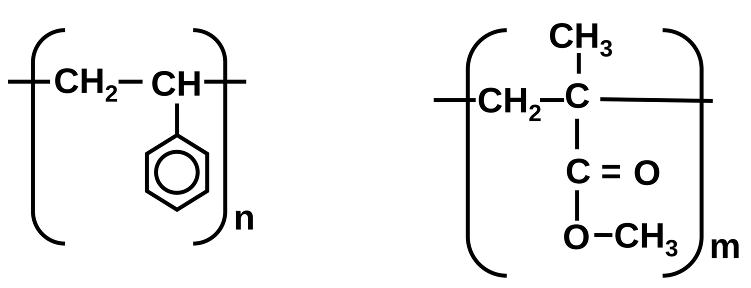
Modeling of block copolymer dry etching for directed self-assembly lithography

Zelalem Belete[a], Eberhard Baer[b], Andreas Erdmann[a b]

[a]Friedrich-Alexander-University of Erlangen-Nuremberg, Chair of Electron Devices, Cauerstrasse 6, 91058 Erlangen, Germany
[b]Fraunhofer Institute for Integrated Systems and Device Technology, Schottkystrasse 10, 91058 Erlangen, Germany

1. Introduction

- This paper presents a model for etching of Directed Self-Assembly (DSA) of block copolymer, polystyrene-block-poly (methyl methacrylate) (PS-*b*-PMMA), using Ar and Ar/O_2 plasma chemistries.
- The etch process to transfer the self-assembled "fingerprint" DSA patterns to the underlying layer is still a challenge.
- A simple generic surface model based on surface site balance is implemented .
- Etching of selected lamella and contact-hole shrink features by Ar/O_2 plasma chemistry was simulated using fitted parameters of the model.
- Application of the model for profile simulation of contact-hole shrink pattern is demonstrated.



Polystyrene **PMMA**

2. Modeling

- Etching in Ar plasma chemistry
  - Only physical sputtering by Ar^+ ions is considered
  - The effect of etching by VUV radiation is neglected because its effect is small at low temperatures..
  - Oxygen flux is zero.
- Etching in Ar/O_2 plasma chemistry
  - Physical sputtering etching by Ar^+ ions and ion-enhanced chemical etching by Ar^+ ions and O_2 neutrals are included in the model.
  - Chemical etching effect is neglected due to the small temperature in the plasma.
  - Physical sputtering is assumed as the main process step before cross-linking and the effect of ion-enhanced chemical etching on the formation of cross-linked layer is neglected.

$$\frac{d\theta_p}{dt} = \frac{1}{\sigma}(\Gamma_i Y_{cl}(1-\theta_p-\theta_o) - \Gamma_i Y_p(1-\theta_{po})\theta_p - \Gamma_i Y_{po}\theta_{po}\theta_p)$$

$$\frac{d\theta_o}{dt} = \frac{1}{\sigma}(\Gamma_o Y_o(1-\theta_p-\theta_o) - \Gamma_i Y_o\theta_o)$$

$$\frac{d\theta_{po}}{dt} = \frac{1}{\sigma}(\Gamma_o S_{po}(1-\theta_{po})\theta_p - \Gamma_i Y_o\theta_{po}\theta_p)$$

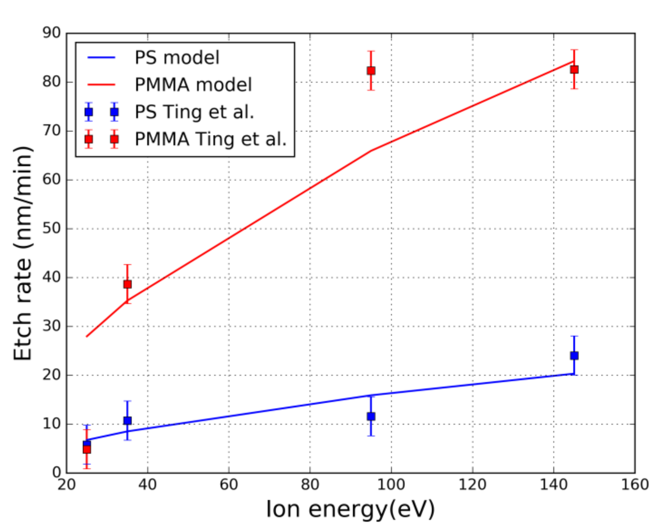
$$ER = \frac{1}{\rho}(\Gamma_i Y_s(1-\theta_p-\theta_o)+\Gamma_i Y_o\theta_o+\Gamma_i Y_p(1-\theta_{po})\theta_p+\Gamma_i Y_{po}\theta_{po}\theta_p)$$

