

MOTIVATION

- Understanding of material Line-Edge Roughness (LER) origins
- Processing effects on LER, especially development
- Understanding of photopolymer dissolution
- Essential need for simulation in micro-scales

IN THIS WORK

Critical Ionization Model [1,2] implemented in 2-dimensions and used to predict :

- 1) dissolution rate
- 2) roughness of flat surface and patterned surface
 - a) various polymerization lengths,
 - b) with and without molecular weight dispersivity and
 - c) various critical ionization fractions.

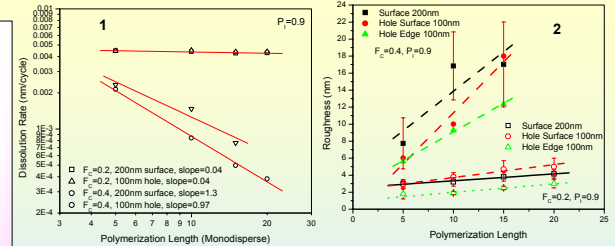
REFERENCES

- [1]. W. Flanagan, V. K. Singh, and C. G. Willson, "Molecular Model of Phenolic Polymer Dissolution in Photolithography", J. Pol. Sci. Part B, 37, 2103 (1999).
- [2]. D. Burns, G. M. Schmid, P. C. Tsiartas, and C. G. Willson, "Advancements to the Critical Ionization Dissolution Model", J. Vac. Sci. Technol. B, 20(2), 537 (2002).
- [3]. G. P. Patsis, N. Glezos, and E. Gogolides, "Monte Carlo simulation of gel formation and surface and line-edge roughness in negative tone chemically amplified resists", J. Vac. Sci. Technol. B, 21, 254 (2003).

Figure 7. RESULTS 1: STUDY OF MOLECULAR WEIGHT – EFFECT OF MONODISPERSE SAMPLE

SIMULATION CONDITIONS

- Material: Homopolymer positive tone photoresist
- Cell size equal to monomer size ~ 1nm
- Lattice: 2D, width=200nm, height=100nm
- Free volume = 10%
- High exposure: All monomers in simulation domain are deprotected and capable of ionizing by the developer molecules with probability $P_i=0.9$.



Graph 1. Effect of polymerization length L critical ionization fraction F_c and patterning on dissolution rate R.

- Increase of L reduces R and the decrease is steepest for higher F_c .
- R for 200nm flat surface and for 100nm hole is the same for $F_c=0.2$.
- R is faster for flat surface than for hole when F_c increases to 0.4.

Graph 2. Effect of polymerization length L and patterning on surface roughness SR and line width roughness LWR.

- Linear increase of SR with L for both flat and patterned surface
- LWR increases linearly but is less than the corresponding SR.
- Steepest increase of SR and LWR with L for increased F_c .

Figure 1. SIMULATION FLOW

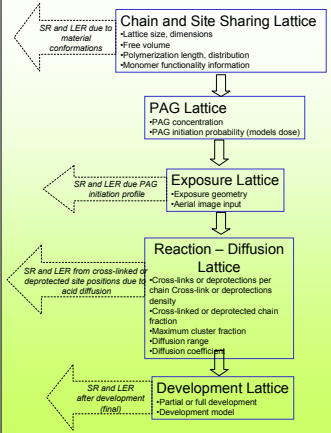


Figure 4. CHAIN INSERTION ALGORITHMS

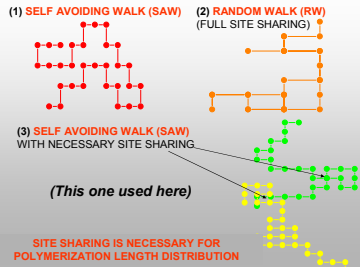
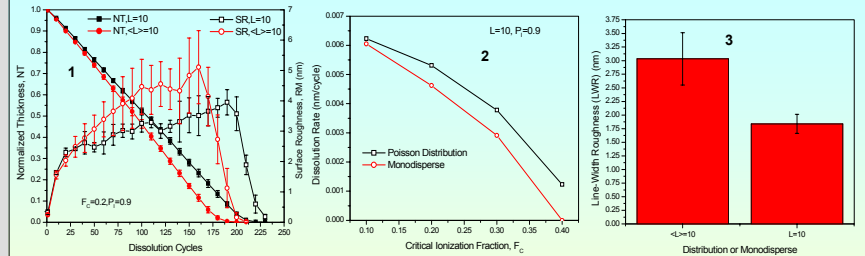


