus = 0.0 mode = 1
stmt 5: sigma = 0.5
stmt 6: mask = 0.3 x 0.3 trans = 0;
stmt 7: cutout = (0.00, 0.00) 0.125 x 0.3 trans = 1;
stmt 35: resist layer = RESIST_LAYER 'film.uvII'
stmt 31: mag = 5 mode = 0;
stmt 32: 50; #table look-up
stmt 10: 0 2;
stmt 14: cutline from (-0.3, 0.0) to (0.3, 0.0)
& with 31 points mode = 1 in 'tsi.RESIST_LAYER'
end 0
```

The last line (stmt 14) tells SPLAT to discretize each layer (0.6um wide) using 31 nodes.

In addition to *splat.tsi* input file, parameters specific to the photoresist being exposed must be specified.

Example UVIIHS photoresist input file (*film.uvII*):

```
4.73 -0.14 1.0 0.0
1.68 20.74 0.2 0.012 5 0.8 90
```

The last 2 numbers on the last line (0.8 90) tells SPLAT to divide a 0.8um thick resist into 90 layers. For more information on other parameters, please

at the explanation given under SPLAT in the Physical Models section of this manual.

To run the above, type:

ws%run.layers ***splat.tsi*** **1 90**

run.layers is a unix script to run many thin-film interference simulations using a single input file. The script searches for the word 'RESIST_LAYER' and replaces it with the current resist layer and then calls SPLAT. Therefore, in this particular simulation there will be 90 different 1D intensity contour files in the current directory. To convert these 1D intensity plots to a 2D contour plot, type:

ws%merge.layers tsi.RESIST_LAYER 1 90 >*tsi.cnt*

merge.layers is another unix script used to merge 2D intensity contour files created using run.layers command. In this example the merged contour file is written to *tsi.cnt*. The output file needs to be edited to reflect the spatial dimensions of the photoresist. **See Tutorial section for example.**

The output file *tsi.cnt* contains the intensity profile information of the resist matrix. Each number in the file (excluding the header lines) is the normalized intensity value at a particular node in the resist. Note that in this particular example, the number of nodes representing the resist matrix is 31X90=2790 nodes. Most uniprocessor machines do not have enough memory resources (> 1 Gigabyte) to run STORM with this many nodes. In most applications, the intensity pattern in the resist is periodic (standing waves in non absorbing resists) or the exposed light is absorbed in the near top region of the resist (TSI resists). In both cases only a small region of the domain can be simulated without much loss of accuracy. In our particular example the top 0.1 micron of the resist can be simulated. Also in most cases, symmetry can be exploited to simulate only half of the selected domain. To select the top 0.1 micron of the resist for BAKE and SILY2D simulation, run the included PERL script file as follows:

ws%sim_region ***tsi.cnt*** 0.1 0.3

This will output the file *splat.out* in the Bake directory

3.2 Running BAKE

BAKE expects an input file from SPLAT output called *splat.out*. Any other image file must be moved to this name for BAKE to execute properly. The PEB parameters must be specified in the parameter file *bake.par*.

Example BAKE parameters input file (*bake.par*):

```
0.45
19.2
0.3
0.011
1e-4
0.27
0.15
3.0
10.0
0.01
100
500
1
90

# I_0 :Initial intensity
# Dose :Exposure Dose
# BaseConc :Base Concentration
# AcidRate :Photolysis Rate Constant
# Diff :Acid diffusion coefficient in free volume
# React :reaction rate
# Loss :Acid loss rate
# Omega :Diffusion model parameter 1
# Nu :Diffusion model parameter 2
# Relax :Polymer relaxation rate constant
# Beta :Polymer shrinkage parameter
# Eta :Polymer Viscosity
# Alpha :Young Modulus?
# FinalTime :Total Post Exposure Bake Time
```

To run BAKE, type:

ws% bake

The program quits executions when it reaches the specified PEB time

A successful BAKE run should output latent image file *bake.ext*, for viewing in MATLAB.

3.3 Running SILY2D

SILY2D expects the input files called *splat.out*. You must make sure that *splat.out* file exists in the SILY2D directory before running SILY2D.Before running SILY2D, the silylation parameter values must be specified in the file *sily.par*.

Example SILY2D parameters input file (*sily.par*)

```
1.0e-4
1.5
1
10.0
20.0
1.0
3.0
100
500
10.0
5.5e-05
0.001
.001
0.55
60

# D:Diffusivity Coefficient
# K_1:Reaction RatRate e Coefficient
# psi:Nonlinear Stress Coupling Coefficient
# omega:Nonlinear Diffusion Coupling Coefficient
# gamma:cross linking coupling parameter
# t_r :Shear stress relaxation time
# tau :Shear stress relaxation time
# eta:Polymer Viscosity
# alpha:Polymer Incompressibility Parameter?
# P:Chamber Pressure
# k_3:Silylation Agent Adsorption rate constant
# k_4:Silylation Agent Desorption rate constant
# E_max: Polymer Swelling Parameter
```

```
# A_max: Polymer Swelling Parameter
# t_final:Total Silylation Time
```

To run SILY2D, type:

ws% **sily**

3.4 Running The Plot Programs.

The results obtained from simulation can be plotted using MATLAB™ or CONTOUR. The plot programs, CONTOUR may be run as independent X-Window programs. They are run by typing the program name followed by the plot data file name. MATLAB scripts are provided for plotting SPLAT, BAKE and SILY2D output data. If you get an error message like "*cannot open display*", you need to set your Unix shell DISPLAY variable by typing:

ws% **setenv DISPLAY** *host:display*

where *host* is the name of your workstation and *display* is the number assigned to your terminal screen.

To exit CONTOUR, DRAWMASK or DRAWPLOT, simply click the mouse in the window or in the QUIT button if one exists. The plotter will then create a PostScript file named *data-plot.ps* and prompt to ask if the file should be sent to the default printer.

4.0 A Tutorial for doing Lithography Simulation

The following section offers a small tutorial for 2D Lithography Simulation. The first tutorial simulates acid diffusion in a DUV resist cross section during PEB. A top view simulation is also presented for completeness. The second tutorial simulates silylation of a positive tone TSI resist. The third tutorial simulates the O_2 RIE dry development of silylated resist. This brief tutorial is meant to help the user get a feel for running simulations in STORM. One can also use this tutorial to check that the software has been installed and is running properly.

4.1 Exposure of DUV Resist Cross Section

The SPLAT input deck initializes various process conditions such as the wavelength, diameter of the numerical aperture, partial coherence factor and the size and geometry of the mask. The following command is used to simulate a thin-film version of SPLAT.

```
stmt 35: resist layer = RESIST_LAYER 'film.uvII'
```

"*film.uvII*" contains the thin-film SPLAT parameter values to be used in this simulation..

The entire SPLAT input file, *splat.uvII,* is shown below. For more information on these commands, please look at the explanation given under SPLAT in the Physical Models section of this manual.