θ_p	cross-linked layer coverage on pristine PMMA/PS
θ_o	oxygen layer coverage on pristine PMMA/PS
θ_{po}	oxygen coverage on cross-linked layer
Y_s	sputtering yield of pristine PMMA/PS
Y_p	sputtering yield of the cross-linked layer
Y_o	Ion-enhanced chemical etching yield of pristine PMMA/PS
Y_{po}	ion-enhanced chemical etching yield of the cross-linked layer

3. Results

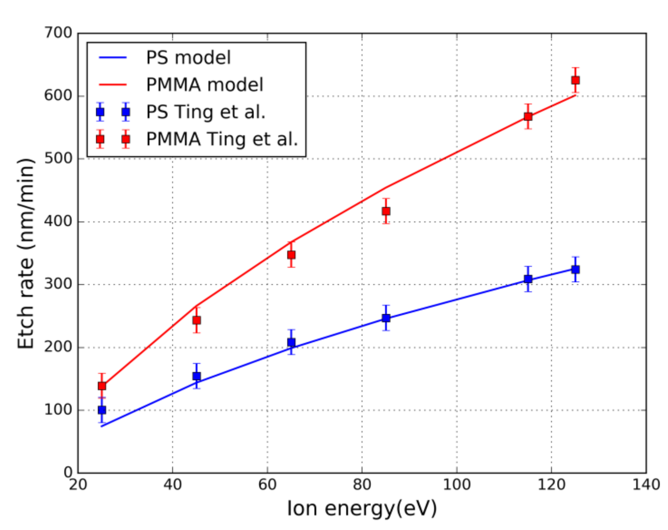
3.1. Etching in Ar and Ar/O_2 chemistry

Ar plasma chemistry



root-mean-square error (RMSE), PS:2.65, PMMA:12.96

Ar/O_2 plasma chemistry



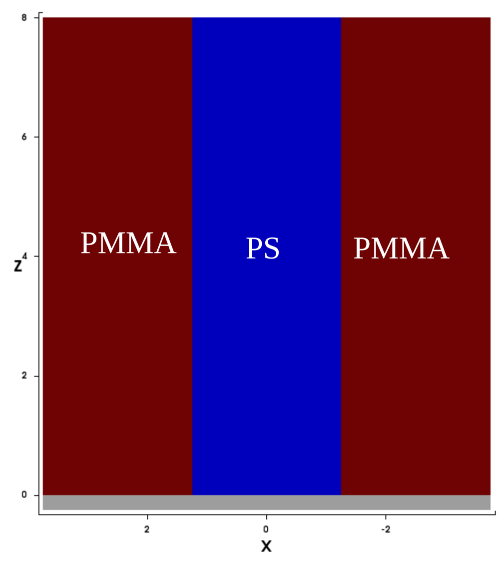
root-mean-square error (RMSE), PS:12.70, PMMA: 21.80

➢ Model calibrated for homopolymer etch rate with Literature data from Ting et. al[1]

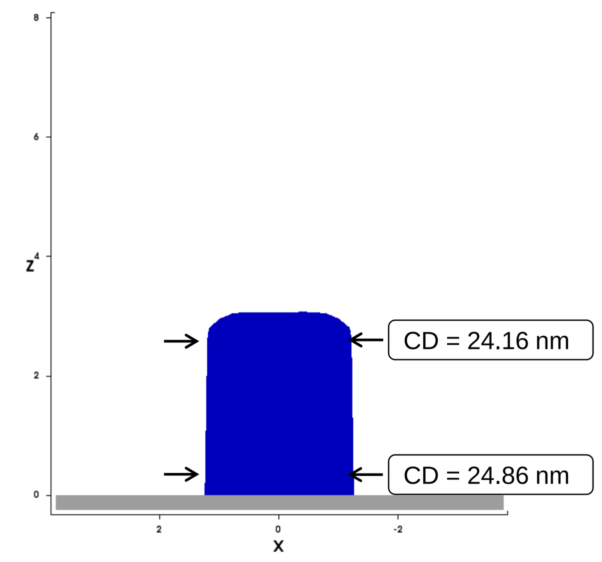
3.2. Profile simulations

- Angular dependence of sputter etching yield by Ar^+ ions is included in the model [2]
- Ion-enhanced chemical etching is assumed to have no angular dependence.
- Monte-Carlo based profile simulation for surface update performed with level set using the Vienna topography simulator ViennaTS [3]

