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*Field Guide to Optical Thin Films*, Ronald R. Willey (FG07)
Field Guide to Optical Lithography

The material in this Field Guide to Optical Lithography is a distillation of material I have been putting together for the last 20 years or so. I have been subjecting students in my graduate-level lithography course at the University of Texas at Austin to my disorganized notes for 14 years, and have published some similar material in my first book *Inside PROLITH* and my column in *Microlithography World* called “The Lithography Expert.” However, the challenge here was not in creating the material for the book but rather deciding what material to leave out and how to make what remained as condensed as possible. As people who know me can attest, I am rarely lacking for words and brevity is not my strong suit (I am a lousy poet). I hope, however, that the kind reader will forgive me when one page on a topic of interest does not satisfy—it is an unavoidable consequence of the Field Guide format, and my own limitations as an overly verbose writer.

I thank Jeff Byers, William Howard, and Rob Jones for their help in reviewing the draft manuscript of this Field Guide. My many mistakes kept them quite busy.

This Field Guide is dedicated to my wife Susan and our daughter Sarah, who have taught me that there is indeed something more fun in this world than lithography.

Chris Mack
chris@lithoguru.com
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x

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## Symbol Glossary

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<th>Description</th>
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<tbody>
<tr>
<td>( a )</td>
<td>Dose-dependent curvature of the CD-through-focus curve; molar absorption coefficient; constant in the Mack 4-parameter dissolution rate model</td>
</tr>
<tr>
<td>( A )</td>
<td>Electric field amplitude; bleachable absorption coefficient</td>
</tr>
<tr>
<td>( A_r )</td>
<td>Arrhenius coefficient</td>
</tr>
<tr>
<td>( B )</td>
<td>Magnetic induction, non-bleachable absorption coefficient</td>
</tr>
<tr>
<td>( c )</td>
<td>Speed of light; concentration</td>
</tr>
<tr>
<td>( C )</td>
<td>Photoresist exposure rate constant</td>
</tr>
<tr>
<td>( CD )</td>
<td>Critical dimension</td>
</tr>
<tr>
<td>( d )</td>
<td>Shifter thickness for a phase-shift mask</td>
</tr>
<tr>
<td>( D )</td>
<td>Electric displacement, photoresist thickness; ARC thickness</td>
</tr>
<tr>
<td>( D_H )</td>
<td>Diffusivity of acid in photoresist</td>
</tr>
<tr>
<td>( DOF )</td>
<td>Depth of focus</td>
</tr>
<tr>
<td>( E )</td>
<td>Electric field, incident exposure dose</td>
</tr>
<tr>
<td>( E_a )</td>
<td>Activation energy</td>
</tr>
<tr>
<td>( E_0 )</td>
<td>Dose to clear</td>
</tr>
<tr>
<td>( E_z )</td>
<td>Exposure dose at depth ( z ) in the resist</td>
</tr>
<tr>
<td>( f_x )</td>
<td>Spatial frequency</td>
</tr>
<tr>
<td>( G_0 )</td>
<td>Initial PAG concentration</td>
</tr>
<tr>
<td>( h )</td>
<td>Planck’s constant; normalized acid concentration in a chemically amplified resist</td>
</tr>
<tr>
<td>( H )</td>
<td>Magnetic field; acid concentration in a chemically amplified resist</td>
</tr>
<tr>
<td>( I )</td>
<td>Intensity of light, aerial image</td>
</tr>
<tr>
<td>( J )</td>
<td>Electric current density</td>
</tr>
<tr>
<td>( k )</td>
<td>Propagation constant, wavenumber; chemical reaction rate constant</td>
</tr>
<tr>
<td>( k_1 )</td>
<td>Normalized Rayleigh resolution</td>
</tr>
<tr>
<td>( k_2 )</td>
<td>Normalized Rayleigh depth of focus</td>
</tr>
<tr>
<td>( L_{\text{eff}} )</td>
<td>Effective gate length</td>
</tr>
<tr>
<td>( m )</td>
<td>Magnification; normalized unreacted site concentration in conventional or chemically amplified resists</td>
</tr>
<tr>
<td>( m_{TH} )</td>
<td>Threshold inhibitor concentration</td>
</tr>
<tr>
<td>( M )</td>
<td>Photoactive compound concentration, unreacted site concentration</td>
</tr>
</tbody>
</table>
Symbol Glossary (cont’d)

\( M_0 \)  Initial PAC concentration
\( n \)  Index of refraction; dissolution selectivity parameter; diffraction order number
\( n_j \)  Complex index of refraction of layer \( j \)
\( N_A \)  Avogadro's number
\( NA \)  Numerical aperture
\( NILS \)  Normalized image log-slope
\( OPD \)  Optical path difference
\( p \)  Pitch
\( P \)  Pupil function; photoresist exposure products; a point in \( x-y-z \) space
\( r \)  Photoresist dissolution rate
\( r_{\text{max}} \)  Dissolution rate of fully exposed positive resist
\( r_{\text{min}} \)  Dissolution rate of unexposed positive resist
\( R \)  Resin concentration; resolution; relative pupil radius position; intensity reflectivity; universal gas constant; photoresist dissolution rate
\( S \)  Solvent concentration
\( t \)  Time, exposure time
\( t' \)  Bake time
\( t_m \)  Mask transmittance function
\( T \)  Transmittance; absolute temperature
\( T_m \)  Fourier transform of the mask transmittance function (diffraction pattern amplitude)
\( U \)  Phasor representation of the sinusoidal e-field
\( v \)  Process variable
\( w \)  Slit width, mask feature width, nominal linewidth
\( x \)  Normalized concentration of reacted sites in a chemically amplified resist; horizontal position
\( X \)  Concentration of reacted sites in a chemically amplified resist
\( Z \)  Zernike polynomial coefficient
\( \alpha \)  Maximum angle of diffraction captured by a lens; absorption coefficient
\( \delta \)  Dirac delta function; defocus distance
\( \varepsilon \)  Dielectric constant
\( \theta \)  Angle; polar angle of pupil position; photoresist sidewall angle
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
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<tbody>
<tr>
<td>( \gamma )</td>
<td>Photoresist contrast</td>
</tr>
<tr>
<td>( \kappa_j )</td>
<td>Imaginary portion of complex refractive index</td>
</tr>
<tr>
<td>( \lambda )</td>
<td>Wavelength (in vacuum)</td>
</tr>
<tr>
<td>( \mu )</td>
<td>Magnetic permeability</td>
</tr>
<tr>
<td>( \rho )</td>
<td>Electric charge density</td>
</tr>
<tr>
<td>( \rho_{ij} )</td>
<td>Reflection coefficient between films ( i ) and ( j )</td>
</tr>
<tr>
<td>( \sigma )</td>
<td>Conductivity; partial coherence factor; diffusion length</td>
</tr>
<tr>
<td>( \tau_{ij} )</td>
<td>Transmission coefficient between films ( i ) and ( j )</td>
</tr>
<tr>
<td>( \Phi )</td>
<td>Phase of an electric field; fraction of absorbed photons producing a chemical change (quantum yield)</td>
</tr>
<tr>
<td>( \omega )</td>
<td>Frequency of monochromatic light; photoresist spin coat speed</td>
</tr>
</tbody>
</table>
The lithography process is fundamental to all of these processes is **lithography**, i.e., the formation of three-dimensional (3D) relief images on the substrate for subsequent transfer of the pattern to the substrate.

The word lithography comes from the Greek *lithos*, meaning stones, and *graphia*, meaning to write. It means quite literally writing on stones. In the case of semiconductor lithography, our stones are silicon wafers and our patterns are written with a light-sensitive polymer called **photore sist**. To build the complex structures that make up a transistor and the many wires that connect the millions of transistors of a circuit, lithography and pattern transfer steps are repeated at least 10 times, but more typically are done 20 to 30 times to make one circuit. Each pattern being printed on the wafer is aligned to the previously formed patterns and slowly the conductors, insulators, and selectively doped regions are built up to form the final device.
Optical lithography is a photographic process by which a light-sensitive polymer, called a photoresist, is exposed and developed to form 3D relief images on the substrate. In general, the ideal photoresist image has the exact shape of the designed or intended pattern in the plane of the substrate, with vertical walls through the thickness of the resist. Thus, the final resist pattern is binary: parts of the substrate are covered with resist while other parts are completely uncovered. This binary pattern is needed for pattern transfer since the parts of the substrate covered with resist will be protected from etching, ion implantation, or other pattern transfer mechanism.

The general sequence of steps for a typical optical lithography process is as follows: substrate preparation, photoresist spin coat, prebake, exposure, post-exposure bake, development, and postbake. A resist strip is the final operation in the lithographic process, after the resist pattern has been transferred into the underlying layer via etching or ion implantation. This sequence is generally performed on several tools linked together into a contiguous unit called a lithographic cluster.
Processing: Substrate Preparation

Substrate preparation is intended to improve the adhesion of the photoresist material to the substrate. This is accomplished by one or more of the following processes: substrate cleaning to remove contamination, baking to remove water, and the addition of an adhesion promoter to keep water from coming back. Substrate contamination can take the form of particulates or a film and can be either organic or inorganic. Particulates result in defects in the final resist pattern, whereas film contamination can cause poor adhesion and subsequent loss of linewidth control. One type of contaminant—adsorbed water—is removed most readily by a high-temperature process called a dehydration bake.

A dehydration bake, as the name implies, removes water from the substrate surface by baking at temperatures of 200°C to 400°C, usually for 30 to 60 minutes. The substrate is then allowed to cool (preferably in a dry environment) and coated as soon as possible. A typical dehydration bake, however, does not completely remove water from the surface of silica substrates (including silicon, polysilicon, silicon oxide, and silicon nitride). Surface silicon atoms bond strongly with a monolayer of water forming silanol groups (SiOH). The preferred method of removing this silanol is by chemical means.

Adhesion promoters are used to react chemically with surface silanol and replace the -OH group with an organic functional group that, unlike the hydroxyl group, offers good adhesion to photoresist. Silanes are often used for this purpose, the most common being hexamethyldisilazane (HMDS). The HMDS can be applied by subjecting the substrate to HMDS vapor, usually at elevated temperature and reduced pressure for about 60 s (called a vapor prime). Performing the dehydration bake and vapor prime in the same oven gives optimal performance. These vapor prime ovens are typically integrated into the photoresist coat/bake tracks.
Processing: Photoresist Spin Coating

A thin, uniform coating of photoresist at a specific, well-controlled thickness is accomplished by the process of **spin coating**. The photoresist, rendered into a liquid form by dissolving the solid components in a solvent, is poured onto the wafer, which is then spun on a turntable at a high speed to produce the film. To achieve the desired thickness and uniformity, there is a choice between static dispense (wafer stationary while resist is dispensed) or dynamic dispense (wafer spinning while resist is dispensed), spin speeds and times, and accelerations to each of the spin speeds. Also, the volume of the resist dispensed and properties of the resist (such as viscosity, percent solids, and solvent composition) play an important role. Practical aspects of the spin operation, such as exhaust, temperature and humidity control, and spinner cleanliness also have significant effects on the resist film.

The photoresist **spin speed curve** is an essential tool for setting the spin speed to obtain the desired resist thickness. The final resist thickness varies inversely with the square root of the spin speed and is roughly proportional to the liquid photoresist viscosity.
After coating, the resulting resist film will contain 20–40% solvent by weight. The post-apply bake process, also called a softbake or a prebake, involves drying the photoresist after spin coating to remove this excess solvent. There are four major effects of removing solvent from a photoresist film: (1) film thickness is reduced, (2) post-exposure bake and development properties are changed, (3) adhesion is improved, and (4) the film becomes less tacky and thus less susceptible to particulate contamination. Typical prebake processes leave 3–8% residual solvent in the resist film, sufficiently small to keep the film stable during subsequent lithographic processing.

For DNQ/Novolak resists, at temperatures greater than about 70°C the photosensitive component (DNQ) will begin to decompose. For chemically amplified resists, residual solvent can significantly influence diffusion and reaction properties during the post-exposure bake, necessitating careful control over the post-apply bake process. Fortunately, these modern chemically amplified resists do not suffer from significant decomposition of the photosensitive components during prebake.

The most popular bake method uses a hot plate in what is called proximity baking. The wafer is brought into close proximity (about a 100 μm gap) to a hot, high-mass metal plate. Due to the high thermal conductivity of silicon, the photoresist is heated quickly to near the hot plate temperature (in about 20 seconds).

When the wafer is removed from the hotplate, baking continues as long as the wafer is hot. The total bake process cannot be well controlled unless the cooling of the wafer is also well controlled. As a result, hotplate baking is always followed immediately by a chill plate operation, where the wafer is brought in close proximity to a cool plate (kept at a temperature slightly below room temperature).
Contact and proximity lithography are the simplest methods of exposing a photoresist through a master pattern called a photomask. Contact lithography offers high resolution, but mask damage and resulting low yield make this process unusable in production environments. Proximity printing reduces mask damage by keeping the mask a set distance above the wafer (e.g., 20 µm). Unfortunately, the resolution limit is increased to greater than 2–4 µm. By far the most common method of exposure is projection printing, where an image of the mask is projected onto the wafer by a lens system.