```
# Fast thin-film SPLAT example for 193nm resist.
stmt 1: print = 3
stmt 2: lambda = 0.193 um
stmt 3: na = 0.6
stmt 4: defocus = 0.0 mode = 1
stmt 5: sigma = 0.5
stmt 6: mask = 1.05 x 0.5 trans = 0;
stmt 7: cutout = (0.15, 0.00) 0.9 x 0.5 trans = 1 ;
stmt 35: resist layer = RESIST_LAYER 'film.uvII'
stmt 31: mag = 5 mode = 0;
stmt 32: 50; #table look-up
stmt 10: 0 2;
stmt 11: (-0.6, 0.00) 1.20 0.5 ;
stmt 14: cutline from (-0.75, 0.0) to (0.75, 0.0)
& with 51 points mode = 1 in 'slr.RESIST_LAYER'
end 0
```

The parameter file, *film.uvII,* is also shown below.

<u>The thin-film SPLAT input file</u>

```
4.73 -0.14 1.0 0.0
1.68 0.74 0.2 0.012 5 0.4 60
```

To run a thin-film SPLAT input deck, type

ws% run.layers ***splat.slr*** **1 60**

This simulation will create 60 different 1D intensity contour files in the current directory.

Now, in order to create a 2D intensity file that is accepted by BAKE, type

ws% merge.layers slr.RESIST_LAYER 1 60 >*slr.cnt*

This will merge the 1D intensity contour files created using the **run.layers** command to create a 2D intensity contour file *slr.cnt.*

The output file needs to be edited to reflect the spatial dimensions of the photoresist. In our example, the x-axis domain is (-1.05, 1.05) and the y-axis domain is (0.0, 0.4) um. The number of x-points is 51 (from stmt 14). To do this, edit *srl.cnt* with your favorite editor (e.g. vi, emacs, etc.) and make the following changes:

```
xmin --> -1.05
xmax --> 1.05
ymin --> 0.0
ymax --> 0.4
nxpts --> 51
```

The nodes approximating the resist domain in the merged contour file are too many for practical Postexposure bake simulation. We can study the effects of Postexposure bake on this profile by simulating the top 0.15um (~3 standing waves) of the 0.4um thick resist. Since the feature is symmetric about the x-axis, we simulate only half of the domain, i.e. (xmin, xmax)=(0.0, 1.05um). Furthermore, the exposed region is only a fraction of the domain. All interesting activities will take place in the exposed region of the domain. Thus, we can trim our simulation region even further by simulating a width of 0.25um. To recap, our simulation region is now (xmin, xmax) = (0, 0.25) instead of (-1.05, 1.05) and (ymin, ymax)= (0.45, 0.6) instead of (0.0, 0.6).. To choose such a domain, type the following:

ws%sim_region ***slr.cnt*** *0.15 0.25*

sim_region is a script that take as an argument the resist thickness from top and width from center (0.15um thick and 0.25um wide in our example). It outputs the file ***splat.out*** (in Bake directory) containing the intensity profile of the specified region for BAKE or SILY2D simulations. You should see the following when you execute the above command:

```
%sim_region slr.cnt .15 .25
Original width    = 0.5
New width         = .25
Input  Thickness = .15
```

```
Actual Thickness = 0.4
Original matrix  = (60 x 51)
New  matrix      = (22 x 13)
Output file is '../Bake/splat.out'
```

4.2 Postexposure Bake of DUV Resist Cross Section

We are now ready to run BAKE. Make sure *splat.out* exists in your Bake directory and choose the following PEB parameters in *bake.par*:

```
1.0e-6
0.5
1
100.0
1.0
3.00
0.001
0.0
100
500
60

# Diff :Acid diffusion coefficient in free volume
# React :Maximum reaction rate
# Psi :nonlinear reaction parameter
# Omega :Diffusion model parameter 1
# Nu :Diffusion model parameter 2
# Relax :Polymer relaxation time
# Beta :Polymer shrinkage parameter
# InitialFreeVol :Initial Free Volume
# Eta :Polymer viscosity
# Alpha :Polymer incompressibility
# FinalTime :Total Post Exposure Bake Time
```

Type:

ws% bake

to run the PEB simulation. You should see the following output:

```
%bake=======Reading Post Exposure Bake Parameters====
```

```
Acid diffusion coefficient in free volume = 1e-06
Maximum reaction rate = 0.5
nonlinear reaction parameter = 1
Polymer relaxation time = 3
Polymer relaxation coefficient = 0.001
Initial Free Volume = 0
Diffusion model parameter 1 = 100
Diffusion model parameter 2 = 1
Total Post Exposure Bake Time = 60


============Finished  Reading Parameters==========

Reading Initial Conditions from SPLAT ...

Simulating the Top 22  Layers of Resist Matrix

Done Reading Initial Conditions ...

Initializing Triangulation ...

Triangulation  Done ...

Allocating Memory for Data Structures ...

Data Structure Set Up Done ...

Starting Systems Solution ...

Total Simulation Time :   1.24891667E+01 minutes

Writing Matlab input file: sil.ext  ...
Writing Matlab input file: stress.ext  ...
Writing Matlab input file: bdf.ext  ...

To visualize silicon concentration in resist
run 'sily' in matlab

To visualize time evolution of silylation variables
run 'bdf2' in matlab
```

```
*****       S       T       O       R       M       ****
```

This simulation takes approximately 12.5 minutes on a DEC Alpha Personal Workstation (600MHz machine).

4.3 SPLAT and BAKE Outputs for DUV Resist Cross section

The final result obtained from running BAKE can be viewed using MATLAB. Type

ws% matlab

In MATLAB, type

>>viewsplat

You will be prompted to input the number of x points per layer. This is the first number in *splat.out* file on line 2. You will then be prompted to enter the simulation region. Make sure you enter this in an array format [ ]. The following output from the above example is shown for illustration:

```
>> viewsplat
The number of xpoints can be found in splat.out file
line 2, first #
Enter this number now : 13
Enter simulation region [xmin xmax ymin ymax] : [0 .25
0 .15]

