# Modeling of two-photon lithography including oxygen diffusion using a generalized compact model

Yuan Yu[a], Valeriia Sedova[a], Christian Schwemmer[a], Jonas Wiedenmann[b], Andreas Erdmann[a]

yuan.yu@iisb.fraunhofer.de

[a]Fraunhofer-Institut für Integrierte Systeme und Bauelementetechnologie IISB, Erlangen, Germany
[b]Heidelberg Instruments Mikrotechnik GmbH (HIMT), Würzburg, Germany

## Introduction

- Modeling the realistic two-photon polymerization (TPP)

**Goal**

Extend the functionality and improve the performance of the compact model[1].

## Model description

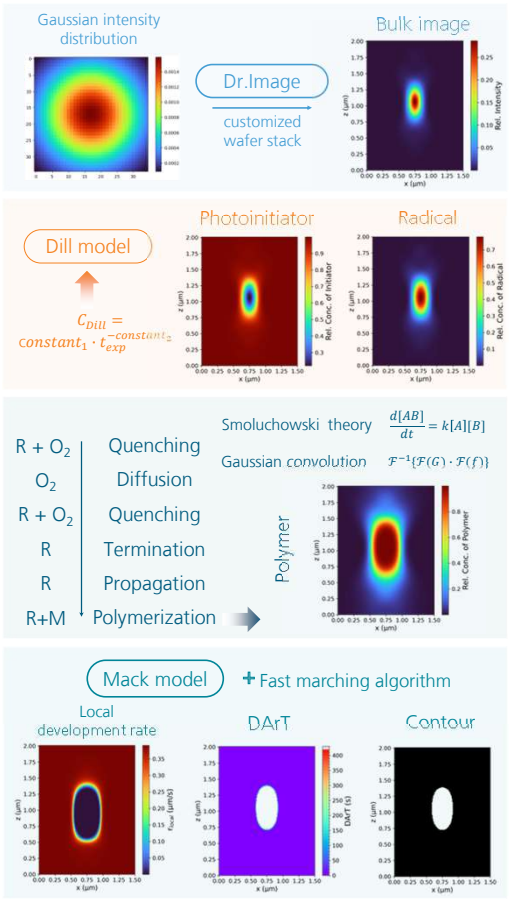


*Figure 1: Four simulation stages of the generalized compact model.*

## Time-dependent Dill model

*Approximation impact of oxygen depletion in exposed areas*

The Dill model for TPP:
$$\frac{\partial[Initiator]}{\partial t} = C_{Dill} \cdot I^2 \cdot [Initiator] \quad (1)$$

The effective dose $D_{eff}$:
$$D_{eff} = C_{Dill} \cdot t_{exp} \cdot I^2 \cdot (R_p t_p) \quad (2)$$

Time-dependent $C_{Dill}$:
$$C_{Dill} = D_{eff} \cdot Area^2 \cdot (R_p t_p) \cdot I_{norm}^{-2} \cdot t_{exp}^{-1} \cdot P_{avg}^{-2} \quad (3)$$

Under identical conditions, $C_{Dill,relative}$ varies with exposure times as:
$$C_{Dill,relative} = constant_1 \cdot t_{exp}^{-constant_2} \quad (4)$$

## Reactions in photoresist

- **Quench** reactive intermediates through oxygen, which inhibits reactions.
- **Diffuse** oxygen between two quenching reactions to capture its impact.
- **Termination** via chain coupling, quenching, and self-trapping.
- **Propagation** through diffusion to mimic chain growth.
- **Polymerization** based on concentrations of reactive sites and monomers.

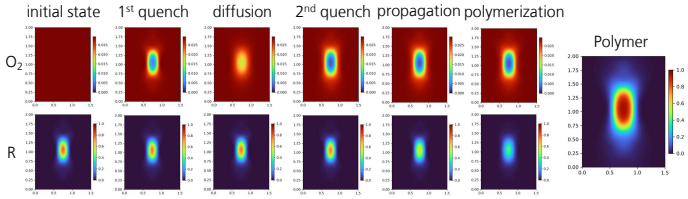


*Figure 2: Simulated cross-sectional profiles of oxygen, radical (R), and the resulting polymer distribution within the photoresist. All axes are in micrometers (µm).*

## Model calibration

- Calibration using a multi-objective genetic optimizer from Dr.LiTHO.

**Calibration results**

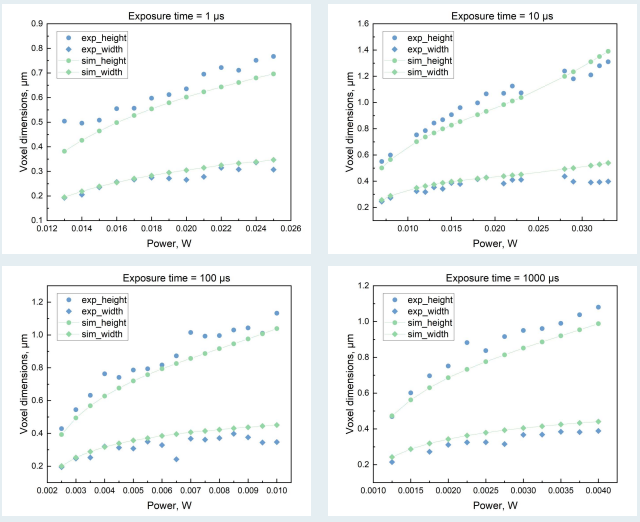


*Figure 3: Voxel dimensions from simulation and experimental measurements[b] plotted against average power at four exposure times at 1 µs, 10 µs, 100 µs, and 1000 µs.*

## Conclusion: Model performance

- Maintains computational efficiency and improves alignment with experimental data across all exposure times.
- Incorporates additional chemical and physical mechanisms.
- Helps to predict outcomes under different setups.

1 Sedova, V., Ogor, F., Rovera, J., Tsilipakos, O., Lemberg, L., Heggarty, K., and Erdmann, A., "Advances in modeling and optimization for two-photon lithography," in [Computational Optics 2024], Smith, D. G. and Erdmann, A., eds., 13023, 1302309, International Society for Optics and Photonics, SPIE (2024).

**This project has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement n° 101091644. UK participants in Horizon Europe Project FABulous are supported by UKRI grant n° 10062385 (MODUS).**