Comparison of coarse-grained and reduced models of directed self-assembly of block copolymers for application for contact shrink process

Przemyslaw Michalak¹, Ulrich Welling², Juan Carlos Orozco Rey³, Mohamed Ismail¹,²,³, Tim Fühner⁴, Marcus Müller⁵, Andreas Erdmann¹
¹Fraunhofer Institute for Integrated Systems and Device Technology, Schottkystrasse 10, 91058 Erlangen, Germany
²Institut für Theoretische Physik, Georg-August-Universität, 37077 Göttingen, Germany
³Friedrich-Alexander-Universität Erlangen-Nürnberg, MAOT

Introduction

• Directed self-assembly (DSA) models applied for double contact shrink process for several ideal guiding patterns (GP)
• Reduced models: Ohta-Kawasaki (OK) and Interface Hamiltonian (IH) [1,2]
• Coarse-grained model: Single Chain in Mean Filed (SCMF) [3]
• IH characteristics: very fast, ideal for designing guiding pattern shapes, only strong segregation limit
• OK characteristics: fast continuum model, dimensionless – all sizes are related to polymer domain spacing $L_0$

\[
\frac{\partial \varphi}{\partial t} = \nabla^2 (\varphi \nabla^2 \varphi - \varphi + \varphi^3) - \alpha(\varphi - \bar{\varphi}) + \psi^2 H_{wall} - \nabla^2 \psi
\]

\[
\begin{array}{|c|c|c|}
\hline
\text{\varphi} & \text{Order parameter, difference between densities of copolymer A and B} \\
\text{\epsilon} & \text{Related to the width of the A-B interface} \\
\text{\alpha} & \text{Long-range interactions, affects domain spacing of copolymers} \\
\text{\bar{\varphi}} & \text{Mean value of the order parameter, \bar{\varphi} \approx (1/\epsilon)} \\
\psi & \text{Volume fraction of phase A in a copolymer melt} \\
H_{wall} & \text{Wall potential, constant non-zero value at borders only, zero elsewhere} \\
\hline
\end{array}
\]

• SCMF characteristics: computationally expensive, chain description on molecular level, chain interactions through molecular field

Modeling strategy

• Target structure definition
  • double contact
  • cylinder CD 20 nm
  • cylinder-to-cylinder distance 37.5 nm
• Copolymer model definition
  • incompatibility parameter $\gamma N = 25$
  • volume fraction 0.31
• CD / cylinder-to-cylinder ratio $0.533 (20/37.5)$ in bulk
• Determining parameters for the OK model (bulk 2D simulations)
  • $\epsilon = 1$
  • $\alpha = 0.015$

• Determining optimum shape of double contact GP (2D IH)
  • constant aspect ratio 1.5

• Modeling directed self-assembly of double contact shrink
  • OK
  • SCMF

Evaluation method and criteria

• Impact of size of optimized GP on:
  • number of cylinders
  • cylinder CD values
  • CD / cylinder-to-cylinder ratio
  • placement error (PE)
• Optimum size of GP in terms of
  • PE value equal to 0
  • CD / cylinder-to-cylinder ratio equal to 0.533

Results (OK & SCMF)

Number of cylinders vs. GP size

CD vs. GP size & CD / cylinder-to-cylinder vs. GP size

PE vs. GP size

Conclusions

• OK & SCMF results in acceptable accordance
• Differences between both models due to:
  • limited scaling accuracy between $\gamma N$ and $\alpha$ parameters
  • different model behavior in unstable regions
• Optimized length of the double contact GP 3.2–3.3 $L_0$
• Results match real dimensions for all block copolymers with given $\gamma N$, volume fraction and CD / cylinder-to-cylinder ratio


Fraunhofer IISB

Lithography Simulation