Figure 8. RESULTS 2: STUDY OF POLYDISPERSE SAMPLE WITH M_w FOLLOWING POISSON DISTRIBUTION



Graph 1. Effect of polydispersity (Poisson distribution in polymerization length L) on dissolution rate R for increasing critical ionization fraction, F_c .

- The polydisperse sample, $\langle L \rangle = 10$ shows:
 - higher R
 - higher SR

Graph 2. Effect of polydispersity on surface roughness SR.

- The polydisperse sample shows higher dissolution rate R in all F_c .

Graph 3. Effect of polydispersity on line-width roughness LWR.

- The polydisperse sample shows higher LWR

Figure 2. PHOTOPOLYMER DISSOLUTION MODELS

- Reptation Model (Peppas et al, Macromolecules 27, 5626 (1994))**
 - Polymer swelling during contact with developer
 - Polymer chain reptation (relaxation) towards developer solution
 - No chemical reaction
- Analytic Model (Tu and Quano, IBM J. Res. Dev. 21, 131 (1977))**
 - Developer diffusion equation
 - Polymer dissolution equation
- Percolation Model (Shih and Reiser, Macromolecules 30, 4353 (1997))**
 - Assumes gel layer
 - Developer diffusion through gel layer is the rate limiting step
 - Developer diffusion in gel layer with random walks
- Critical Ionization Model (1,2)**
 - Dissolution criterion is the critical ionization fraction, F_c
 - Layer-by-layer dissolution
 - Chain ionization is the rate limiting step

Figure 5. DEFINITION OF SR AND LWR

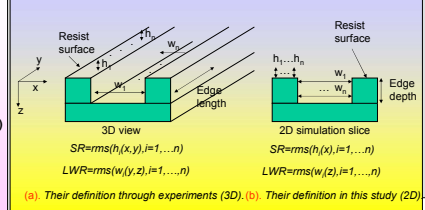


Figure 3. DISSOLUTION WITH THE CRITICAL IONIZATION MODEL OF A POSITIVE TONE RESIST

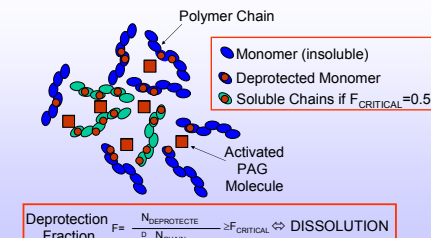
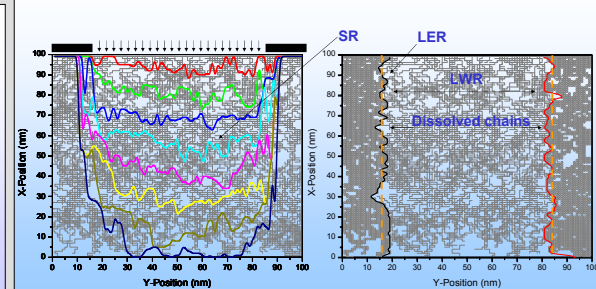


Figure 6. EXAMPLE OF DISSOLUTION WITH CRITICAL IONIZATION MODEL



CONCLUSIONS

Simulation showed:

- Dissolution rate R: a) decreases with polymerization length L, b) decreases with patterning, c) increases with polydispersity
- Surface roughness SR: a) increases linearly with L, b) increases with patterning only in easily dissolved polymers (low F_c). The reverse is true for dissolvable polymers (high F_c), c) increases with polydispersity
- Line-width roughness LWR: a) Increases linearly with L, b) increases with polydispersity, c) shows lower values than corresponding SR
- Strong effect of critical ionization fraction F_c (polymer model) on R (stronger decrease), SR and LWR (both show steepest increase)
- Agreement with experimental observations
- Simulator able to reproduce the microscopic physics-chemistry

FUTURE WORK → Extension to 3D