The major classes of projection lithography tools are scanning and step-and-repeat systems. Scanners project a slit of light from the mask onto the wafer as the mask and wafer are moved simultaneously by the slit. Step-and-repeat cameras (called steppers for short) expose the wafer one rectangular section (called the image field) at a time. A hybrid step-and-scan approach uses a fraction of a normal stepper field (for example, 25 mm × 8 mm), then scans this field in one direction. The wafer is then stepped to a new location and the scan is repeated.
Monochromatic light, when projected onto a wafer, strikes the photoresist surface over a range of angles, approximating plane waves. This light travels down through the photoresist and, if the substrate is reflective, is reflected back up through the resist. The incoming and reflected light interfere to form a standing wave pattern of high and low light intensity at different depths in the photoresist. After development, this pattern is replicated in the photoresist, causing undesirable ridges in the sidewalls of the resist feature. One method of reducing the standing wave effect is called the post-exposure bake (PEB). The high temperatures used (100–130°C) cause diffusion of the photoproducts within the photoresist, thus smoothing out the standing wave ridges. It is important to note that the detrimental effects of high temperatures on photoresist during post-apply baking also apply to the PEB. The rate of diffusion is dependent on the prebake conditions—the presence of solvent enhances diffusion during a PEB.

For a conventional resist, the main reason for the PEB is to remove standing waves. For chemically amplified resists the PEB is an essential part of the chemical reactions that create a solubility differential between exposed and unexposed parts of the resist. For these resists, exposure generates a small amount of a strong acid that does not itself change the solubility of the resist. During the post-exposure bake, this photogenerated acid catalyzes a reaction that changes the solubility of the polymer resin in the resist.
Once exposed, the photoresist must be developed. Most photoresists use aqueous bases as developers. In particular, tetramethyl ammonium hydroxide (TMAH) is used at a concentration of 0.26 N. Often, surfactants are included in the developer to improve wafer wetting during development. The characteristics of the resist-developer interactions determine to a large extent the shape of the photoresist profile and, more importantly, the linewidth control.

The method of applying developer to the photoresist is important in controlling the development uniformity and process latitude. During spin development wafers are spun, using equipment similar to that used for spin coating, and developer is poured onto the rotating wafer. The wafer is also rinsed and dried while still spinning. Another technique, spray development, has been shown to have good results using developers specifically formulated for this dispensing method. Using a process identical to spin development, the developer is sprayed (rather than poured) onto the wafer by using a nozzle that produces a fine mist. This technique reduces developer usage and gives more uniform developer coverage. Another in-line development strategy is called puddle development. Again using developers specifically formulated for this process, the developer is poured onto a stationary wafer that is then allowed to sit motionless for the duration of the development time. The wafer is then spin rinsed and dried. Note that all three in-line processes can be performed in the same piece of equipment with only minor modifications, and combinations of these techniques are frequently used.
A **postbake** (also called a hard bake) is used to harden the final resist image so that it will withstand the harsh environments of pattern transfer. High temperatures (110–150°C) crosslink the polymer resin in the photoresist, thus making the image more thermally stable. If the temperature used is too high, the resist will soften and flow, causing degradation of the image. While postbake is common for Novolak-based resists, 248-nm resists are only a little improved by a postbake, and these bakes are never used for 193-nm resists. Exposure to high-intensity deep-UV light can be used to crosslink the resin at the surface of the resist forming a tough skin around the pattern, allowing the photoresist to withstand temperatures in excess of 200°C. Plasma treatments and electron beam bombardment have also been shown to effectively harden photoresist. For 193-nm resists, no treatment or plasma treatments are the most common.

After the postbake, the hardened resist is often subjected to a resist etching step called a **descum etch**. During descum, a thin layer (about 20 nm) of the photoresist is removed. This is principally done to open areas of the wafer that have been unintentionally covered with small amounts of resist “scum.” Because photoresists are largely made of organic compounds, descum is often accomplished using an oxygen-containing plasma, and is thus similar to **resist stripping** or ashing.

After the lithographic printing is complete, the resulting patterns must be transferred into the substrate. There are three basic pattern transfer approaches: subtractive transfer (etching), additive transfer (selective deposition), and impurity doping (ion implantation).

**Etching** is the selective removal of material from a surface, and is the most common pattern transfer approach. A uniform layer of the material to be patterned is deposited on the substrate. Lithography is then performed such that the areas to be etched are left unprotected (uncovered) by the photoresist. Etching is performed either with wet
chemical baths, or by plasma processing. Because plasma etching takes place in a dry environment, it is often called dry etching. In chemical etching (wet or dry), material is removed by direct chemical reaction between the etchants and the substrate. Chemical etching, unfortunately, is isotropic; it removes material from the surface uniformly in all directions—even from under the photoresist. Dry sputter etching was developed to alleviate this problem. The wafer is placed on an electrode in the plasma reactor where ions extracted from the plasma are directed toward it at high energy and nearly vertical angles. Material is removed from the surface through mechanical collisions and is thus highly anisotropic, though not very selective. Using reactive gases in the plasma reactor gives a combination of chemical and mechanical etching. This is called reactive ion etching (RIE), and it gets the best of both behaviors—selectivity from chemical reactions and anisotropy from sputtering.

For additive processes, the lithographic pattern is used to open areas where the new layer is to be grown (by electroplating, in the case of copper). Stripping of the resist then leaves the new material in a negative version of the patterned photoresist.

Finally, doping involves the addition of controlled amounts of contaminants that change the conductive properties of a semiconductor. Ion implantation uses an accelerated beam of dopant ions directed at the photoresist-patterned substrate. The resist blocks the ions, but the areas unprotected by resist are embedded with ions, creating the selectively doped regions.
Light is an **electromagnetic wave** with coupled electric and magnetic fields ($\mathbf{E}$ and $\mathbf{H}$) traveling through space. These fields can interact with a material to give rise to four other quantities: the electric displacement $D$, the magnetic induction $B$, the electric current density $J$, and the electric charge density $\rho$, as described by Maxwell’s Equations (shown here in CGS units):

$$\vec{\nabla} \times \vec{H} - \frac{1}{c} \frac{\partial \vec{D}}{\partial t} = \frac{4\pi}{c} \vec{J}$$

$$\vec{\nabla} \times \vec{E} + \frac{1}{c} \frac{\partial \vec{B}}{\partial t} = 0$$

$$\vec{\nabla} \cdot \vec{D} = 4\pi \rho$$

$$\vec{\nabla} \cdot \vec{B} = 0$$

where $c$ is the speed of light in vacuum and the dot notation is used for the time derivative. The first two equations show how a time-varying electric field (or displacement) causes a change in the magnetic field (or induction). The second two equations show how static charge affects the electric field and that there are no magnetic charges. The properties of the materials involved provide relationships between the current density and the electric field, the electric displacement and the electric field, and the magnetic induction and the magnetic field. If the material that the electromagnetic radiation is propagating through is **isotropic**, and is moving slowly relative to the speed of light, and the fields involved are time-harmonic, then the three material equations become

$$\vec{J} = \sigma \vec{E}$$

$$\vec{D} = \varepsilon \vec{E}$$

$$\vec{B} = \mu \vec{H}$$

where $\sigma$ is the **conductivity** of the material, $\varepsilon$ is its **dielectric constant**, and $\mu$ is the **magnetic permeability**. Over the range of electric and magnetic field strengths of interest here, these three material properties can be considered constants. In general, the materials of interest to the lithographer are non-magnetic, and $\mu = 1$. Also note that for transparent materials (also called **dielectrics**), $\sigma = 0$. Thus, absorption in a material is related to the generation of current density under the influence of an electric field (i.e., conduction).
The Plane Wave and the Phasor

A general harmonic electric field $E$ (due to monochromatic light of frequency $\omega$) at any point $P$ and time $t$ can be described by a deceptively simple sinusoidal equation:

$$E(P, t) = A(P) \cos(\omega t + \Phi(P))$$

where $A$ is the amplitude and $\Phi$ is the phase, both of which are position dependent, in general. As an example, consider a “plane wave” of light traveling in the $+z$ direction. The term plane wave refers to the shape of the wavefront, i.e., the shape of the function $\Phi(P) = \text{constant}$. Thus, a plane wave traveling in the $+z$ direction would require a constant phase in the $x$-$y$ plane. Such a plane wave would be described by the equation

$$E(P, t) = A \cos(\omega t - kz)$$

where $k$ is a constant called the propagation constant or the wave number. Plane waves are especially important in optics because more complex wave functions can be expressed as a superposition of different plane waves.

Although the first equation completely describes an arbitrary time-harmonic electromagnetic field, a more compact representation is possible based on the assumption that the frequency of the light does not change (a good assumption under normal optical conditions). A sinusoid can be related to a complex exponential by

$$E(P, t) = A(P) \cos(\omega t + \Phi(P)) = \text{Re}\left\{U(P)e^{-i\omega t}\right\}$$

where

$$U(P) = A(P)e^{-i\Phi(P)}$$

and $U(P)$ is called the phasor representation of the sinusoidal electric field $E(P, t)$. Notice that this phasor representation shows no time dependence. Since the time dependence of the electric field typically does not change as light travels, interferes, and interacts with matter, phasor representations have become quite common in the mathematical analysis of optical systems. Fields that satisfy this assumption are called time-harmonic fields.
Basic Imaging Theory

A generic projection system consists of a light source, a condenser lens, the mask, the objective lens, and finally the resist-coated wafer. The combination of the light source and the condenser lens is called the illumination system. The purpose of the illumination system is to deliver light to the mask (and eventually into the objective lens) with sufficient intensity, the proper directionality and spectral characteristics, and adequate uniformity across the field. The mask consists of a transparent substrate on which a pattern has been formed. This pattern changes the transmittance of the light and in its simplest form is just an opaque film. The light then passes through the clear areas of the mask and diffracts on its way to the objective lens. The purpose of the objective lens is to pick up a portion of the diffraction pattern and project an image onto the wafer which, one hopes, will resemble the mask pattern.

However, the objective lens, being only of finite size, cannot collect all of the light in the diffraction pattern. Typically, lenses used in microlithography are circularly symmetric and the entrance to the objective lens can be thought of as a circular aperture. Only those portions of the mask diffraction pattern that fall inside the aperture of the objective lens go on to form the image. The loss of diffraction information is the ultimate limiter of image quality and resolution.
Diffraction

Diffraction is usually thought of as the bending of light as it passes by an edge. More correctly, diffraction theory simply describes how light propagates. This propagation includes the effects of the surroundings (boundaries).

A simple interpretation of the physical principle behind diffraction is best captured by Huygen’s Principle: any wavefront can be thought of as a collection of radiating point sources. The new wavefront at some later time can be constructed by summing up the wavefronts from all of the radiated spherical waves. Joseph Fresnel formed a mathematical theory of diffraction by turning this summation into an integral and including the phase of the light when adding together the propagating spherical waves. This scalar diffraction theory was put on a more rigorous footing by the mathematician Gustav Kirchhoff, who required the diffracting waves to satisfy the Helmholtz equation and conservation of energy. Fresnel’s formulas are in fact a simplification of Kirchhoff’s formulation for the case when the distance away from the diffracting plane (that is, the distance from the mask to the objective lens) is much greater than the wavelength of light. Finally, if the distance to the objective lens is very large, or if the mask is illuminated by a spherical wave which converges to a point at the entrance to the objective lens, Fresnel diffraction simplifies to Fraunhofer diffraction.

![Diagram of diffraction regions](image-url)
Fraunhofer Diffraction: Examples

For Fraunhofer diffraction, the diffraction pattern (i.e., the electric field distribution as it enters the objective lens) is just the Fourier transform of the mask pattern (the electric field transmittance of the mask).

Two mask patterns—one an isolated space, the other a series of equal lines and spaces—result in mask transmittance functions, \( t_m(x) \), that look like a square pulse and a square wave, respectively. The Fourier transforms are

- **Isolated space:**
  \[
  T_m(f_x) = \frac{\sin(\pi w f_x)}{\pi f_x}
  \]

- **Dense space:**
  \[
  T_m(f_x) = \frac{1}{p} \sum_{n=-\infty}^{\infty} \frac{\sin(\pi w f_x)}{\pi f_x} \delta\left(f_x - \frac{n}{p}\right)
  \]

where \( \delta \) is the Dirac delta function, \( w \) is the spacewidth, and \( p \) is the pitch (the linewidth plus the spacewidth), and \( f_x \) is the spatial frequency, a scaled diffraction plane coordinate. The isolated space gives rise to a sinc function diffraction pattern, and the equal lines and spaces yield discrete diffraction orders.