Etching of lamella by Ar/O_2



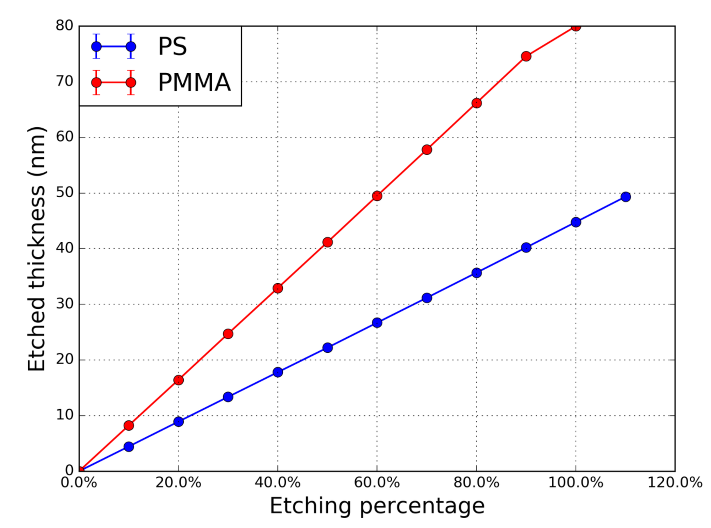
Initial geometry (scale = 0.1)
CD for PS (red)
and PMMA (blue) = 25 nm



Ar/O_2 plasma etched profile (scale = 0.1)

<u>Literature data</u> [1]
- Final PS CD = 24.24 nm
- Etch selectivity = 2.04

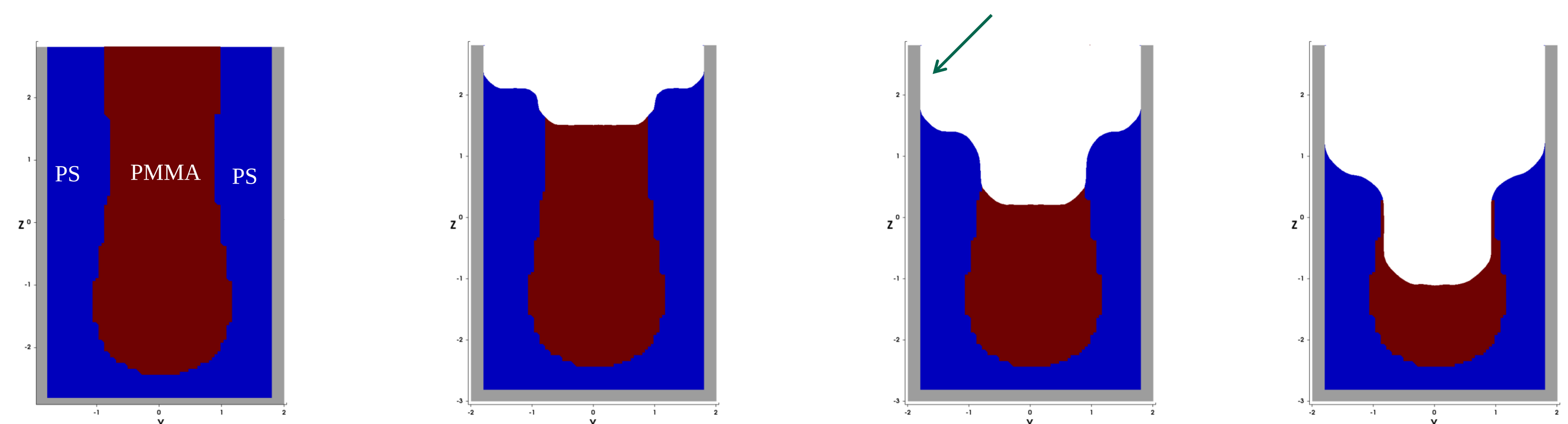
<u>Simulation result</u>
- Final PS CD
  - 24.86 nm at z = 3.41 nm
  - 24.16 nm at z = 25.72 nm
- Etch selectivity = 1.85