Warning: Duplicate x-y data points detected: using
average of the z values
> In /usr/sww/matlab-5.0/toolbox/matlab/polyfun/grid-
data.m at line 60
 In /home/ebo/SRC/backup/Bake/viewsplat.m at line 53
```

The following two commands plot the output of BAKE.

>>viewacid

>>viewbake

The three plots generated should look like those in Figure 1.

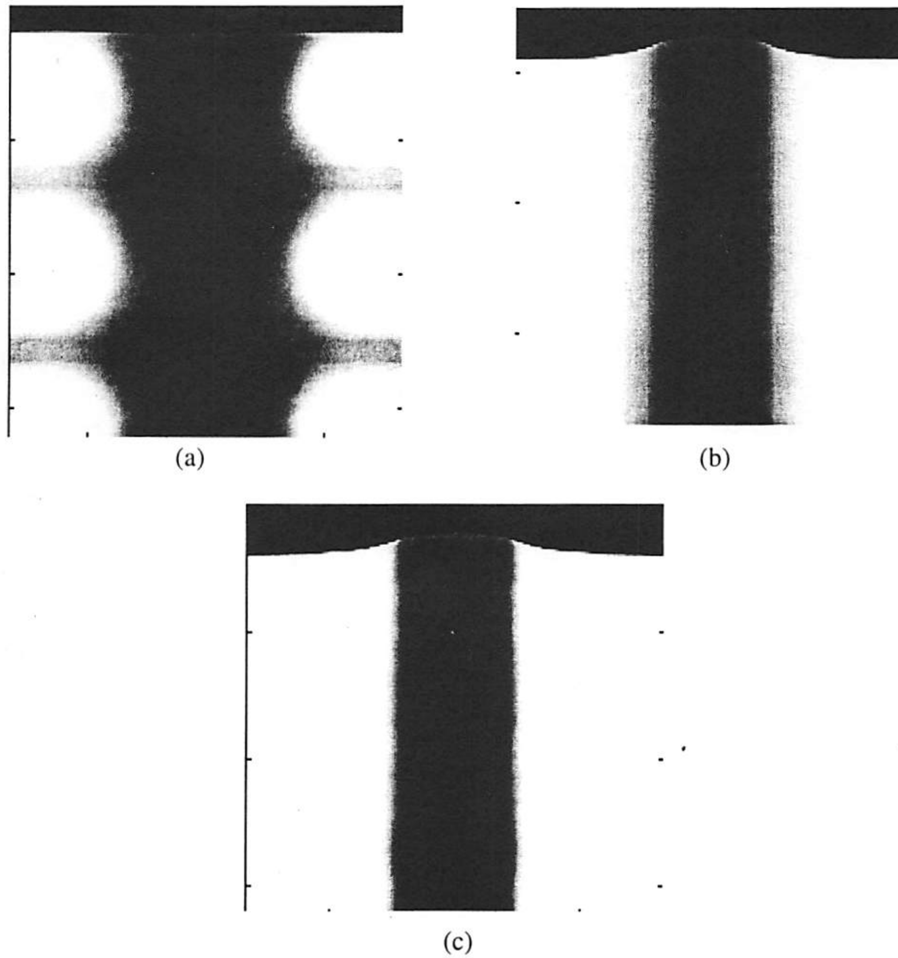


Figure 1. Cross section simulation of CAR process (a) initial acid concentration. (b) acid profile after PEB. (c) latent image after PEB.

4.4 Exposure Bake of DUV Resist Top View

The following command is used to simulate a top view version of SPLAT. The entire SPLAT input file, *les,* is shown below. For more information on these commands, please look at the explanation given under SPLAT in the Physical Models section of this manual.

```
# top view SPLAT example for 193nm resist.
2: wavelength=0.193 microns;
3: NA=0.60;
4: defocus=0.0 microns;
5: partial coherence=0.7;
6: simulated region 3.8 x 3.8 um at 1 transmittance;

        7:      0.000   0.000   3.000   0.180   -1
        7:      0.600   0.360   0.150   2.690   -1
        7:      0.600   3.050   2.840   0.150   -1
        7:      1.350   0.360   0.150   0.880   -1
        7:      1.350   1.420   0.150   0.880   -1
        7:      1.350   2.300   1.030   0.150   -1
        7:      2.560   2.300   0.880   0.150   -1
        7:      2.100   0.360   0.150   1.190   -1
        7:      2.100   1.550   1.340   0.150   -1
        7:      3.620   0.800   0.180   3.000   -1
        7:      0.585   0.360   0.180   0.100   -1
        7:      3.340   3.035   0.100   0.180   -1
        7:      1.335   0.360   0.180   0.100   -1
        7:      1.335   1.140   0.180   0.100   -1
        7:      1.335   1.420   0.180   0.100   -1
        7:      2.280   2.285   0.100   0.180   -1
        7:      2.560   2.285   0.100   0.180   -1
        7:      3.340   2.285   0.100   0.180   -1
        7:      2.085   0.360   0.180   0.100   -1
        7:      3.340   1.535   0.100   0.180   -1

10;
11: (1.5,1.7) 2.3 2.1 13 13 'les.cnt';
0: end;
```

This SPLAT input file generates the line-end shortening (LES) mask shown in Figure 2.

To run a top view SPLAT input deck, type

ws% splat < *les*

This simulation will create a 2D intensity contour files called *les.cnt* in the current directory.

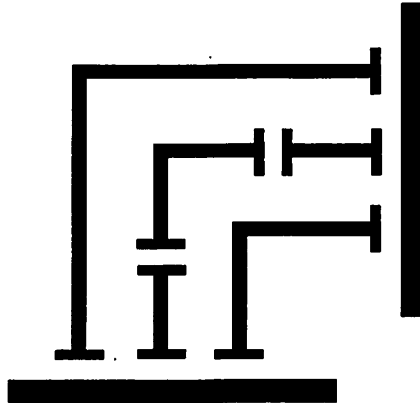


Figure 2. DRAWMASK output for line-end shortening mask.

4.5 Postexposure of DUV resist (top view)

We are now ready to run BAKE. Make sure to move *les.cnt* to *splat.out* in your Bake directory and choose the following PEB parameters in *bake.par*:

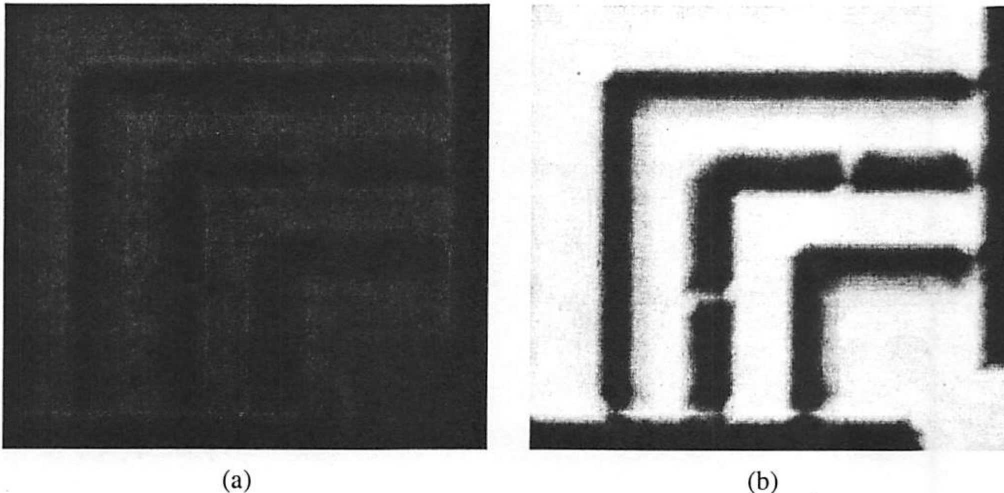
```
0.45
19.2
0.3
0.011
1e-4
0.27
0.15
3.0
10.0
0.01
100
500
1
90

# I_0 :Initial intensity
# Dose :Exposure Dose
# BaseConc :Base Concentration
# AcidRate :Photolysis Rate Constant
```

```
# Diff :Acid diffusion coefficient in free volume
# React :reaction rate
# Loss :Acid loss rate
# Omega :Diffusion model parameter 1
# Nu :Diffusion model parameter 2
# Relax :Polymer relaxation rate constant
# Beta :Polymer shrinkage parameter
# Eta :Polymer Viscosity
# Alpha :Young Modulus?
# FinalTime :Total Post Exposure Bake Time
```

Type:

ws% bake

to run the PEB simulation. The MATLAB plots of this simulation is shown in Figure 3.:



(a) (b)

Figure 3. (a) initial acid concentration after SPLAT simulation. (b) latent image after PEB

4.6 Exposure of Positive Tone TSI Resists

The remaining sections of this chapter give an example of simulating the TSI Lithography process. We will simulate the Exposure, silylation and dry development processes.

The following command is used to simulate thin-film exposure using SPLAT.