![Diagram of a mask and its diffraction pattern](image)

It is interesting to consider how different these two diffraction patterns are. The isolated space results in a continuous distribution of energy in the form of a sinc function. The dense array of spaces produces discrete points of light, whose amplitude follows the sinc function envelope.
The Numerical Aperture

Light passing through the mask (the object plane) is diffracted at various angles. Given a lens of a certain size placed at a certain distance from the mask, there is some maximum angle of diffraction $\alpha$ for which the diffracted light just makes it into the lens. Light emerging from the mask at larger angles misses the lens and is not used in forming the image. The most convenient way to describe the size of the lens aperture is by its **numerical aperture**, defined as the sine of the maximum half-angle of diffracted light that can enter the lens times the index of refraction of the surrounding medium: $NA = n \sin \alpha$.

A large numerical aperture means that a larger portion of the diffraction pattern is captured by the objective lens. For a small numerical aperture, much more of the diffracted light is lost. The diffraction pattern for a repeating mask pattern is a series of discrete diffraction orders. The numerical aperture controls the number of diffraction orders that are used to form the image, and thus the quality of the image. For a lens with magnification, there is an object side and an image side numerical aperture, and the ratio of the two is the **magnification factor**.
The goal of imaging is to create an image that resembles the mask pattern. Since diffraction gives the Fourier transform of the mask, if the lens could give the inverse Fourier transform of the diffraction pattern, the resulting image would resemble the mask pattern. In fact, lenses are designed to behave precisely in this way. Does an ideal lens produce a perfect image? No. Because of the finite size of the numerical aperture, only a portion of the diffraction pattern enters the lens. Thus, even an ideal lens cannot produce a perfect image unless the lens is infinitely big. Since in the case of an ideal lens the image is limited only by the diffracted light that does not make it through the lens, we call such an ideal system diffraction-limited.

The objective lens pupil function $P$ of an ideal lens simply describes what portion of light enters the lens: it is one inside the aperture and zero outside.

$$P(f_x, f_y) = \begin{cases} 
1, & \sqrt{f_x^2 + f_y^2} < NA/\lambda \\
0, & \sqrt{f_x^2 + f_y^2} > NA/\lambda 
\end{cases}$$

Thus, the product of the pupil function and the diffraction pattern ($T_m$) describes the light entering the objective lens. Combining this with our description of how a lens behaves gives us our final expression for the electric field at the image plane (that is, at the wafer):

$$E(x, y) = F^{-1}\{T_m(f_x, f_y)P(f_x, f_y)\}$$
Spatial Coherence and Oblique Illumination

Spatial coherence describes the range of angles used to illuminate the mask. Coherent illumination means simply that the light striking the mask arrives from only one direction. Generally it is assumed that coherent illumination on the mask is normally incident. The result is a diffraction pattern that is centered in the entrance to the objective lens. What would happen if we changed the direction of the illumination so that the light struck the mask at some angle $\theta'$? The effect is simply to shift the position of the diffraction pattern with respect to the lens aperture (in terms of spatial frequency, the amount shifted is $(\sin\theta')/\lambda$). Since only the portion of the diffraction pattern passing through the lens aperture is used to form the image, it is quite apparent that this shift in the position of the diffraction pattern can have a profound effect on the resulting image.

Sometimes, tilting the illumination can make the image better (allowing another diffraction order to enter the lens), and sometimes it will make the image worse (an order no longer enters the lens), depending on the pitch of the pattern. Thus, adjusting the tilt of the illumination to improve printing will be pitch dependent.
Partial Coherence

Light arriving at the mask from only one angle is called **coherent illumination**. If the illumination of the mask is composed of light coming from a range of angles, the illumination is called **partially coherent**. If one angle of illumination causes a shift in the diffraction pattern, a range of angles will cause a range of shifts, resulting in broadened diffraction orders.

One can characterize the range of angles used for the illumination in several ways, but the most common is the **partial coherence factor** $\sigma$ (also called the degree of partial coherence, the pupil-filling function, or just the partial coherence). The partial coherence is defined as the sine of the half-angle of the illumination cone divided by the objective lens numerical aperture. It is thus a measure of the angular range of the illumination relative to the angular acceptance of the lens. Finally, if the range of angles striking the mask extends from $-90$ to $90^\circ$ (that is, all possible angles), the illumination is said to be **incoherent**.

Coherent light has $\sigma = 0$, incoherent light has $\sigma = \infty$, with partially coherent being between (although normally $\sigma < 1$).
**Aberrations**

An **aberration** is any deviation from the ideal, “diffraction-limited” imaging performance of a lens. In practice, aberrations come from three sources—aberrations of design, aberrations of construction, and aberrations of use.

An “aberration of design” does not mean mistakes or problems caused by the designer of the lens. Aberrations are fundamental to the nature of imaging and it is the goal of the lens designer to “design out” as many of these aberrations as possible. The aberrations of design are those aberrations, inserted into the imaging system by the nature of light, that the designer was not able to extract through clever design.

In terms of geometrical optics, the goal of imaging can be stated very simply: light emanating in all directions from some point on the object should be collected by the lens and focused to its ideal image point. Thus, a ray of light coming from the object point should pass through the lens and arrive at the image point, regardless of its angle.

Some typical examples of aberrations are tilt, defocus, coma, astigmatism, spherical aberration, and chromatic aberration.
The aberration behavior of a lens can be predicted using lens design software, or measured using interferometry, resulting in a map of the phase error of the light exiting from the lens for a given point in the field. Aberrations will vary as a function of field position, typically taking 25–50 measurements across the field to fully characterize a lithographic lens.

For a given point in the field, a map of the phase error across the exit pupil is curve-fit to a function such as a high-order polynomial. By carefully choosing the form of the polynomial, the coefficients themselves can take on physically meaningful interpretations. By far the most common such polynomial is the Zernike polynomial. This orthogonal polynomial series has an infinite number of terms, but is typically cut off after 36 terms, with powers of the relative pupil radius position and trigonometric functions of the polar angle $\theta$. The Zernike polynomial is formulated so that each term in the expansion has physical significance, such as coma, spherical, and astigmatism.
## Aberrations: Zernike Examples

<table>
<thead>
<tr>
<th>Term</th>
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<td>$Z_0$</td>
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<tr>
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</tr>
<tr>
<td>$Z_6$</td>
<td>$(3R^2 - 2)R \cos \theta$</td>
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</tr>
<tr>
<td>$Z_7$</td>
<td>$(3R^2 - 2)R \sin \theta$</td>
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</tr>
<tr>
<td>$Z_8$</td>
<td>$6R^4 - 6R^2 + 1$</td>
<td>3rd-Order Spherical</td>
</tr>
<tr>
<td>$Z_9$</td>
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<td>$Z_{10}$</td>
<td>$R^3 \sin 3\theta$</td>
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<tr>
<td>$Z_{11}$</td>
<td>$(4R^2 - 3)R^2 \cos 2\theta$</td>
<td>5th-Order Astigmatism</td>
</tr>
</tbody>
</table>

![Diagram](image-url)
Chromatic Aberration

Since the index of refraction of all materials varies with wavelength (a property called \textit{dispersion}), lens elements will focus different wavelengths differently. This fundamental problem, called \textit{chromatic aberration}, can be alleviated by using two different glass materials with different dispersions such that the chromatic aberrations of one lens element cancels the chromatic aberrations of the other. As with all aberrations, this cancellation is not perfect, meaning that all lenses will have some level of residual chromatic aberrations.

The effects of chromatic aberrations depend on two things: the degree to which the Zernike polynomial coefficients vary with wavelength (the magnitude of the chromatic aberrations), and the range of wavelengths used by the imaging tool. For example, a typical i-line stepper might use a range of wavelengths on the order of 10 nm, whereas a KrF-excimer-laser-based deep-UV stepper may illuminate the mask using light with a wavelength range of 1 pm. A typical deep-UV lens makes no attempt at chromatic correction since only fused silica is used for all the elements in the lens. As a result, chromatic aberrations are a concern in deep-UV lithographic lenses even when extremely narrow bandwidth light sources are used.

For lenses with no chromatic corrections, the plane of best focus shifts nearly linearly with changes in wavelength. Since the center wavelength of most excimer lasers is adjustable over a large range, this effect can be readily measured, with typical KrF lenses showing 100–500 nm of focus shift for every 1 pm of wavelength shift. Each wavelength in the laser spectrum will be projected through the imaging lens, forming an \textit{aerial image} shifted in focus according to the wavelength response characteristic for that lens. The total aerial image will be the sum of all of the images from all the wavelengths in the source, resulting in a final aerial image that is somewhat smeared through focus.
Horizontal-Vertical (H-V) Bias

**H-V bias** is the systematic difference in linewidth between horizontally and vertically oriented resist features that, other than orientation, should be identical. One main cause of H-V bias is **astigmatism**—a difference in best focus as a function of feature orientation. The pupil phase error due to 3rd order astigmatism is $2\pi Z_{\text{astig}} R^2 \cos \theta$. For a $y$-oriented vertical pattern the diffraction pattern will spread across the $x$-axis of the pupil ($\theta = 0^\circ$ and $180^\circ$). For horizontally oriented lines, the diffraction pattern will be along the $y$-axis of the pupil ($\theta = \pm 90^\circ$) and the astigmatism will cause a phase error of opposite sign compared to the vertical patterns.

The pupil phase error due to defocus is also quadratic with pupil radius $R$:

$$\text{phase error} \approx \frac{\pi \delta NA^2}{\lambda} R^2$$

where $\delta$ is the defocus distance, $\lambda$ is the wavelength, and $NA$ is the numerical aperture. Thus, astigmatism will cause the vertically oriented lines to shift best focus, with the horizontal lines shifting focus by the same magnitude but in the opposite direction. To first order, CD has a quadratic dependence on focus: $CD \approx CD_{\text{best focus}} + a\delta^2$, where $a$ is the dose-dependent curvature of the CD-through-focus curve. If best focus is shifted due to astigmatism, we can calculate the CD of the vertical and horizontal features, and the resulting H-V bias is just the difference in these two CDs.

$$H - V \text{ bias} \approx \frac{8a\delta Z_{\text{astig}} \lambda}{NA^2}$$
**Defocus**

The impact of focus errors on the resulting aerial image can be described as equivalent to an aberration of a sort. By viewing the actual wavefront as having an error in curvature relative to the desired wavefront (i.e., the one that focuses on the wafer), we can quantify the effect of defocus. The distance between wavefronts is called the **optical path difference (OPD)**. Describing the position within the exit pupil by an angle $\theta$, the optical path difference is given by

$$OPD = \delta(1 - \cos \theta)$$

A Taylor expansion in terms of $\sin \theta$ gives

$$OPD = \delta(1 - \cos \theta) = \frac{1}{2} \delta \left( \sin^2 \theta + \frac{\sin^4 \theta}{4} + \frac{\sin^6 \theta}{8} + \cdots \right)$$

For small angles (that is, small numerical apertures), the impact of defocus is approximately

$$OPD \approx \frac{1}{2} \delta \sin^2 \theta$$

Defocus causes a phase error that is zero at the center of the pupil and approximately quadratic across the pupil.
Flare

Within a lens, reflections at an interface, scattering caused by particles or surface roughness, or scattering caused by glass inhomogeneity all result in stray light called **flare**. Defects such as these occur during lens manufacturing, or can arise due to lens degradation (aging, contamination, etc.).

Measuring flare is reasonably straightforward. Consider the imaging of an isolated island feature whose dimension is extremely large compared to the resolution limits of the imaging tool (say, a 100 µm square island in positive resist). In the absence of flare, the imaging of such a large feature will result in very nearly zero light energy at the center of the image of the island. The presence of flare, on the other hand, will provide light to this otherwise dark region on the wafer. The dose to clear ($E_0$) is defined as the minimum dose required to completely remove the photore sist during development for a large open frame exposure. A related concept is the island dose to clear ($E_{0\text{-island}}$), the minimum dose required to completely wash away a large island structure during a normal development process. By measuring both of these quantities, the amount of flare can be determined as

$$Flare = \frac{E_0}{E_{0\text{-island}}}$$

For example, if the dose to clear of a resist is 15 mJ/cm$^2$, then an imaging tool with 5% flare would mean that a large island will clear with a dose of about 300 mJ/cm$^2$. 
Vector Nature of Light

Light is an electromagnetic wave. Electric and magnetic fields oscillate at some characteristic frequency while traveling at the speed of light. These fields have a magnitude, phase, and direction. It is the direction (also called the polarization) of the electric field that defines its vector nature, and a key property of an electromagnetic wave is that its electric and magnetic field vectors are at right angles to each other, and at right angles to the direction of propagation. Two plane waves, approaching a wafer at different angles, will interfere to form fringe patterns of light and dark. The intensity of light $I$ is the square of the magnitude of the electric field $E$. If the two electric fields do not interfere, the total intensity is the sum of the individual intensities.

$$I = |E_1|^2 + |E_2|^2$$

If, however, the two electric fields interfere completely, the total intensity will be

$$I = |E_1 + E_2|^2$$

Two electric fields interfere with each only to the extent that their electric fields oscillate in the same direction. If the electric fields are at right angles to each other, there will be no interference. To determine the amount of interference between two electric fields, one must first determine the amount of directional overlap between them.