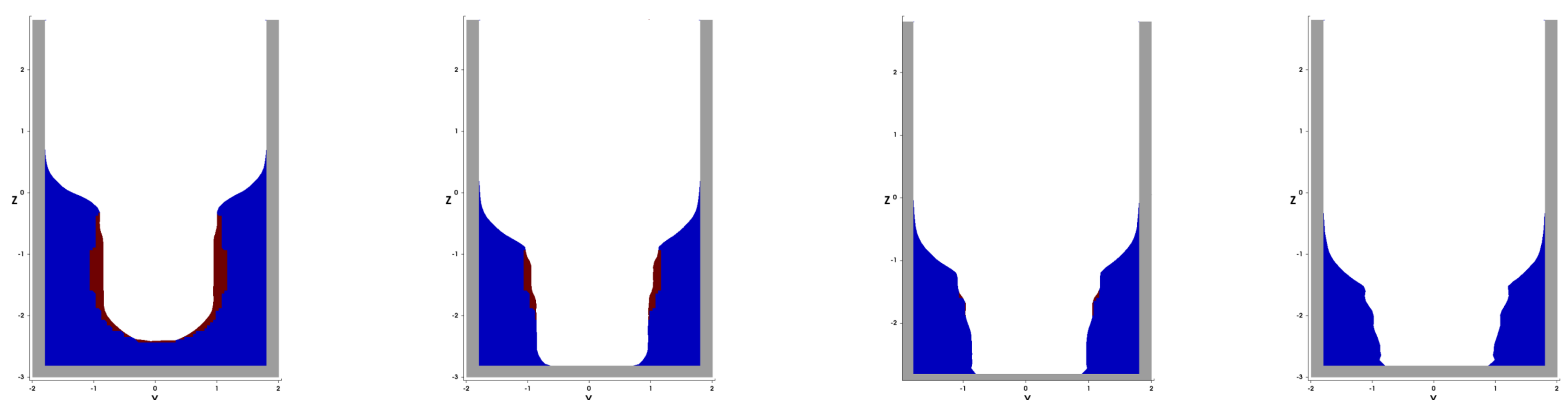
Etching percentage - the etch time normalized to the time required to etch the initial PMMA thickness completely at normal angle of incidence.
- Initial PMMA thickness = 80 nm

Etching of contact-hole shrink by Ar/O_2

photoresist-guiding pattern
etch rate = 0.0



Initial geometry (scale = 0.1) | 20% etch time | 40% etch time | 60% etch time



80% etch time | 100% etch time | 110% etch time | 120% etch time

Etch profiles (cross section through the center) at time steps for 115 eV ion energy, percentage etch time is the etch time normalized with time until PS is etched through in the center (52.93 nm PMMA + 5.6 nm PS). The initial structure generated by self-assembly of block copolymers was simulated with Dr.LiTHO[4].

4. Conclusions

- The etch rates of PS and PMMA homopolymers can be approximated by a simple model.
- Profile simulations using model parameters extracted by fitting the model with homopolymer etch rates can give results which well agree with literature data.
- The remaining PS thickness and CD loss can be investigated with the model for profile simulations.
- Further investigations with more experimental data will provide a better understanding of VUV etching, chemical etching and cross-linking effects.

[1] Ting, Y.-H., Park, S.-M., Liu, C.-C., Liu, X., Himpsel, F. J., Nealey, P. F. and Wendt, A. E., J. Vac. Sci. Technol. B 26(5), 1684 (2008).
[2] Mouchtouris, S. and Kokkoris, G., , Plasma Process. Polym. 14 (2017)
[3] Ertl, O. and Selberherr S., Computational Physics Communications, 180 (2009) pp1242–50
[4] Fuehner, T., Erdmann, A., Farkas, R., Tollkuehn, B., and Kokai, G., Proc. of SPIE 6520 (2007)

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