Direct Link Between DUV-Induced a-SiO_2 Compaction and Lens Aberration Drift: From Atomic-Scale Modeling to Field Optical Validation in Photolithography

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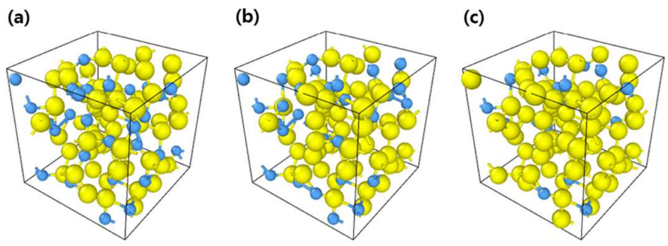
This study presents a comprehensive characterization of the dynamic interplay between atomistic interface evolution in amorphous SiO_2 projection optics and device-scale optical performance drift under deep ultraviolet (DUV, 193nm) exposure. By integrating large-scale molecular dynamics (MD) simulations with machine learning force fields and density functional theory (DFT) calculations, we unveil how DUV-induced local compaction and defect evolution at interfacial regions modulate both refractive index (n) and wavefront aberrations in operational lithography systems. Specifically, our results demonstrate a quantitative correlation between MD-tracked Si-Si bond fraction/density metrics and DFT-calculated optical constants, establishing a structure-property relationship essential for device-level transport and optical characterization.

Fleet-scale, in-field monitoring of photolithography scanners confirms that progression of Y-direction Zernike coma (WFE, Coma-Y) is aligned with simulation-predicted compaction-driven refractive index shifts, cementing the impact of interface-level atomic changes on macroscopic optical device performance. Notably, the transition from elastic to plastic compaction regimes leads to nonlinear escalation in WFE drift slopes, providing actionable thresholds for predictive maintenance and device calibration.

This work bridges atomistic simulation and high-volume manufacturing field data to deliver direct, actionable insights for the characterization and management of light transport, wavefront propagation, and functional reliability in advanced optical devices.



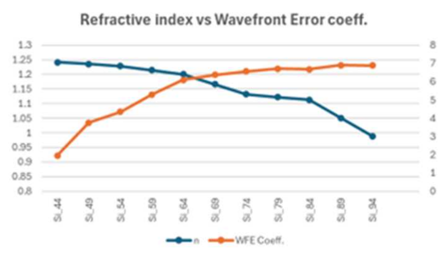


Figure 1. Visualization of amorphous SiO_2 models showing an increasing Si fraction from left to right under DUV radiation [Si:O count ratios - a) 34:68, b) 64:38, c) 84:18].

Figure 2. Refractive index (n) decreases while wavefront error coefficient (WFE) increases with progressive compaction, illustrating the inverse correlation between optical property degradation and structural densification in amorphous SiO_2.