The standard head-to-tail method of geometrically adding two vectors can be used to determine interference. If the two vectors are at right angles to each other so that the
head-to-tail construction forms a simple right triangle, the length of the resultant vector is given by the familiar Pythagorean theorem: the intensities add together (there is no interference). At the other extreme (the middle example in this figure), two vectors in the same direction add directly and the electric fields will add (they interfere completely). Finally, the bottom example shows an intermediate case. Working through the trigonometry of the vector sum shows that the portion of the two vectors that overlap will interfere, and the portion of the vectors that are at right angles will add in quadrature.

For two plane waves approaching the wafer, the transverse electric or TE fields (the electric field pointing out of the page of the drawing) are always 100% overlapped regardless of the angle between the plane waves. For the transverse magnetic or TM field (the electric field pointing in the page of the drawing), the extent of overlap between the two vectors grows smaller as the angle between the plane waves grows larger.
Polarization

The direction of the electric field of an electromagnetic wave, and how that direction varies in time or space, is called its polarization. Since an electromagnetic wave travels through time and space, there are two useful and equivalent ways of looking at the direction of the electric field: the variation of the electric field direction in space at an instant in time, or the variation of the electric field direction in time at a fixed point in space.

The simplest type of polarization is called linear polarization. At an instant in time, the electric field $E$ is always pointing in one direction for all points in space. At one point in space, the electric field changes magnitude sinusoidally through time, but always points in the same direction.

Other types of polarization include circular polarization, elliptical polarization, and random polarization (often called unpolarized).

Linear

Circular

Elliptical

Random
The Optical Invariant

**Snell’s Law** says that light traveling through material 1 with refractive index \( n_1 \) striking a surface with angle \( \theta_1 \) relative to the normal to that surface will be transmitted into material 2 (with index \( n_2 \)) at an angle \( \theta_2 \): 
\[
    n_1 \sin \theta_1 = n_2 \sin \theta_2.
\]
This simple law applied to a film stack made up of any number of thin parallel layers means that Snell’s law can be applied repeatedly. The quantity \( n \sin \theta \) is *invariant* as a ray of light travels through this stack of parallel films.

We find another, related invariant when looking at how an imaging lens works. The **Lagrange invariant** (often just called the **optical invariant**) relates the angles entering and exiting the lens to the magnification \( m \):
\[
    m = \frac{n_o \sin \theta_o}{n_i \sin \theta_i}
\]
where \( n_o \) is the refractive index of the media on the object side and \( n_i \) is the image side refractive index.

Taking into account the magnification scale factor, the quantity \( n \sin \theta \) for a diffracted order is constant from the time it leaves the mask to the time it combines inside the resist with other diffraction orders to form an image of the mask.
Immersion Lithography: Resolution

If the air between the lens and the wafer is replaced with water, the optical invariant says that the angles of light inside the resist will be the same. There are two impacts on lithography: the maximum possible angle of light that can reach the resist is increased (increasing the maximum potential resolution), and the phase of that light is changed, causing an improvement in depth of focus.

The maximum value of the optical invariant will be limited by the material in the film stack above and including the resist with the smallest refractive index. If one of the layers is air (with a refractive index of 1.0), this will become the material with the smallest refractive index and the maximum possible value of the invariant will be 1.0. If the air is replaced with a fluid of a higher refractive index, but still smaller than the index of the photoresist, the maximum possible value of the invariant will be $n_{\text{fluid}}$, and the maximum possible angle of light inside the resist will be greater: $\sin \theta_{\text{max, resist}} = n_{\text{fluid}}/n_{\text{resist}}$. At a wavelength of 193 nm, resists have refractive indices of about 1.7 and water has a refractive index of about 1.44. The fluid does not make the angles of light larger, but it enables those angles to be larger. If one were to design a lens to emit larger angles, immersion lithography will allow those angles to propagate into the resist. The numerical aperture of the lens (defined as the maximum value of the invariant $n \sin \theta$ that can pass through the lens) can be made to be much larger using immersion lithography, with the resulting improvements in resolution one would expect.

Immersion lithography is now in use and is expected to allow lenses to be made with numerical apertures greater than 1.0. Lenses with NAs above 1.2 or 1.3 seem likely. If an immersion fluid with a refractive index closer to that of the photoresist can be found, numerical apertures of up to 1.5 might be possible.
Immersion Lithography: Depth of Focus

For a given diffraction order (and thus a given angle of the light inside the resist), the angle of the light inside an immersion fluid will be less than if air were used. These smaller angles will result in smaller optical path differences between the various diffracted orders when out of focus, and thus a smaller degradation of the image for a given amount of defocus. In other words, for a given feature being printed and a given numerical aperture, immersion lithography will provide a greater depth of focus (DOF).

The high NA version of the Rayleigh depth of focus criterion (which assumes we are imaging a small binary pattern of lines and spaces of pitch \( p \)) is

\[
DOF = k_2 \frac{\lambda}{2 n_{\text{fluid}} (1 - \cos \theta)}
\]

where \( n_{\text{fluid}} \sin \theta = \lambda/p \). Combining these equations, one can see how immersion will improve the depth of focus of a given small feature:

\[
\frac{DOF(\text{immersion})}{DOF(\text{dry})} = \frac{1 - \sqrt{1 - (\lambda/p)^2}}{n_{\text{fluid}} - \sqrt{(n_{\text{fluid}})^2 - (\lambda/p)^2}}
\]

Fluid index = 1.44
Standing Waves: Definition

When a thin dielectric film placed between two semi-infinite media (e.g., a thin coating on a thick substrate in air) is exposed to monochromatic light, standing waves are produced in the film. Standing waves occur whenever two waves, traveling in opposite directions and with a fixed phase relationship to each other, combine in an interference pattern along the direction of propagation. In lithography, light passing through the photoresist is reflected off the substrate. This reflected light wave interferes with the light wave traveling down to produce the standing wave pattern.

Standing waves always have a negative impact on lithography. If not removed through a post-exposure bake diffusion process, standing waves will print on the sidewalls of the photoresist features to cause scalloped edges.
Standing Waves: Mathematics

Consider the propagation of light (a monochromatic plane wave of wavelength \( \lambda \) normally incident on the resist) through a film stack of air (layer 1) on resist (layer 2) on a substrate (layer 3). The transmission coefficient and reflection coefficient between layers \( i \) and \( j \) are given by

\[
\tau_{ij} = \frac{2n_i}{n_i + n_j} \quad \rho_{ij} = \frac{n_i - n_j}{n_i + n_j}
\]

where \( n \) is the complex refractive index of the material.

A plane wave traveling through material \( i \) in the \(+z\) direction is

\[
E(z) = e^{-ik_zz} = e^{-i2\pi n_iz/\lambda}
\]

The internal transmittance of resist of thickness \( D \) is

\[
\tau_D = e^{-i2\pi n_2 D/\lambda}
\]

Thus, an incident wave \( (E_i) \) will propagate into and through the resist (being absorbed along the way), reflect off the substrate, and bounce up and down inside the resist an infinite number of times, creating the final electric field inside the resist of

\[
E_{total}(z) = \frac{\tau_{12}E_i(e^{-i2\pi n_2 z/\lambda} + \rho_{23}\tau_2^2 e^{i2\pi n_2 z/\lambda})}{1 + \rho_{12}\rho_{23}\tau_2^2}
\]

The relative intensity inside the resist is then given by

\[
I(z) = \frac{n_2|E(z)|^2}{n_1|E_i|^2}
\]

The result is a sinusoidal variation of intensity with Period = \( \lambda/2n_2 \). The amplitude of the standing waves is determined by the reflectivity of the substrate (\( \rho_{23} \)) and the amount of absorption in the resist (\( e^{-\alpha D} \)).
Consider light intersecting the plane interface between two materials, numbered 1 and 2, with an incident electric field $E_i$, a reflected electric field $E_r$, and a transmitted electric field $E_t$. The transmission and reflection coefficients are functions of the angle of incidence and the polarization of the incident light. If $\theta_i$ is the incident (and reflected) angle and $\theta_t$ is the transmitted angle, then the electric field reflection and transmission coefficients are given by the Fresnel formulæ.

\[
\rho_{12\perp} = \frac{n_1 \cos(\theta_i) - n_2 \cos(\theta_t)}{n_1 \cos(\theta_i) + n_2 \cos(\theta_t)}
\]

\[
\rho_{12\parallel} = \frac{n_1 \cos(\theta_t) - n_2 \cos(\theta_i)}{n_1 \cos(\theta_t) + n_2 \cos(\theta_i)}
\]

\[
\tau_{12\perp} = \frac{2n_1 \cos(\theta_i)}{n_1 \cos(\theta_i) + n_2 \cos(\theta_t)}
\]

\[
\tau_{12\parallel} = \frac{2n_1 \cos(\theta_t)}{n_1 \cos(\theta_t) + n_2 \cos(\theta_i)}
\]

where $n_j = n_j + i\kappa_j$ is the complex index of refraction of material $j$. Here, $\parallel$ represents an electric field vector that lies parallel to the plane defined by the direction of the incident light and a normal to the material interface. Other names for $\parallel$ polarization include $p$ polarization and TM (transverse magnetic) polarization. The polarization denoted by $\perp$ represents an electric field vector that lies in a plane perpendicular to that defined by the direction of the incident light and a normal to the surface. Other names for $\perp$ polarization include $s$ polarization and TE (transverse electric) polarization. Note that

\[
\rho_{21} = -\rho_{12}, \quad \tau_{21} = \frac{n_2 \cos(\theta_t)}{n_1 \cos(\theta_i)} \tau_{12}
\]
Swing Curves

Generically, a swing curve is the sinusoidal variation of some lithographic parameter (e.g., linewidth, dose to clear, or reflectivity) with resist thickness.

The same thin-film interference effects that cause standing waves also give rise to swing curves. Interference between $E_{r0}$ and $E_{r1}$ can be constructive or destructive depending on the thickness of the resist. The reflectivity of the film stack is given by

$$R = \frac{|\rho_{12}|^2 + |\rho_{23}|^2 e^{-\alpha D} + 2|\rho_{12}\rho_{23}| e^{-\alpha D} \cos(4\pi n_2 (D/\lambda) - \phi_{12} - \phi_{23})}{1 + |\rho_{12}\rho_{23}|^2 e^{-2\alpha D} + 2|\rho_{12}\rho_{23}| e^{-\alpha D} \cos(4\pi n_2 (D/\lambda) - \phi_{12} - \phi_{23})}$$

From this equation, one can see that swing curves can be reduced by reducing substrate reflectivity ($\rho_{23}$) by using a bottom ARC, reducing resist reflectivity ($\rho_{12}$) by using a top ARC, or by increasing resist absorbance ($\alpha D$) by using a dyed photoresist.
A top antireflection coating (TARC) can be used to reduce swing curves. For simplicity, consider air (layer 1) on TARC (layer 2) on an infinitely thick photoresist (layer 3). The filmstack reflectivity is reduced when

\[ R_{\text{total}} = |\rho_{\text{total}}|^2 = \left| \frac{\rho_{12} + \rho_{23} \tau_D^2}{1 + \rho_{12} \rho_{23} \tau_D^2} \right|^2 = 0 \text{ when } \rho_{12} + \rho_{23} \tau_D^2 = 0 \]

A classic solution to this equation works very well when the materials 1 and 3 are not very absorbing: \( \tau_D^2 = -1 \) and \( \rho_{12} = \rho_{23} \). The requirement that \( \tau_D^2 = -1 \) means that two passes of the light through the ARC causes a 180° phase change with no absorption (the magnitude is one). To get \( \tau_D^2 = -1 \), the ARC thickness \( D \) must be adjusted to a “quarter wave”:

\[ D = \frac{\lambda}{4n_2} \]

The requirement that \( \rho_{12} = \rho_{23} \) will be satisfied when the index of refraction of the ARC is made to be

\[ n_2 = \sqrt{n_1 n_3} \]

Further, since the ARC does not absorb (a consequence of \( \tau_D^2 = -1 \)), the imaginary part of its index is zero. Thus, the perfect TARC can only be achieved if both materials 1 and 3 have no imaginary parts to their indices of refraction (i.e., when materials in question are transparent). For a resist with a refractive index of 1.7 at a wavelength of 193 nm (in air), the optimum TARC will have a refractive index of about 1.30 and a thickness of 37 nm.

Since in reality, resist will always be somewhat absorbing, a perfect TARC is not possible. Also, it is very difficult to find practical materials with refractive indices low enough to make a nearly ideal TARC. Additionally, top coatings are also used for environmental protection, keeping airborne base contaminants away from chemically amplified resists and water away from immersion resists.
Reflections from the substrate can cause unwanted variations in the resist profile (standing waves) and swing curve effects. One possible solution is the bottom antireflection coating (also called bottom ARC or BARC).