```
stmt 35: resist layer = RESIST_LAYER 'film.tsi'
```

"*film.tsi*" contains the thin-film SPLAT parameter values to be used in this particular simulation.. The parameters are chosen so as to limit the exposure to the near top region of the resist.

The entire SPLAT input files *isoline* is shown below. For more information on these commands, please look at the explanation given under SPLAT in the Physical Models section of this manual.

```
# Fast thin-film SPLAT example for TSI resist.
# isoline
stmt 1: print = 3
stmt 2: lambda = 0.193 um
stmt 3: na = 0.33
stmt 4: defocus = 0.0 mode = 1
stmt 5: sigma = 0.68
stmt 6: mask = 1.05 x 0.5 trans = 0 ;
stmt 7: cutout = (0.15, 0.00) 0.9 x 0.5 trans = 1 ;
stmt 35: resist layer = RESIST_LAYER 'film.tsi'
stmt 31: mag = 5 mode = 0;
stmt 32: 50; #table look-up
stmt 10: 0 2;
stmt 11: (-0.6, 0.00) 1.20 0.5 ;
stmt 14: cutline from (-0.75, 0.0) to (0.75, 0.0)
& with 101 points mode = 1 in 'tsi.RESIST_LAYER'
end 0
```

```
The thin-film SPLAT input file
4.73 -0.14 1.0 0.0
1.68 10.00 0.2 0.012 50 0.8 200
```

To run a thin-film SPLAT input deck use the **run.layers** command. Type

ws% run.layers ***splat.tsi*** **1 200**

This simulation will create 200 different 1D intensity contour files in the current directory.

Now, in order to create a 2D intensity file that is accepted by BAKE, type

ws% merge.layers tsi.RESIST_LAYER 1 200 >*tsi.cnt*

This will merge the 1D intensity contour files created using the **run.layers** command to create a 2D intensity contour file *tsi.cnt.*

The output file needs to be edited to reflect the spatial dimensions of the photoresist. In our example, the x-axis domain is (-1.05, 1.05) and the y-axis domain is (0.0, 0.8) um. The number

of x-points is 101 (from stmt 14). To do this, edit *tsi.cnt* with your favorite editor (e.g. vi, emacs, etc.) and make the following changes:

```
xmin --> -1.05
xmax --> 1.05
ymin --> 0.0
ymax --> 0.8
nxpts --> 101
```

We choose the following domain for our simulation (xmin, xmax) = (0, 0.3) and (ymin, ymax) = (0.4, 0.8) by typing:

ws%get_region *tsi.cnt 0.3 0.4 15*

get_region is another script that take as an argument the resist thickness from top, width from center (0.4um thick and 0.3um wide in our example) and the number of rows to select from the given thickness (15 in our example). It outputs the file splat.out containing the intensity profile of the specified region for BAKE or SILY2D simulations. You should see the following:

```
%get_region bake.in .3 .4 15
Output file: splat.out
Original width    = 1.05
New width         = .3
Input  Thickness = .4
Actual Thickness = .8
Original matrix  = (200 x 101)
New  matrix      = (15 x 14)
Selecting from top 100 rows
Output file is splat.out
```

This will outputs the file *splat.out* containing the intensity contours of the specified region.

4.7 Positive tone silylation

SILY2D needs the input files called *splat.out* (**get_region** output) to execute properly.

To run SILY2D, the silylation parameter values must be specified in the file *sily.par.*

Example SILY2D parameters input file (*sily.par*)

```
1.0e-4
1.5
1
10.0
20.0
```

```
1.0
3.0
100
500
10,0
5.5e-05
0.001
.001
0.55
60

# D: Diffusivity Coefficient
# K_1: Reaction RatRate e Coefficient
# psi: Nonlinear Stress Coupling Coefficient
# omega: Nonlinear Diffusion Coupling Coefficient
# gamma: cross linking coupling parameter
# t_r Shear stress relaxation time
# tau Shear stress relaxation time
# eta: Polymer Viscosity
# alpha: Polymer Incompressibility Parameter?
# P: Chamber Pressure
# k_3: Silylation Agent Adsorption rate constant
# k_4: Silylation Agent Desorption rate constant
# E_max: Polymer Swelling Parameter
# A_max: Polymer Swelling Parameter
# t_final: Total Silylation Time
```

Type:

ws% sily

to run SILY2D.

4.8 Viewing SILY2D outputs

The final result obtained from running SILY2D can be viewed using MATLAB. Type

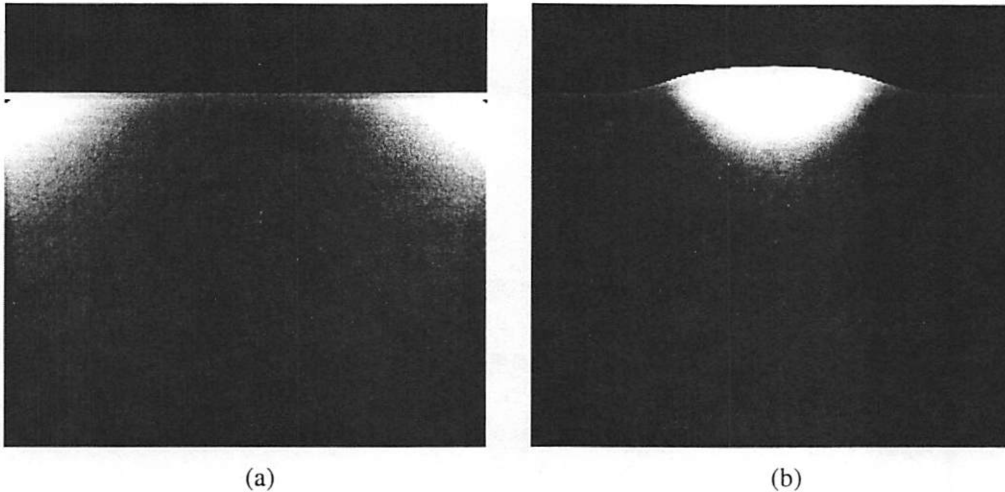
%matlab

In MATLAB, type

>>viewsplat

>>viewsily

This will generate the plots similar to the one shown in Figure 4. The left figure is SPLAT out-



(a) (b)

Figure 4. Simulation results for positive tone silylation scheme. (a) exposure simulation results is supposed to represent the extent of crosslinking in the film after exposure. (b) silylated profile

put and is supposed to represent the extent of crosslinking in the resist after exposure. This crosslinked region inhibits the mobility of the silylating agent as it diffuses into the resist polymer, resulting in the positive tone image (right figure).

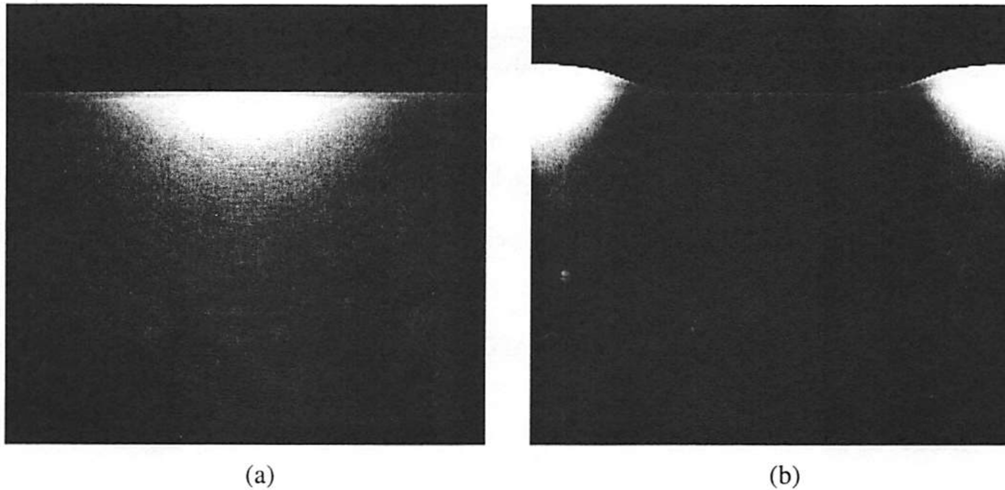
A similar simulation for the isolated space case gives the outputs in Figure 5.

4.9 O_2 reactive ion etching

SILY2D outputs the files silicon.node and silicon.ele needed for O2ETCH simulations. To run O2ETCH, the etching parameter values must be specified in the file *etch.par.*

Example O2ETCH parameters input file (*etch.par*)