When optimizing a litho process for reflectivity, there are three basic tasks: 1) optimize the BARC, 2) optimize the resist thickness (from a swing curve perspective), and 3) understand the sensitivity to BARC, resist, and film stack variations. For the first task, there are two classes of BARC problems:

- BARC on metal (absorbing substrate): the goal is to reduce the reflectivity (the thickness of the metal or what’s underneath doesn’t matter)
- BARC on oxide (transparent substrate): reduce the sensitivity to oxide thickness variations (while also keeping reflectivity low)

There are three BARC parameters available for optimization: the thickness of the BARC, and the real and imaginary parts of its refractive index. For the simplest use case, a BARC is given and the goal is just to optimize its thickness.

When all three parameters can be optimized, there is a family of solutions available, given by the equation

\[ D = \frac{\lambda}{4\pi k_2} \ln \left| \frac{\rho_{23}}{\rho_{21}} \right| = \frac{\lambda}{4\pi n_2} (\theta_{23} - \theta_{21}) \text{ where } \rho_{ij} = |\rho_{ij}| e^{i\theta_{ij}} \]

The situation is more complicated when non-normal incidence of the light is included.
Novolak/DNQ Resists

For g-line (436 nm) and i-line (365 nm) lithography, the most common resists are of the Novolak/DNQ variety. These positive photoresists (meaning the exposed region becomes more soluble in developer) are made up of three major components; a base Novolak resin that gives the resist its structural properties and etch resistance, a photoactive compound or sensitizer called a diazonaphthoquinone (DNQ), and a solvent that renders these components into liquid form for spin coating.

By themselves, Novolak resins are moderately soluble in aqueous base developers. But the DNQ acts as a strong inhibitor to dissolution. Exposure converts the inhibiting DNQ into a soluble carboxylic acid, rendering the resist soluble in developer.

DNQ molecules are photosensitive in the 350–450 nm range. Since Novolak resins are reasonably transparent over this wavelength range as well, the combination makes for a good resist for g-line and i-line light sources.
Chemically Amplified Resists

Unlike conventional resists, such as the diazonaphthoquinone/Novolak systems, chemically amplified resists require two separate chemical reactions in order to change the solubility of the resists. First, exposure turns an aerial image into a latent image of exposure reaction products (acids). Although very similar to conventional resists, the reaction products of exposure for a chemically amplified resist do not significantly change the solubility of the resist. Instead, a second reaction during a post-exposure bake is catalyzed by the exposure reaction products. The result of the post-exposure bake reaction is a change in the solubility of the resist.

The defining characteristic of a chemically amplified resist is that this reaction is catalyzed by the acid so that the acid is not consumed by the reaction. A base polymer such as polyhydroxystyrene (PHS) is used that is very soluble in an aqueous base developer. It is the hydroxyl groups that give the PHS its high solubility, so by “blocking” these sites (by reacting the hydroxyl group with some longer chain molecule) the solubility can be reduced. A t-butoxycarbonyl group (t-BOC) can be used as the blocker, resulting in a very slowly dissolving polymer. In the presence of a strong acid and heat, the t-BOC blocked polymer will undergo acidolysis (a deblocking reaction) to generate the soluble hydroxyl group.

\[
\begin{align*}
\text{CH}_2-\text{CH} & \quad \xrightarrow{H^+} \quad \text{CH}_2-\text{CH} \\
\text{O} & \quad \xrightarrow{\Delta} \quad \text{O} \\
\text{C}=\text{O} & \quad \xrightarrow{\Delta} \quad + \text{CH}_2 = \text{C} + \text{CH}_3 + \text{CO}_2 \\
\text{CH}_3-\text{C}=\text{CH}_3 & \quad \xrightarrow{\Delta} \quad \text{CH}_3 \\
\text{OH} & \quad \xrightarrow{\Delta} \quad + \text{CH}_3 + \text{CH}_3 + \text{CO}_2
\end{align*}
\]
Absorption of Light

The basic law of absorption is the empirical Lambert law:

\[
\frac{dI}{dz} = -\alpha I,
\]

which gives

\[
I(z) = I_0 e^{-\alpha z}
\]

where \( I \) is the intensity of light traveling in the \( z \)-direction through a medium, and \( \alpha \) is the absorption coefficient of the medium and has units of inverse length. The integrated form (right equation) is only applicable in a homogeneous medium (i.e., \( \alpha \) is not a function of \( z \)).

The propagation of an electric field through some material can implicitly account for absorption by using a complex index of refraction \( n \) for the material such that \( n = n - i\kappa \). The imaginary part of the index of refraction is related to the absorption coefficient by

\[
\alpha = 4\pi \kappa / \lambda
\]

Beer's law is much less accurate than Lambert's law (though often still useful) and says that for dilute solutions or mixtures the absorption coefficient is proportional to the concentration of the absorbing species in the solution.

\[
\alpha_{solution} = \alpha c
\]

where \( \alpha \) is the molar absorption coefficient (sometimes called the molar extinction coefficient) of the absorbing species and \( c \) is the concentration. The stipulation that the solution be dilute expresses a fundamental limitation of Beer's law. At high concentrations, where absorbing molecules are close together, the absorption of a photon by one molecule may be affected by a nearby molecule. Since this interaction is concentration dependent, it causes deviation from the linear relation. For an \( N \)-component homogeneous solid, the absorption coefficient becomes

\[
\alpha_T = \sum_{j=1}^{N} a_j c_j
\]
A resist is made up of a resin $R$, the photoactive compound $M$, the solvent $S$, and a fourth component that appears during exposure: exposure products $P$ generated by the reaction of $M$ with ultraviolet light. Applying Beer’s Law, the absorption coefficient $\alpha$ is then

$$\alpha = a_M M + a_P P + a_R R + a_S S$$

If $M_o$ is the initial PAC concentration (i.e., with no UV exposure), the stoichiometry of the exposure reaction gives $P = M_o - M$. The absorption coefficient can then be expressed as $\alpha = A m + B$ where $A = (a_M - a_P)M_o$, $B = a_P M_o + a_R R + a_S S$, and $m = M/M_o$.

$A$ and $B$ are called the bleachable and non-bleachable absorption coefficients, respectively, and make up the first two Dill parameters. Other non-bleachable components of the photoresist (such as a dye) are added to $B$.

The quantities $A$ and $B$ are experimentally measurable and can be related to typical resist absorbance curves, measured using a UV spectrophotometer. When the resist is fully exposed, $M = 0$ and $\alpha_{\text{exposed}} = B$. Similarly, when the resist is unexposed, $m = 1$ ($M = M_o$) and $\alpha_{\text{unexposed}} = A + B$. From this, $A$ may be found by $A = \alpha_{\text{unexposed}} - \alpha_{\text{exposed}}$. Thus, $A(\lambda)$ and $B(\lambda)$ may be determined from the UV absorbance curves of unexposed and completely exposed resist.
Exposure Kinetics

The absorption of UV light by the photoactive compound (PAC) leads to the chemical conversion of PAC $M$ to exposure product $P$.

$$M \xrightarrow{UV} P$$

This concept is stated in the first law of photochemistry: only the light that is absorbed by a molecule can be effective in producing photochemical change in the molecule. Simple kinetics can be applied to the proposed mechanism assuming first order reactions.

$$\frac{dm}{dt} = -CIm$$

where the relative PAC concentration $m (= M/M_o)$ has been used and $C$ is the standard exposure rate constant and the third Dill parameter. A more thorough microscopic analysis of the exposure process allows this exposure rate constant to be broken down into the product of the absorption cross-section of the PAC and the quantum yield of the reaction (the fraction of absorbed photons that produce the chemical change, $\Phi$):

$$C = \frac{\Phi a \lambda \lambda}{N_A h c}$$

where $N_A$ is Avogadro’s number, $h$ is Planck’s constant, and $c$ is the speed of light.

A solution to the exposure rate equation is simple if the intensity within the resist is constant throughout the exposure (no photoresist bleaching):

$$m = e^{-CIt}$$

This result illustrates an important property of first-order kinetics called reciprocity. The amount of chemical change is controlled by the product of light intensity and exposure time, called the exposure dose or exposure energy.
Measuring the Dill ABC Parameters

The photoresist to be measured is coated on a non-reflecting transparent substrate. The resist is then exposed by a normally incident parallel beam of light at the wavelength of measurement. At the same time, the intensity of the light transmitted through the substrate is measured continuously. The output of the experiment, transmitted intensity as a function of exposure time, is then analyzed to determine the resist ABC parameters.

Note that the effectiveness of this measurement technique rests with the nonzero value of $A$. If the photoresist does not change its optical properties with exposure, measuring transmittance will provide no insight on the exposure reaction.

The ABC parameters can be obtained from the transmittance curve by measuring the initial transmittance $T(0)$, the final (completely exposed) transmittance $T(\infty)$, the initial slope of the curve, and resist thickness $D$.

$$A = \frac{1}{D} \ln \left( \frac{T(\infty)}{T(0)} \right), \quad B = -\frac{1}{D} \ln \left( \frac{T(\infty)}{T_{12}} \right)$$

$$C = \frac{A + B}{AT(0)(1 - T(0))T_{12}} \left. \frac{dT}{dE} \right|_{E=0}, \quad T_{12} = 1 - \left( \frac{n_{\text{resist}} - 1}{n_{\text{resist}} + 1} \right)^2$$
Chemically Amplified Resist Kinetics

Chemically amplified resists require two separate chemical reactions in order to change the solubility of the resists. First, exposure turns an aerial image into a latent image of exposure reaction products with first-order kinetics identical to conventional resists. A second deblocking reaction during a post-exposure bake is catalyzed by the acid exposure reaction product. Using $M$ as the concentration of some reactive site, these sites are consumed (i.e., are reacted) according to kinetics of first order in acid concentration $H$ and first order in $M$:

$$\frac{dM}{dt'} = -kMH$$

where $k$ is the amplification rate constant and $t'$ is the bake time. Assuming $H$ is constant, this equation can be solved for the concentration of reacted sites $X$:

$$X = M_0 - M = M_0(1 - e^{-kHt'})$$

It is useful here to normalize the concentrations to initial values. This results in a normalized acid concentration $h$ and normalized reacted and unreacted sites $x$ and $m$:

$$h = \frac{H}{G_o} \quad x = \frac{X}{M_0} \quad m = \frac{M}{M_0}$$

$$h = 1 - e^{-CIt} \quad m = 1 - x = e^{-Kamp'Clt}$$

where $K_{amp} = G_o k$ and $G_o$ is the initial PAG concentration. The result of the PEB is an amplified latent image $m(x)$, corresponding to an exposed latent image $h(x)$, resulting from the aerial image $I(x)$.

Consider the quite common case of a small exposure dose ($It \ll 1/C$) so that the amount of acid generated is small.

$$h \approx CIt \quad \text{and} \quad m = 1 - x \approx e^{-K_{amp}'CIt}$$

If we define the thermal dose as $K_{amp}'CIt$, then there is a reciprocity between exposure dose and thermal dose.
Diffusion in Chemically Amplified Resists

For chemically amplified resists, the photogenerated acid and the base additives diffuse during the post-exposure bake. In one dimension, the standard diffusion equation (taking acid diffusion as the example) is

$$\frac{\partial H}{\partial t'} = \frac{\partial}{\partial z} \left( D_H \frac{\partial H}{\partial z} \right)$$

where $D_H$ is the diffusivity of acid in the photoresist. Solving this equation requires two boundary conditions for each dimension, one initial condition, and a knowledge of the diffusivity as a function of position and time.

The diffusivity is a strong function of temperature and, most probably, the extent of amplification. Since the temperature is changing with time during the bake, the diffusivity will be time dependent. The concentration dependence of diffusivity results from an increase in free volume for typical positive resists: as the amplification reaction proceeds, the polymer blocking group evaporates resulting in a decrease in film thickness but also an increase in free volume (and probably a change in the glass transition temperature as well). Since the acid concentration is time and position dependent, the diffusivity must be determined as a part of the overall reaction kinetics solution.

The temperature dependence of the diffusivity can be expressed in a standard Arrhenius form:

$$D_H(T) = A_re^{-E_a/RT}$$

where $A_r$ is the Arrhenius coefficient, $E_a$ is the activation energy, $R$ is the universal gas constant (1.98717 cal/mole-°C or 8.31431 J/mole-°C), and $T$ is absolute temperature. In general, the activation energy of diffusion will differ from the reaction activation energies, making the balance between reaction and diffusion very sensitive to PEB temperature.
Acid Loss Mechanisms

Through a variety of mechanisms, acid formed by exposure of the resist film can be lost and thus not contribute to the catalyzed reaction to change the resist solubility. There are two basic types of acid loss—loss that occurs between exposure and post-exposure bake, and loss that occurs during the post-exposure bake. The first type of loss leads to post-exposure delay time effects—the resulting lithography is affected by the delay time between exposure and post-exposure bake. The typical mechanism for delay-time acid loss is the diffusion of atmospheric base contaminants into the top surface of the resist. Another possible delay-time acid loss mechanism is base contamination from the substrate.

Acid loss during the PEB could occur by other mechanisms. For example, as the acid diffuses through the polymer, it may encounter sites that “trap” the acid, rendering it unusable for further amplification. Acid can also be lost at the top surface of the resist due to evaporation. The amount of evaporation is a function of the size of the acid and the degree of its interaction with the resist polymer.

Most modern formulations of chemically amplified resists include the addition of a base quencher. Loaded at concentrations of 5–20% of the initial PAG loading, this base quencher is designed to neutralize any photogenerated acid that comes in contact with it. The main purpose of the base quencher is to neutralize the low levels of acid that might diffuse into the nominally unexposed regions of the wafer, thus making the final resist linewidth less sensitive to acid diffusion.
Baking a resist may have many purposes, from removing solvent to causing chemical amplification. In addition to the intended results, baking may also cause numerous unintended outcomes. For example, the light-sensitive component of the resist may decompose at temperatures typically used to remove solvent. The solvent content of the resist can impact diffusion and amplification rates for a chemically amplified resist. And all aspects of baking will probably affect the dissolution properties of the resist.

For conventional resists, sensitizer decomposition during post-apply bake (PAB) can be significant but can be monitored as a change in the bleachable absorption coefficient $A$. For chemically amplified resists, the PAG does not readily decompose.

Residual solvent in the film after baking can have two significant effects on the lithographic performance of a photoresist. Residual solvent increases the free volume and thus the diffusivity of acid during PEB. For a chemically amplified resist, especially when baking in a diffusion-controlled temperature regime, this increase in acid diffusivity can have quite a large impact. Secondly, residual solvent can impact resist dissolution rates, affecting both the average dissolution rate and the variation of dissolution rate with exposure dose. Also, solvent profiles with depth into the resist can cause surface inhibition during development.
Photoresist Development Kinetics

The chemistry of photoresists is designed to turn a spatial distribution of energy (the aerial image) into a spatial distribution of resist solubility. Ultimately, the dissolution process turns the continuous energy distribution of the projected aerial image into a binary resist image: either the resist is dissolved or it remains on the wafer.

**Photoresist dissolution** involves three processes: diffusion of the active component of the developer from the bulk solution to the surface of the resist, reaction of the developer with the resist, and diffusion of the product back into the solution. A simple but useful kinetic model is called the Mack 4-parameter dissolution rate model:

\[
r = r_{\text{max}} \left( \frac{a + 1}{a + (1 - m)^n} \right) + r_{\text{min}} \quad \text{where} \quad a = \frac{(n + 1)}{(n - 1)}(1 - m_{\text{TH}})^n
\]

where \( m_{\text{TH}} \) is the threshold inhibitor concentration, \( r_{\text{max}} \) is the dissolution rate of fully exposed resist, \( r_{\text{min}} \) is the dissolution rate of unexposed resist, and \( n \) is the dissolution selectivity parameter controlling the contrast of the resist.

![Graph showing the dissolution rate model with different values of n and m_{TH}](image-url)
Surface Inhibition

The basic kinetics of dissolution give the development rate of the resist as a function of the photoactive compound concentration remaining after the resist has been exposed to UV light. The most notable deviation from the kinetic theory is the surface inhibition effect. The inhibition, or surface induction, effect is a decrease in the expected development rate at the surface of the resist.

Several factors have been found to contribute to the surface inhibition effect. Baking of the photoresist can produce surface inhibition, and two possible mechanisms are thought to be likely causes. One possibility is an oxidation of the resist at the resist surface, resulting in reduced development rate of the oxidized film. Alternatively, the induction effect may be the result of reduced solvent content near the resist surface, which also results from baking the resist. Quite commonly, surface inhibition can be induced with the use of surfactants in the developer. Chemically amplified resists open a wide array of mechanisms for surface inhibition due to reduced amplification near the resist surface (caused, for example, by acid evaporation, base contamination, or reduced acid diffusion in the low solvent surface region).

Slower development of the top of the resist can lead to less resist loss for lines and profiles with sharper, more square tops. Proper magnitude and depth of surface inhibition can be used to counteract effects of absorption. Too much inhibition can lead to T-top-shaped profiles and a loss of linewidth control.

![Graph showing Relative Development Rate vs Relative Depth into Resist](image-url)
Developer Temperature and Concentration

The temperature of the developer solution during development can have a significant impact on resist performance. The speed (i.e., overall development rate) varies in a complicated way with temperature, usually resulting in the counterintuitive result of a “faster” resist process (i.e., a process requiring lower exposure doses) at lower developer temperatures. The shape of the development rate versus dose (or versus sensitizer concentration) curve will also vary considerably with temperature, leading to possibly significant performance differences. Since tight control of developer temperature is necessary, most development is done close to room temperature for easier control.

As one would expect, developer normality (the concentration of base) also impacts dissolution rates greatly. In general, higher normality produces higher dissolution rates. The important dissolution selectivity parameter $n$ (which is proportional to resist contrast) tends to have an optimum, essentially going to zero at very high and very low normalities. The combined impact of temperature and normality on the dissolution selectivity $n$ is quite complicated. A solution of 0.26N (2.38 weight percent) TMAH in water has become an industry standard, used by almost all resists. It is not at all clear that this is the optimum normality for every resist, but most resists have been designed with this normality in mind.
The development path can be generated by tracing the position of the resist surface through the development time. The path must always be perpendicular to the surface of the resist throughout the development cycle. Although the path begins vertically (since the resist surface is horizontal), a photore sist image is formed when the path turns to a nearly horizontal direction (for a 90° sidewall, the end of the path must be horizontal). It is the behavior of the horizontal part of the development path that determines the behavior of the resist profile (including the final dimension of the feature and the resist sidewall angle). As one might expect, the horizontal path is strongly affected by the exposure dose variation caused by the aerial image.

Good profile control is obtained when the development rate at the beginning of the path is much greater than the development rate at the end of the path. In other words, thinking of the path as segmented into vertical followed by horizontal development, good development spends very little time developing vertically, and most of the total development time going horizontally. To a good approximation, in the absence of surface inhibition, the final sidewall angle $\theta$ can be related to the development rates at the beginning and end of the path by

$$\cos \theta \approx \frac{\text{rate at path end}}{\text{rate at path start}}$$
NILS: The Normalized Image Log-Slope

The transition from bright to dark within an aerial image is the source of the information as to where the photore sist edge should be. The steeper the intensity transition, the better the edge definition of the image, and as a result the better the edge definition of the resist pattern. If the lithographic property of concern is the control of the photore sist linewidth, then the image metric that affects this lithographic result is the slope of the aerial image intensity near the desired photore sist edge \( \frac{dI}{dx} \). However, to be useful it must be properly normalized. Dividing the slope by the intensity will normalize out the effect of dose. The result is called the image log-slope (ILS):

\[
\text{Image Log-Slope} = \frac{1}{I} \frac{dI}{dx} = \frac{d \ln(I)}{dx}
\]

where this log-slope is measured at the nominal (desired) line edge position.

Since variations in the photore sist edge positions (line- widths) are typically expressed as a percentage of the nominal linewidth, the position coordinate \( x \) can also be normalized by multiplying the log-slope by the nominal linewidth \( w \) to give the normalized image log-slope (NILS).

\[
\text{NILS} = w \frac{d \ln(I)}{dx}
\]

The NILS is usually the best single metric to judge the lithographic usefulness of an aerial image.
NILS: The Log-Slope Defocus Curve

Since the **NILS** is a measure of image quality, it can be used to investigate how optical parameters affect image quality. One of the most obvious examples is **defocus**. The effects of focus on an image are quite familiar: as an image goes out of focus, it gets blurry. Specifically, the edges become blurred so that it is harder to distinguish the exact point where the image transitions from bright to dark. In other words, the slope of the aerial image at the edge between bright and dark features (the **NILS**) is reduced as we go out of focus.

By plotting **NILS** versus focus, the sensitivity of the image to defocus can be quantified. An estimate of the minimum acceptable **NILS** (the smallest value of **NILS** that still allows the feature to be printed with acceptable quality) can lead to an estimate of the depth of focus. Using the log-slope defocus curve, image parameters (for example, numerical aperture or partial coherence) can be optimized for maximum depth of focus.
NILS: Image Optimization

To see how the log-slope defocus curve can be used to understand imaging, consider the effects of wavelength and numerical aperture on the focus behavior of an aerial image. The first figure shows how the NILS of a 0.25 μm line-space pattern degrades with defocus for three different wavelengths (365 nm, 248 nm, and 193 nm). It is clear from the plot that the lower wavelength provides better image quality for the useful range of defocus. For a given minimum acceptable value of NILS, the lower wavelength will allow acceptable performance over a wider range of focus.

The impact of numerical aperture (NA) is a bit more complicated. The log-slope defocus curves for three different numerical apertures (again, a 0.25 μm line-space pattern is shown here) cross each other. If one picks some minimum acceptable NILS value, there will be an optimum NA that gives the maximum depth of focus (for example, a minimum NILS value of 2.5 has the best depth of focus when NA = 0.6).
The aerial image, through the process of exposure, transfers its information into a latent image, a spatial distribution of exposed and unexposed resist. For a resist with first-order kinetics whose optical properties do not change with exposure dose (commonly the case for chemically amplified resists), the latent image \( m(x, y, z) \) is related to the aerial image \( I(x, y) \) by
\[
m(x, y, z) = e^{-CE_zI(x,y)}
\]
where \( C \) is the exposure rate constant and \( E_z \) is the exposure dose at a depth \( z \) into the resist that would result for an open frame exposure of incident dose \( E \).

The slope or gradient of the latent image is a good metric of latent image quality. By taking the derivative of the above equation,
\[
\frac{\partial m}{\partial x} = m \ln(m) \frac{\partial \ln I}{\partial x}
\]
Thus, the latent image gradient is directly proportional to the image log slope (and thus the normalized latent image gradient is proportional to NILS).

The term \( m \ln(m) \) is exposure dependent (\( m \) being the relative amount of resist sensitizer that has not been exposed at the point where the latent image gradient is being described). A plot of \( -m \ln(m) \) versus \( m \) shows that there is one exposure dose (one value of \( m \)) that will maximize the latent image quality. When \( m = e^{-1} \approx 0.37 \), the value of \( -m \ln(m) \) reaches its maximum and the full information of the aerial image is transferred into the resist during exposure.

Often, dose is used as just a “dimension dial,” adjusting dose to obtain the desired feature size. If the dose is near the optimum, this approach is valid. If, however, the dose used is significantly off from optimum (say, very underexposed), changing dose will affect both dimension and overall latent image quality.
NILS: PEB Optimization

Diffusion during PEB will spread out the latent image, degrading the information present in the image and decreasing the gradient near the line edge. The change in the latent image gradient (LIG) due to diffusion can be described approximately by

$$\frac{\partial m^*}{\partial x} \approx \frac{\partial m}{\partial x} e^{-\sigma^2/2L^2}$$

where $\sigma$ is the diffusion length and $L$ is a characteristic length related to the width of the edge region (the range over which the original latent image gradient is nonzero). For a pattern of small lines and spaces, $L$ is about equal to the half pitch of the pattern. Obviously, increased diffusion (indicated by a larger diffusion length) results in a greater degradation of the latent image gradient. Also, smaller features (smaller values of $L$) are more sensitive to diffusion, showing a greater fractional decline in the latent image gradient for a given diffusion length.

For chemically amplified resists, diffusion during PEB is accompanied by a reaction that changes the photogenerated acid latent image into a latent image of blocked and deblocked polymer. Since reaction and diffusion occur simultaneously, rigorous evaluation of the impact on the latent image gradient requires full lithography simulation approaches. However, a simple approach can give important insights into the trade-offs.

Ignoring acid loss before or during the PEB, a simple mechanism for a first-order chemical amplification gives

$$m^*(x) = e^{-\alpha[1-m(x)]}$$
where $\alpha$ is the amplification factor, proportional to the PEB time and exponentially dependent on PEB temperature. For a given level of required amplification, thermal and exposure doses can be exchanged so long as $\alpha(1-m)$ is kept constant. The gradient of this new latent image after amplification is then

$$\frac{\partial m^*}{\partial x} = -m^* \ln(m^*) \left( \frac{1}{1-m} \frac{\partial m}{\partial x} \right)$$

$$= -m^* \ln(m^*) \left[ \frac{m \ln(m)}{1-m} \right] \frac{\partial \ln I}{\partial x}$$

For a given latent image after exposure [given $m(x)$], the optimum latent image after amplification occurs when $m^* = e^{-1}$, giving $\alpha(1-m) = 1$.