```
1.0e-4
10
0.00
2
2
```



(a) (b)

Figure 5. Simulation results for positive tone silylation scheme. (a) exposure simulation results is supposed to represent the extent of crosslinking in the film after exposure. (b) silylated profile

```
0
10
1
0
10
10.0
5.0e-2
30.0
5.5e-05
0.001
11

# Diff :Diffusivity Coeff [um^2/sec]
# React_Oxy :Oxidation Reaction Rate Const
# React_Carb :Carbon Resist Reaction Rate Const
# React_Ion :Ion Resist Reaction Rate Const
# React_Ash :Ashing Resist Reaction Rate Const
# SputRate :Silicon Sputtering Yield Const
# Omega :Nonlinear Diffusion Coeff [1/Normalize conc]
# MeanEnergy :Ion Mean Energy [1/Normalize conc]
# Sigma :Ion Standard deviation  [1/Normalize conc]
# Gamma :Adsorption Inhibition [1/Normalize conc]
```

```
# Alpha :
# BarThresh :Barrier Threshold
# Pressure :Chamber Pressure [Torr]
# K3press :Silylation gas Adsorption rate const
# K4si :Silylation gas Desorption rate const
# FinalTime :Total Silylation Time [sec]
```

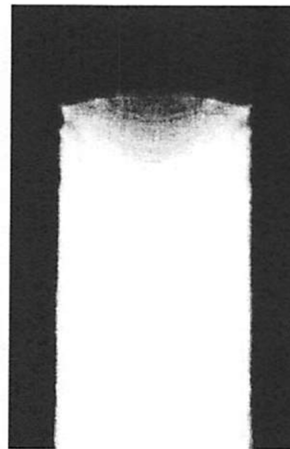
To simulate the dry etching process, type:

ws% etch

After the simulation, the following MATLAB commands can be used to generate the plots in Figure 6:

>>viewsily

>>viewetch



(a) (b)

Figure 6. (a) initial silylated resist profile (b) silylated profile after O_2 RIE dry development

5.0 Physical Models in STORM

This section presents an overview of the physical models in STORM. The presentation moves from optical applications to postexposure bake and silylation.. For more information, see the references listed in the appendix.

5.1 Optical Image Models and Algorithms - SPLAT

The optical image simulation is carried out by SPLAT version 5.0. This thin-film version of SPLAT allows high NA images to be calculated within the resist layer.

The algorithm is based on Hopkin's approach as extended by Michael Yeung to include thin-film effects in the pupil function. SPLAT version 5.0 also allows aberrations to be specified in Zernike polynomials or wave front maps. Modified illuminations in the form of quadrupole, annular or illumination maps can be specified. Phase shift masks and inlens filtering are also included.

The program is capable of simulating the effects of lens aberrations, apodization, spatial filtering, focus and magnification effects for high NA, and modified illumination, and the five primary lens aberrations: coma, astigmatism, distortion, spherical aberration, and curvature or defocus. Apodization schemes, such as the Hitachi spatial filter, can be added to the illumination system. Annular, offaxis and quadrupole illumination sources can be also be simulated. As mentioned before, the latest version of SPLAT (version 5.0) which comes with this release is also capable of modelling thin-film interference effects.

Here are a few of the more commonly used SPLAT commands from the SPLAT user guide:

[STATEMENT] 1 *printlevel*

STATEMENT 1 sets the level of diagnostic output generated by the program. PRINTLEVEL=1 produces no diagnostic output, while PRINTLEVEL=2 causes the program to echo the input lines to the output. PRINTLEVEL=3, on the other hand, is primarily for interactive/diagnostic use and causes the program to report when statement execution is completed by displaying the input parameters. The default value of PRINTLEVEL is 1.

[STATEMENT] 2 *wavelength*

This statement sets the wavelength, in micrometers, of the light used to illuminate the mask. Currently, the program is set up to accept only a single wavelength. The default is WAVELENGTH = 0.436 μm.

[STATEMENT] 3 *numerical.aperture*

The imaging system is projection-type, with an imaging lens numerical aperture equal to NUMERICAL.APERTURE. Default NUMERICAL.APERTURE is 0.28.

[STATEMENT] 4 *defocus[mode]*

The image can be calculated at a plane other than the plane of best focus. The distance from the plane of best focus, DEFOCUS, is measured in micrometers and defaults to 0.0 Mm. Positive DEFOCUS is defined as being below the gaussian plane, while negative DEFOCUS is above it.MODE is an integer flag used to specify the type of defocus. MODE = 1 specifies that true defocus ($\sqrt{1-\rho^2}$) will be used and is the default mode. MODE = 0 specifies that approximate defocus ($1-\rho^2/2$) will be used.

[STATEMENT] 5 *sigma [sigma_in]*

STATEMENT 5 sets the partial coherence factor, SIGMA, of the imaging system. Only values of partial coherence that lie between 0.0 (full coherence) and 1.0 (partial coherence) are accepted by the program. SIGMA defaults to 0.7, a value common to most projection printers. SIGMA_IN is used for annular illumination schemes. It indicates the radius of the illumination cone which will be blocked out. The actual illumination occurs only in the annulus from SIGMA_IN to SIGMA. SIGMA_IN defaults to 0.0.

[STATEMENT] 6 *xlength ylength [transmittance [scale]]*

The working area is the size of the mask which is to be imaged and is specified by XLENGTH and YLENGTH in micrometers. This specified area is actually only the first quadrant in Cartesian coordinates. The total/unfolded area is bounded by the coordinates (-XLENGTH,-YLENGTH), (- XLENGTH,YLENGTH), (XLENGTH,YLENGTH), (XLENGTH,-YLENGTH), and a periodic extension in both the X and Y directions is assumed. The optional TRANSMITTANCE is the initial transmittance of the mask (usually either 1 for transparent or 0 for opaque). The image calculation time is approximately proportional to the square of the imaged area, and to avoid long computation times, field sizes with total areas greater than 16 micrometers squared should be avoided. One way to do this is to take advantage of symmetry - see STATEMENT 7 for details. The default for TRANSMITTANCE is 0, while XLENGTH and YLENGTH both default to 2.0 micrometers. SCALE is a positive real number that can be used to scale the mask. This scale factor will also apply to any STATEMENTs 7, 8, 27, and 28 that come after a STATEMENT 6.

[STATEMENT] 7 *xcoord ycoord xlen ylen transmittance [phase]*

This statement is used to add a rectangular feature to the mask. The rectangle specified is mirrored across the x and y axes. Rectangles may overlap other rectangles - it is the user's responsibility to make sure no part of the mask has transmittance greater than 1 or less than 0.

XCOORD = x coordinate of lower left corner of rectangle

YCOORD = y coordinate of lower left corner of rectangle

XLEN = length of rectangle in x direction

YLEN = length of rectangle in y direction

TRANSMITTANCE= transmittance of the rectangle relative to the current transmittance of the mask where it is to be placed.

PHASE = phase angle (normally 0 degrees). This option is used for phase shifted masks.

As an example, to specify a 2 µm x 2 µm transparent square in a 5 µm x 5 µm opaque mask, the following statements could be used:

STATEMENT 6: 5 um x 5 um at 0 transmittance;

STATEMENT 7: (2.0,2.0) 2.0 um x 2.0 um at 1 transmittance;

However, symmetry can and should be utilized to reduce the computation time by locating the center of the rectangle at the origin of the coordinate system in the following manner:

STATEMENT 6: 2 um x 2 um at 0 transmittance;

STATEMENT 7: (0.0,0.0) 1.0 um x 1.0 um at 1 transmittance;

In the last two input statements above, a 1 µm x 1 µm transparent square is defined in a 2 µm x 2 µm opaque mask. Because the program automatically makes even periodic extensions in the x and y directions, the region specified by the user is actually only the first quadrant in the cartesian coordinate system; the other three quadrants are the mirror images of the first, reflected across the x and y-axes respectively. Therefore, the 1 µm x 1 µm square defined above is actually only part of a 2 µm x 2 µm square, with the center of symmetry of that larger square located at the origin. In a similar manner, an opaque square on a transparent mask can be defined using the statements below, where the transmittance is 1 for the background, and -1 for the square.

STATEMENT 6: 2 um x 2 um at 1 transmittance;

STATEMENT 7: (0.0,0.0) 1.0 um x 1.0 um at -1 transmittance;

[STATEMENT] 8 *xcoord ycoord xlen ylen transmittance [phase]*; or

[STATEMENT] 8 *x1 y1 x2 y2 x3 y3 transmittance [phase]*;

Add a triangular aperture to the mask. The triangle specified is mirrored across the x and y axes. Triangles may overlap other triangles and rectangles - it is the user's responsibility to make sure no part of the mask has transmittance greater than 1 or less than 0. The triangle can be specified in two ways - as a right-angled triangle defined by the corner (right angle) point, base and height or as a general triangle defined by three points. Again, even periodic extensions in the x and y directions are assumed. Please note that if only six arguments are provided, the program assumes that the triangle being defined is a right- angled triangle.

XCOORD = x coordinate of corner of right-angled triangle

YCOORD = y coordinate of corner of right-angled triangle

XLEN = base length of right-angled triangle (may be negative to flip triangle)

YLEN = height of right-angled triangle (may be negative to flip triangle)

X1 = x coordinate of point defining general triangle

Y1 = y coordinate of point defining general triangle

X2 = x coordinate of point defining general triangle

Y2 = y coordinate of point defining general triangle

X3 = x coordinate of point defining general triangle

Y3 = y coordinate of point defining general triangle

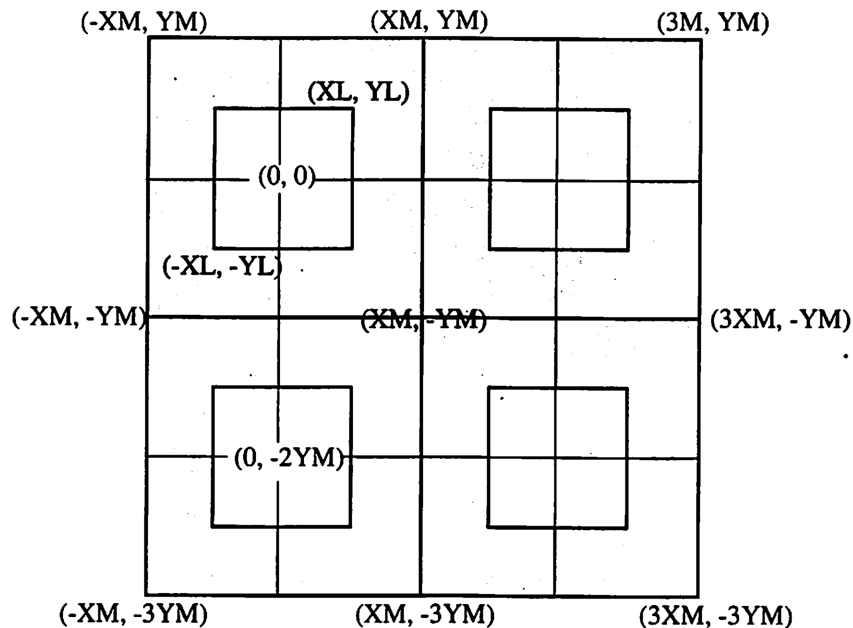
TRANSMITTANCE= transmittance of the triangle relative to the current transmittance of the mask where it is to be placed.

PHASE = phase angle (normally 0 degrees). This option is used for phase shifted masks.

Input Statements:

Statement 6: XM x YM @0;

Statement 7: (0,0) (XL,YL) @1;



[STATEMENT] 9 *nx ny [mode [xllc yllc xlen ylen [difflag]]] ['filename'];*

STATEMENT 9 is used to calculate the transmittance profile of the mask. The transmittance at any point is the sum of the working area(mask) transmittance (see STATEMENT 6) and the transmittances of all rectangles or triangles defined by STATEMENTs 7 and 8 that cover that point. The output file consists of a list of transmittances at points on a grid defined by NX and NY. The default is to calculate for the entire working area, but the user can specify a smaller (or larger) area. MODE defines the type of output obtained from this statement. MODE = 0 produces output to a specified file, MODE = 1 sends a crude contour plot to the terminal, while MODE = 2 does both.

NX = number of divisions along x axis (default = 20)

NY = number of divisions along y axis (default = 20)

MODE = type of output desired

XLLC = x coordinate of lower left corner of rectangle to be plotted

YLLC = y coordinate of lower left corner of rectangle to be plotted

XLEN = length of rectangle in x direction

YLEN = length of rectangle in y direction

DIFFLAG = 1 to limit spatial frequencies (normally not used)

FILENAME= name of file into which to store the calculated intensities.

[STATEMENT] 10 *[mode [force]] ['filename']*;

STATEMENT 10 orders the program to calculate the transmission cross-coefficients (TCCs) as well as the Fourier coefficients of the image intensity profile. This statement can take a long time to execute. MODE = 1 stores the TCCs in *binary* form in the file FILENAME. FORCE is an integer flag which forces the program to choose which of the 3 integration routines should be used for TCC calculation. FORCE = 0 is the default, FORCE = 1 uses a 1-dimensional integration routine, while FORCE = 2 uses a 2-dimensional integration scheme. When aberrations other than approximate defocus are used or when magnification is set, FORCE = 2 is used automatically.

[STATEMENT] 11 *[xllc yllc xlen ylen [nx ny]] ['filename']*;

This statement calculates the image intensity within a rectangle specified by XLLC, YLLC, XLEN, YLEN. The intensities are calculated at each point of a rectilinear NX by NY equally spaced grid within that rectangle. (Note: Maximum NX*NY is 10000) This output file may be used with a 3-dimensional plotting package to provide either a 3- dimensional intensity profile or an intensity contour plot. The parameters are:

XLLC = x coordinate of lower left corner of rectangle to be plotted

YLLC = y coordinate of lower left corner of rectangle to be plotted

XLEN = length of rectangle in x direction