If we approximate the actual reaction-diffusion system with a simplified acid diffusion (without reaction) followed by amplification (without diffusion) mechanism, the solution can be easily found by combining the above equations and setting the exposure dose to be always adjusted to give the optimum final gradient for any amount of amplification [i.e., by setting $\alpha(1-m) = 1$]. The result is an optimum amount of bake that balances the benefits of more amplification with the detriments of more diffusion.
NILS: Development Optimization

The fundamental chemical response of interest is the change in dissolution rate as a function of the exposure dose seen by the resist. A plot of development rate $R$ versus exposure dose $E$ on a log-log scale is called a Hurter-Driffield (H-D) curve and allows for the definition of the photoresist contrast, $\gamma$. Quite simply, the photoresist contrast is the maximum slope of the development rate H-D curve.

$$\gamma \equiv \left. \frac{\partial \ln R}{\partial \ln E} \right|_{\text{max}}$$

To be a bit more general, a photoresist contrast function $\gamma(E)$ can be defined as the slope of the H-D curve at any point.

The photoresist contrast is a measure of the discrimination of the resist with respect to exposure. Higher contrast means that a given change in dose will result in a greater change in development rate. This point can be seen clearly using the lithographic imaging equation, derived from the definition of photoresist contrast:

$$\frac{\partial \ln R}{\partial x} = \gamma(E) \frac{\partial \ln I}{\partial x}$$

The contrast turns the image log-slope into a gradient of development rate.
NILS: Total Process Optimization

It is useful to think about lithography as a sequence of information transfer steps. A designer lays out a desired pattern in the form of simple polygon shapes. This layout data drives a mask writer so that the information of the layout becomes a spatial variation of transmittance (chrome and glass, for example) of the photomask. Next, the mask is used in a projection imaging tool to create an aerial image of the mask. However, due to the diffraction limitations of the wavelength and lens numerical aperture, the information transmitted to the wafer is reduced. The aerial image, through the process of exposure, transfers its information into a latent image, followed by PEB, development and etch. At each step of the process, information is lost.

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<td></td>
<td>Profile (CD, sidewall angle, resist loss)</td>
<td>latitude</td>
</tr>
</tbody>
</table>
Defining Photoresist Linewidth

A cross-section of a photoresist profile has, in general, a very complicated 2D shape. In order to compare the shapes of two different profiles, one must find a convenient description for the shapes of the profiles that somehow reflects their salient qualities. The most common description is to model the resist profile as a **trapezoid**. Thus, three numbers can be used to describe the profile: the width of the base of the trapezoid (linewidth \( w \)), its height (profile thickness \( D \)), and the angle that the side makes with the base (sidewall angle \( \theta \)). Obviously, to describe such a complicated shape as a resist profile with just three numbers is a great, though necessary, simplification. The key to success is to pick a method of fitting a trapezoid to the profile that preserves the important features of the profile, is numerically practical, and as a result is not overly sensitive to slight changes in the profile.

The trapezoidal feature model can cause an inherent uncertainty in the measurement of a resist feature whenever the actual resist shape differs significantly from a trapezoid, as is often seen when imaging out of focus.

![Focus below and above the resist](image-url)
Critical Dimension Control

Fundamentally, errors in the final dimension of a feature are the result of errors in the tools, processes, and materials that affect the final critical dimension (CD). Suppose the influence of each input variable on the final CD were expressed in a mathematical form, such as

\[ CD = f(v_1, v_2, v_3, \ldots) \]

where \( v_i \) are the input (process) variables. Given an error in each process variable \( \Delta v_i \), the resulting CD error can be computed from a Taylor expansion. Ignoring the higher-order terms (that is, assuming a linear response), as well as the cross terms,

\[ \Delta CD = \Delta v_1 \frac{\partial CD}{\partial v_1} + \Delta v_2 \frac{\partial CD}{\partial v_2} + \cdots \]

Each \( \Delta v_i \) represents the magnitude of a process error. Each partial derivative \( \frac{\partial CD}{\partial v_i} \) represents the process response, the response of CD to an incremental change in the variable. This process response can be expressed in many forms; for example, the inverse of the process response is called process latitude.

The linear error equation above can be modified to account for the nature of the errors at hand. In general, CD errors are specified as a percentage of the nominal CD. For such
a case, the goal is usually to minimize the relative CD error, $\Delta CD/CD$:

$$\frac{\Delta CD}{CD} = \Delta v_1 \frac{\partial \ln CD}{\partial v_1} + \Delta v_2 \frac{\partial \ln CD}{\partial v_2} + \cdots$$

Also, many sources of process errors result in errors that are a fraction of the nominal value of that variable (for example, illumination nonuniformity in a stepper produces a dose error that is a fixed percentage of the nominal dose). For such error types, it is best to use a relative process error, $\Delta v_i/v_i$:

$$\frac{\Delta CD}{CD} = \frac{\Delta v_1}{v_1} \frac{\partial \ln CD}{\partial v_1} + \frac{\Delta v_2}{v_2} \frac{\partial \ln CD}{\partial v_2} + \cdots$$

These equations are simple, but reveal a very important truth about error propagation and the control of CD. There are two distinct ways to reduce $\Delta CD$: reduce the magnitude of the individual process errors ($\Delta v_i$), or reduce the response of CD to that error ($\partial CD/\partial v_i$). Reducing the magnitude of process errors is generally considered a process control activity. Reducing the process response is a process optimization activity.

A note of caution: the derivation of the above equations assumed that the process errors were small enough to be linear and independent in their influence on CD. This will not always be the case in a real lithographic process. One need only consider the two variables of focus and exposure to see that the response of CD is certainly nonlinear and the two variables are highly dependent on each other. Usually, a linear expansion is most useful as a guide to understanding rather than as a computational tool.
Critical Dimension Control: Effect on Devices

A classic example of the influence of CD control is at the polysilicon gate level of standard CMOS logic devices. Physically, the polysilicon gate linewidth controls the effective gate length $L_{eff}$, which is directly proportional to the switching time of the transistor. Thus, narrower gates tend to make transistors that can switch on and off at higher clock speeds. But transistors are designed for a specific gate length. As the gate length gets smaller than this designed value, the transistor “leaks” current when it should be off, causing an increase in power consumption.

When printing a chip with millions of transistor gates, the gate lengths take on a distribution of values across the chip. This across-chip linewidth variation (ACLV) produces a range of transistor behaviors. The overall speed with which an operation can be performed (i.e., the fastest clock speed) is limited by the slowest (largest gate CD) transistor in the critical path for that operation. On the other hand, the reliability of the chip is limited by the smallest gate CDs on the chip due to leakage current resulting in high power consumption.
Overlay Control

An integrated circuit is built up layer by layer to create a complex, 3D structure of many different materials. Anywhere from 20 to 30 separate lithography steps are performed on a wafer to create a modern chip. When printing a small pattern, one must not only get the size of that feature correct, one must place that feature on the wafer at just the right spot so that it can work correctly with the patterns defined by previous lithography steps. Overlay is the measure of how well one pattern is placed on a wafer relative to a previously defined pattern.

Overlay errors have a definite impact on how small we can make the circuit device. Given a certain expected amount overlay error, the chip must be designed with enough room between the various components in order to tolerate these errors without causing device failure. As a result, the transistors are not as small and are not packed as tightly together as they might otherwise be. The biggest impact of adding tolerance for overlay errors is a decrease in packing density and a subsequent increase is chip size. Thus, overlay control affects price per function and functions per chip. Continuously improving our ability to control overlay is almost as important as improving our ability to control CD.
Line Edge Roughness

When variations in the width of a resist feature occur quickly over the length of the feature, this variation is called linewidth roughness. When examining these variations along just one edge it is called line edge roughness (LER). LER becomes important for feature sizes on the order of 100 nm or less, and can become a significant source of linewidth control problems for features below 50 nm. LER is caused by a number of statistically fluctuating effects at these small dimensions such as shot noise (photon flux variations), statistical distributions of chemical species in the resist such as photoacid generators, the random walk nature of acid diffusion during chemical amplification, and the nonzero size of resist polymers being dissolved during development. It is unclear which process or processes dominate in their contribution to LER.

LER is usually characterized as the $3\sigma$ deviation of a line edge from a straight line, though a more complete frequency analysis of the roughness can be valuable as well. For 193-nm lithography, LER values of 4 nm and larger are common. LER is inversely proportional to the normalized image log-slope (NILS), so LER generally gets worse as an image goes out of focus and for higher resolution patterns.

The impact of LER on device performance depends on the specific device layer and specific aspects of the device technology. For lithography generations below 100 nm, typical specifications for the $3\sigma$ LER are about 5% of the nominal CD. It is possible that LER will become the main limiter of CD control below 65-nm production.
Metrology: Critical Dimension

In the early days of semiconductor processing, optical microscopes were used to measure the dimensions of important features on the wafer. Today, feature sizes are too small for precise optical measurements. The most common metrology tool for CD measurement is the scanning electron microscope (SEM). A sample is scanned by a focused beam of fairly low-energy electrons. Secondary and/or backscattered electrons are then detected as a function of beam position to form an image. The resolution of the image is a function of the beam size and the electron scattering range inside the materials being imaged. Charging of the resist pattern can also cause blurring of the image and inaccuracies in the measurement.

Steps in the height of the materials (such as the edge of a photoresist feature) produce increased electron production to the detector, making edges of the features appear brighter. Analysis of the image along a cross-section gives a linescan of grayscale values. Various algorithms can be used to detect the edges and measure the width of the feature.

A higher-accuracy alternative to the SEM is the slower and more expensive atomic force microscope (AFM). A special narrow tip of silicon is brought so close to the sample that atomic forces attract or repel the tip. By detecting the height of the tip to produce a constant force, a map of the surface height of the sample is obtained.
Metrology: Overlay

Overlay control requirements are, as a rule of thumb, about one third of the minimum feature size. Typically, any control application requires metrology precision equal to one tenth to one fifth of the control requirement. Thus, overlay measurement precision requirements today are just a few nanometers, and are always shrinking.

Most overlay today is measured using optical imaging of wafer patterns printed with two different lithography steps. The box-in-box structure is the most common, where features are big enough (about 2 µm) to be readily imaged in a broadband microscope of moderately high numerical aperture. Edge detection finds small difference in right-left and top-bottom gaps between the two boxes, which are translated into overlay error vectors.

Errors in overlay measurement come from odd aberrations in the measurement optics, such as coma (giving rise to TIS, tool-induced shift) and asymmetries in the physical shape of the measurement target (giving rise to WIS, wafer-induced shift).

Analysis of overlay data is fit to models of typical overlay error sources, such as translation and rotation of the reticle or the wafer, and magnification errors. Model coefficients are then used to correct these error sources for subsequent wafers.
The Process Window

Since the effect of focus is dependent on exposure, the only way to judge the response of the process to focus is to simultaneously vary both focus and exposure in a focus-exposure matrix. Plotting linewidth as a function of focus for different exposures is called a Bossung plot. Of course, one output as a function of two inputs can be plotted in several different ways. For example, the Bossung curves could also be plotted as exposure latitude curves (linewidth versus exposure) for different focus settings. Probably the most useful way to plot this 2D data set is a contour plot—contours of constant linewidth versus focus and exposure.

The contour plot form of data visualization is especially useful for establishing the limits of exposure and focus that allow the final image to meet certain specifications. Rather than plotting all of the contours of constant CD, one could plot only the two CDs corresponding to the outer limits of
The Process Window (cont’d)

acceptability—the CD specifications. Because of the nature of a contour plot, other variables can also be plotted on the same graph. The figure below shows an example of plotting contours of CD (nominal ±10%), 80° sidewall angle, and 10% resist loss all on the same graph. The resulting overlapping region is called the process window—the region of focus and exposure that keeps the final resist profile within all three specifications.

The focus-exposure process window is one of the most important plots in lithography since it shows how exposure and focus work together to affect linewidth, sidewall angle, and resist loss. The process window can be thought of as a process capability—how the process responds to changes in focus and exposure. An analysis of the error sources for focus and exposure in a given process will give a process requirement. If the process capability exceeds the process requirements, yield will be high. If, however, the process requirement is too large to fit inside the process capability, yield will suffer.

The process window is used to measure the depth of focus (DOF).
Depth of Focus

To measure the size of a focus-exposure process window, the first step is to graphically represent errors in focus and exposure as a rectangle on the same plot as the process window. The width of the rectangle represents the built-in focus errors of the processes, and the height represents the built-in dose errors. The problem then becomes one of finding the maximum rectangle that fits inside the process window. However, there is no one answer to this question. There are many possible rectangles of different widths and heights that are “maximum,” i.e., they cannot be made larger in either direction without extending beyond the process window. The result is a very important trade-off between exposure latitude and depth of focus (DOF).

If all focus and exposure errors were systematic, then the proper graphical representation of those errors would be a rectangle. If, however, the errors were randomly distributed, then a surface of constant probability of occurrence is an ellipse.