YLEN = length of rectangle in y direction

NX = number of grid-points in the x direction (default is 50)

NY = number of grid-points in the y direction (default is 50)

FILENAME= name of file into which to store the calculated intensities.

[STATEMENT] 12 *'filename'*

Save the Fourier coefficients that describe mask transmittance and image intensity. This input line will produce a relatively large (approx. 30 kbytes) binary output file, which contains the Fourier coefficients as well as the imaging system parameters - numerical aperture, wavelength, coherence factor, mask size. The coefficients can be reloaded with STATEMENT 13 to generate more plot files of the same mask pattern.

[STATEMENT] 13 *'filename'*

STATEMENT 13 is used to load the Fourier mask and image coefficients previously saved with STATEMENT 12. Therefore, for a given set of imaging system parameters (N.A., wavelength, sigma, mask size and pattern), the intensity profile need only be calculated once with STATEMENT 10. STATEMENT 12 saves the data computed by STATEMENT 10 for later use, and STATEMENT 13 reloads this data. Note that the TCCs saved via STATEMENT 10 can be used for any mask pattern, as long as the field size remains con-

stant. On the other hand, STATEMENT 12-13 saves the Fourier coefficients only, so these can be used only for one particular mask pattern.

[STATEMENT] 14 *xi yi xf yf [npts [mode]] ['filename'];*

Calculate the image intensity profile along the line joining points (XI,YI) and (XF,YF). The number of points along that profile and is optionally specified by NPTS, which defaults to 50. The intensity profile is output in the same format as a SAMPLE f77punch7 file. The 'x' values in the file represent the distance along the line from the point (XI,YI), while the 'y' values represent the light intensity normalized to 1.00. Again, MODE is an integer flag, normally 0, used to specify the format of the intensity profile. MODE = 1 outputs the intensities with 5 decimal spaces (as compared to 3 with MODE = 0). This option is particularly useful for analysis of small patterns such as defects, where the intensity is very low.

XI = x coordinate of initial plot point

YI = y coordinate of initial plot point

XF = x coordinate of final plot point

YF = y coordinate of final plot point

NPTS = number of points (default is 50, maximum is 500)

MODE = accuracy flag (defaults to 0)

[STATEMENT] 30 *spot_radius Jx Jy*

STATEMENT 30 allows entry of a single illumination spot. The SPOT_RADIUS is the radius of the illumination spot while (Jx,Jy) indicate its coordinates in the entrance. pupil of the system. The radius of the entrance pupil is normalized to 1. Multiple illumination spots are specified by using up to 10 of these statements. For example, the following commands define a quadrupole illumination scheme for a system with a partial coherence of 0.695. The system partial coherence is computed automatically as the smallest sigma which will overlap all illumination spots.

STATEMENT 30: Spot_radius = 0.2 at (0.35, 0.35);

STATEMENT 30: Spot_radius = 0.2 at (-0.35, 0.35);

STATEMENT 30: Spot_radius = 0.2 at (0.35,-0.35);

STATEMENT 30: Spot_radius = 0.2 at (-0.35,-0.35);

[STATEMENT] 31 *magnification [mode]*

This statement is used to include magnification effects in the calculation of the aerial image. MAGNIFICATION (or more precisely demagnetization) is defined as the object height divided by the image height. MODE = 0, the default mode, specifies that the mask image will be calculated using the mask dimensions at the mask plane. MODE = 1 specifies that the mask image will be calculated using the mask dimensions scaled down by MAGNIFICATION. This statement must be called prior to STATEMENT 6.

[STATEMENT] 32 *[grid_pts [symmetry]]*

This statement turns on the use of the table lookup routines when calculating the TCCs. Instead of recalculating the pupil function every time, the values are stored in a table and subsequently looked up. The main use of this feature is to speed up the thin-film calculations (STATEMENT 35) and it does not provide any speedup for systems with only few aberrations. The number of columns and rows of the lookup table is initialized with dimension *grid_pts* X *grid_pts*. A good number of grid points is 50 for the thin film cases--the results differ by less than 1% from those when not using the table. The maximum number of grid points is 400 and the default is 50. The *symmetry* parameter refers to the use of symmetry in the calculation of the TCCs (STATEMENT 10) which normally reduces the computation time. When *symmetry* = 0, symmetry in the TCC calculation is turned off. This will speed up the simulation time when the mask area is very small since the determination of the symmetry dominates the simulation time. Explicitly disabling the symmetry is only permitted in conjunction with STATEMENT 35. By default *symmetry* = 1 which is the state of normal operation.

[STATEMENT] 35 *resist_layer 'thin-film_data_file'*

Statement 35 allows the image to be calculated within the photoresist. The resist is split up into many thin layers as specified in the *'thin-film_data_file'*. The format of the thin-film input file is given below. The correct number of parameters must be listed on each line and any number of spaces (but no tabs) may be used to separate them.

Thin-film Data File Input Format

substrate_n subsrtate_k medium_n medium_k wavelength

resist_n A B C dose thickness layers

layer1_n layer1_k thickness

layer2_n layer2_k thickness

...

layer12_n layer12_k thickness

The first four parameters are the real and imaginary parts of refractive index of the substrate and medium (Air) respectively. The fifth parameter is the wavelength in the initial medium. The next line specifies the resist properties: the real part of the index of refraction; the resist A, B, C parameters, used to calculate the imaginary part of the index of refraction; dose; thickness; and number of layers. Any lines following the resist parameters specify the real and imaginary parts of the index of refraction of layers under the photoresist and their thicknesses. Up to 12 layers may be specified.

Thin-film Utilities

The following UNIX scripts and or C programs have been created:

run.layers - a unix script to run many thin-film interference simulations using a single input file

Usage: *run.layers splat_input_file start_layer end_layer*

The script searches for the word 'RESIST_LAYER' and replaces it with the current resist layer and then calls SPLAT. At the end of the simulation there will be end_layer 1D intensity files in your current directory. Since this script calls SPLAT, it must be accessible from your current directory.

merge.layers - a unix script used to merge the 1D intensity files created using run.layers into a 2D intensity contour file

Usage: *merge.layers filename_RESIST_LAYER.plot start_layer end_layer*

merge.contours - a unix script used to merge the 2D intensity contour files created using run.layer into 3D intensity file for input in SAMPLE-3D

Usage: *merge.layer filename_RESIST_LAYER.ctr start_layer end_layer*

For an illustration of these scripts please refer to the tutorial on Lithography Simulation in section 3.1 of this document.

5.2 Postexposure bake, Reaction and Diffusion - BAKE

The BAKE program coverts the aerial image and/or the cumulative energy deposited per unit volume to acid sites concentration under appropriate process effects. When an initial aerial image is specified the effect of acid diffusion during the exposure can be calculated.

It is common in resist models to describe the exposure by converting an exposure dose to an initial acid concentration through Dill's ABC parameters. The PEB both diffuses the acid and drives the reaction to alter the solubility of the film. Dissolution models then predict development as a function of extent of reaction in order to arrive at a final resist profile.

The PEB modeling is based on the chemical and physical mechanisms that govern the latent image formation and takes the following form:

$$\frac{\partial A}{\partial t} = k_r(1-A)H \quad (1)$$

$$\frac{\partial H}{\partial t} = -k_l HB + \nabla(D\nabla H) \quad (2)$$

$$\frac{\partial B}{\partial t} = -k_l HB \quad (3)$$

$$\frac{\partial F}{\partial t} = k_r(1-A)H - k_x F \quad (4)$$

$$D = D_0 \exp\left(\frac{\omega F}{1+\upsilon F}\right) \quad (5)$$

Eq. 1 describes the deprotection (A) rate during the thermally induced cleavage of the normalized protecting groups (1-A) by the photogenerated acid (H). Eq. 2 tracks changes in the acid concentration due to free volume (F) enhanced diffusion (Eq. 5) and acid loss from base neutralization. Eq. 3 and 4 track the base concentration and free volume generation/elimination respectively. In the absence of diffusion, the above equations yield the following analytical solution for the extent of deprotection as a function of exposure dose and time.

$$A(t) = 1 - \exp(-k_r Ht) \quad (6)$$

$$H(t) = C_1 \tanh(C_1 k_l t - C_2) + C_1 \quad (7)$$

$$B(t) = C_1 \tanh(C_1 k_l t - C_2) - C_1 \quad (8)$$

$$C_1 = \frac{H_0 - B_0}{2}$$

$$C_2 = \tanh^{-1}\left(\frac{H_0 + B_0}{B_0 - H_0}\right)$$

This simplification allows for reaction rate and acid loss parameters to be extracted from open frame exposure experiments to within a few percent, provided that the initial acid (H_0) and base (B_0) concentrations are known.

5.3 Resist Silylation - SILY2D

The silylation model implemented in STORM is described by the following set of nonlinear differential equations:

$$\frac{\partial S}{\partial t} = -k_{ads}k_r SH + \nabla(D\nabla S)$$

$$\frac{\partial H}{\partial t} = -k_{ads}k_r SH$$

$$\frac{\partial R}{\partial t} = k_{ads}k_r SH$$

$$\frac{\partial}{\partial t}Vol = \beta k_{ads}k_r SH$$

$$D = D_0 \exp\left(\frac{\omega R}{1+R} - \gamma C\right)$$

$$k_{ads} = \left(1 - \exp\left(-\alpha\frac{S}{t_r}\right)\right)$$

$$k_r = A\exp\left[-\frac{(Ea_1 + \sigma_n)}{RT}\right]$$

where S is the concentration of the silylating agent, H is the concentration of bonding sites, R is the concentration of reacted sites, Vol is the volume of the resist film. k_{ads} is the adsorption probability. Stress dependence is introduced through the reaction rate $k_r = \text{Aexp}(-(\sigma + E_a)/RT)$, where σ_n is the resultant normal stress as calculated from the induced surface tractions and body forces in the film.The nonlinear diffusion model captures the sharp boundary experimentally observed between silylated and unsilylated areas and near linear uptake with processing time. C is the crosslinking concentration which inhibits the diffusivity of the silylating agent.

5.4 O_2 Reactive Ion Etching

The following set of equations describe the O_2 RIE dry development model:

$$\frac{\partial O}{\partial t} = -k_{ox}OS - k_{th}OC + \nabla(D\nabla O)$$

$$\frac{\partial S}{\partial t} = -k_{ox}OS - Y_S k_{ion}IS$$

$$\frac{\partial B}{\partial t} = k_{ox}OS - Y_B k_{ion}IB$$

$$\frac{\partial C}{\partial t} = -k_{th}OC - Y_{OC}k_{ion}IOC$$

$$\frac{\partial P}{\partial t} = k_{th}OC + Y_{OC}k_{ion}IOC$$

$$D = D_0 \exp\left(\frac{\omega P}{1 + \upsilon P}\right)$$

where k_{ox} is the oxidation rate constant, k_{ads} is the adsorption rate constant, k_{ther} is the thermal desorption rate constant, Y_{CO}, Y_S and Y_B are the yield of CO, S and B molecules desorped or sputtered per ion incident, and k_{ion} is proportional to the ion bombardment energy. The following describes the assumptions that let to the above model. During the dry development step, O atoms (activated neutrals) diffuse to the resist surface to react with the carbon (C) and silicon (S) while energetic ions (I) bombard the exposed surface. The reaction of the O with S result in a SiO_x etch barrier (B). The adsorption O by C surface and subsequent reaction results in isotropic etching (ashing) of the resist. The ion enhances the etching rate at the surface by increasing the desorption rate of the etched products. The rate-limiting step is assumed to be desorption of CO gas. Energetic ions can also sputter the silicon before it forms a barrier or can sputter the barrier. The absence of resist material after etching means the fresh O atoms can be quickly transported to the new exposed surface. We consider this as an enhancement of the local diffusivity at the etched sites.