Using either a rectangle for systematic errors or an ellipse for random errors, the size of the errors that can be tolerated for a given process window can be determined. Taking the rectangle as an example, one can find the maximum rectangle that will fit inside the processes window. Every maximum rectangle is determined and its height...
Depth of Focus (cont'd)

(the exposure latitude) is plotted versus its width (depth of focus, DOF). Likewise, assuming random errors in focus and exposure, every maximum ellipse that fits inside the processes window can be determined. The horizontal width of the ellipse would represent a 3σ error in focus, while the vertical height of the ellipse would give a 3σ error in exposure. A plot of the height versus the width of this family of maximal error shapes gives the exposure latitude versus DOF curve.

The exposure latitude versus DOF curve provides the most concise representation of the coupled effects of focus and exposure on the lithography process. Each point on the exposure latitude vs. DOF curve is one possible operating point for the process. The user must decide how to balance the trade-off between DOF and exposure latitude. One approach is to define a minimum acceptable exposure latitude and then operate at this point. This has the effect of maximizing the DOF of the process. In fact, this approach allows for the definition of a single value for the DOF of a given feature for a given process. The depth of focus of a feature can be defined as the range of focus that keeps the resist profile of a given feature within all specifications (linewidth, sidewall angle, and resist loss) over a specified exposure range.
**Resolution**

**Resolution** is the smallest feature that you are able to print (with a given process, tool set, etc.) with sufficient quality. For a production engineer, the manufacturable resolution is the smallest feature size that provides adequate yield for a device designed to work at that size.

In practice, process variations limit resolution since smaller features have inherently less process latitude. It is common to use focus and exposure dose as representative process variables, so that resolution is defined as the smallest feature of a given type that can be printed with a specified **depth of focus**.

For contact holes, the **point spread function** of the lens forms a good measure of resolution. For dense lines and spaces, the smallest pitch is limited by how many **diffraction orders** can pass through the lens (and thus is limited by $\lambda/NA$). For an isolated feature, there is no hard resolution cut-off. Instead, linewidth control is the limiter.
The easiest (though not the only) way to derive the Rayleigh resolution criterion is with the imaging of equal lines and spaces. For a pitch \( p \), the diffraction pattern will be discrete diffraction orders at spatial frequencies that are multiples of \( 1/p \). The lens allows a portion of the diffraction pattern to pass through and be used to form the image. The largest spatial frequency that can make it through the lens is \( NA/\lambda \).

In order to form an image, at least two diffraction orders must go through the lens. Assuming coherent illumination, this means the zero order and the two first orders must go through the lens. The smallest pitch that allows this to happen would put the first diffraction orders exactly at the edge of the lens:

\[
\frac{1}{p_{\text{min}}} = \frac{NA}{\lambda}
\]

For equal lines and spaces, the resolution is one half of this minimum pitch:

\[
R = \frac{p_{\text{min}}}{2} = 0.5 \frac{\lambda}{NA}
\]

Since the above criterion for resolution is fairly specific (equal lines and spaces with coherent illumination), it is common in lithography applications to generalize somewhat and simply say that resolution is directly proportional to \( \lambda/NA \), using \( k_1 \) as the proportionality factor:

\[
R = k_1 \frac{\lambda}{NA}
\]
Rayleigh Criteria: Depth of Focus

Defocusing of a wafer is equivalent to causing an aberration—an error in curvature of the actual wavefront relative to the desired wavefront. The distance from the desired to the “defocused” wavefront is called the optical path difference (OPD). Describing the position within the exit pupil by an angle $\theta$, the optical path difference is

$$OPD = \delta(1 - \cos \theta) = \frac{1}{2} \delta \left( \sin^2 \theta + \frac{\sin^4 \theta}{4} + \frac{\sin^6 \theta}{8} + \ldots \right)$$

The diffraction pattern of an array of small lines and spaces is a set of discrete diffraction orders, points of light entering the lens spaced regularly depending only on the wavelength of the light $\lambda$ and the pitch $p$ of the mask pattern. The angle of the first diffracted order is $\sin \theta = \lambda/p$.

For small lens numerical apertures, the largest angles going through the lens are also quite small and the higher-order terms in the Taylor series for OPD can be ignored.

$$OPD \approx \frac{1}{2} \delta \sin^2 \theta$$

If the OPD were set to a quarter of the wavelength, the zero and first diffracted orders would be exactly 90° out of phase with each other. At this much OPD, the zero order would not interfere with the first orders and no pattern would be formed. The true amount of tolerable OPD must be less than this amount (as indicated by the factor $k_2$).

$$OPD_{\text{max}} = k_2 \frac{\lambda}{4}, \text{ where } k_2 < 1.$$ Thus,

$$DOF = 2\delta_{\text{max}} = k_2 \frac{\lambda}{\sin^2 \theta} = k_2 \frac{\lambda}{NA^2}$$

where the last expression on the right applies only at the resolution limit, so that the first diffracted orders are at the edge of the lens. Note that this Rayleigh DOF criterion applies only to low numerical apertures when imaging dense patterns at the resolution limit.
**Mask Error Enhancement Factor (MEEF)**

For “linear” imaging, mask critical dimension (CD) errors translate directly into wafer CD errors (taking into account the reduction factor of the imaging tool). If, however, the features of interest are near the edge of the linear resolution limit, the assumption of linear imaging falls apart. Near the resolution limit, small errors in the mask dimension can cause large errors in the final resist CD. This amplification of mask errors is characterized by the **mask error enhancement factor (MEEF)**. The MEEF is defined as the change in resist CD per unit change in mask CD:

\[
\text{MEEF} = \frac{\partial \text{CD}_{\text{resist}}}{\partial \text{CD}_{\text{mask}}}
\]

where again the mask CD is in wafer dimensions. Regions where the MEEF is significantly greater than 1 are regions where mask error may come to dominate CD control on the wafer.

Optical proximity correction techniques allow us to lower the linear resolution, but without improving the MEEF.
Attempts to improve the process window by optical means (sometimes called optical “tricks”) include:

- Optimization of the mask pattern shape (optical proximity correction, OPC)
- Optimization of the angles of light illuminating the mask (off-axis illumination, OAI)
- Adding phase information to the mask (phase-shift masks, PSM)
- Control of the polarization of the illumination

Collectively, these optical approaches are known as resolution enhancement technologies (RETs). While some techniques improve feature resolution at the expense of pitch resolution, many of the RET approaches can improve pitch resolution and increase the process window simultaneously. However, the most promising RETs (especially the best PSMs techniques) require a revolution in chip layout design that has yet to occur.
Phase-Shift Masks

Phase-shift masks (PSMs) work by adding phase information to the mask in addition to amplitude information. A binary chrome-on-glass mask encodes the information about where to position resist edges using chrome (with zero amplitude transmittance) and glass (with 100% amplitude transmittance). A phase-shift mask relies on the fact that light passing through a transparent media will undergo a phase change as a function of its optical thickness, the refractive index times the physical thickness. Thus, light passing through a certain thickness of quartz will have a different phase transmittance than light passing through the same thickness of air. By adjusting the thickness of the quartz, any phase difference can be obtained.

By setting the phase shift to be $180^\circ$, high-resolution imaging with good depth of focus can be obtained. Light from shifted and unshifted parts of the mask, when combined, will interfere and cancel out at the image plane due to the $180^\circ$ phase shift. If the shifted and unshifted light is of equal quantity the cancellation will be complete. A $0–180^\circ$ phase edge on a mask will print as a narrow dark line. An array of these edges will print patterns of lines and spaces with widths as low as $0.25\lambda/NA$. Common types of PSMs are alternating (pictured here) and attenuated PSMs. Practical implementation of PSMs is limited by phase termination problems and mask fabrication difficulties.
Phase-Shift Masks: Alternating

**Alternating phase-shift masks** (AltPSM) are used to print narrow lines in positive photoresist by making the clear areas on either side of the line of opposite phase. Thus, the phase cancellation effect of light diffracted from either side of the line will keep the line dark and narrow, even when out of focus. AltPSM is a “strong” PSM that can maximize resolution and depth of focus.

AltPSM suffers from two very important drawbacks. On the mask fabrication side, a subtractive etch to create the phase-shifted space results in reduced amplitude transmittance and non-perfect 180° phase transmittance, both of which vary with the width of the shifted space. Biasing the etched spaces wider and allowing the etch to undercut the chrome can alleviate but not eliminate the problem.

The second difficulty is called the **phase conflict** problem. Attempting to phase shift an arbitrary layout of lines will invariably lead to phase conflicts: no phase shift where you do want it, and a phase shift where you don’t want it. The first type results in a lack of phase shift across a critical feature when there is an odd wrapping of phase assignments. This “non-shifted” feature will not properly print. The second type is also called the termination problem since it usually occurs at the end of a line. Alternating phase across each side of a line will result in those two phases meeting at the line end. Whenever two opposing phases meet, a dark interference line is created causing an unwanted resist line to print. Generally, a second “trim” exposure is required to remove unwanted phase prints.
Phase-Shift Masks: Attenuated

Attenuated phase-shift masks (also called the embedded phase-shift masks, or EPSM) have been very widely adopted for contact hole and via printing, and are becoming fairly mainstream for other critical lithography layers as well. This type of PSM is generally called a “weak” shifter—it provides only a portion of the full resolution and depth of focus potential of alternating PSM. Its great advantage is the simplicity and low cost of replacing chrome on glass (COG) masks, the non-phase shift alternative. Essentially, an existing design based on COG can be converted to an EPSM by simply recalibrating the optical proximity correction (OPC) models used to apply OPC to the design. Mask manufacturing, while certainly more difficult than COG, is not dramatically different (the chrome is replaced by a more complex absorber such as molybdenum silicon) and only somewhat more costly. In short, the transition from COG to EPSM-based lithography presents no major hurdles.

Typical EPSM materials have 6% intensity transmittance and a 180° phase shift, though higher transmittance masks are sometimes used. The resulting 0–180° phase edge makes the aerial image edges steeper and better defined. The overall background transmittance of 6% can cause problems when nearby features interact constructively to produce sidelobes, unwanted regions of high intensity. If the intensity in the sidelobe becomes too high, it could print as an unwanted hole in the photoresist.

While EPSM on its own does not provide the resolution and depth of focus enhancement that can come with AltPSM, the combination of EPSM with off-axis illumination can be optimized to give very good results.
Optical Proximity Effects

Proximity effects are the variations in the linewidth of a feature (or the shape for a 2D pattern) as a function of the proximity of other nearby features. The simplest example of an optical proximity effect is the difference in printed linewidth between an isolated line and a line in a dense array of equal lines and spaces, called the iso-dense print bias.

The proximity effect is very feature size dependent. For large features, the diffraction patterns for isolated and dense lines are similar, giving very little differences in the aerial images. As feature size shrinks, the differences grow. Since the iso-dense print bias is predominantly an optical effect, the optical parameters of the imaging tool affects the magnitude of the bias.

Proximity effects are more completely characterized by measuring resist linewidth versus pitch for different mask CDs. More complex proximity effects include line end shortening and corner rounding.
For a given lithography process, the difference between the “as drawn” designed feature sizes and the actual printed wafer dimensions can be characterized and corrected by biasing the mask (i.e., changing the actual feature width on the mask to be different from the desired resist width). This type of geometry-dependent mask biasing is commonly referred to as optical proximity correction (OPC), although a more descriptive name might be “mask shaping.”

There are three basic styles of OPC. The simplest and most important is geometry biasing—changing the feature sizes on the mask. To reduce line edge shorting and to improve corner fidelity, serifs can be added to the corners and endcaps (hammerheads) to the line ends. Finally, sub-resolution assist features (SRAFs) can be added to make isolated features behave more like dense features.

Automated OPC software can take an entire design and, using rules and/or lithography models, adjust the edge positions of the design to achieve a better match to the desired printed shapes.
**Off-Axis Illumination**

**Off-axis illumination** refers to any illumination shape that significantly reduces or eliminates the “on-axis” component of the illumination, that is, the light striking the mask at near normal incidence. By tilting the illumination away from normal incidence, the diffraction pattern of the mask is shifted within the objective lens. Placing those diffraction orders that make it through the lens evenly about the center of the lens leads to improved depth of focus (DOF). Thus, the main advantage of off-axis illumination is an increase in depth of focus for small pitch patterns.

The distance between diffraction orders in sigma space is $\frac{\lambda}{(pNA)}$. To center the zero and first orders about the center of the lens, the zero order must by shifted by $\frac{\lambda}{(2pNA)}$ in sigma space. Thus, this becomes the optimum illumination tilt to give maximum depth of focus. Tilting in both positive and negative directions produces an illumination called dipole and adds the desirable effect of reducing sensitivity to lens aberrations such as image placement error. Note that the optimum illumination tilt is pitch dependent.

If both vertical and horizontal lines are to be imaged together on the same mask, an illumination shape must be used that provides optimum tilts for both geometries. The simplest shape that provides this optimum tilt for both horizontal and vertical line/space patterns is called *quadrupole illumination*. In sigma space, the radial position of
the center of each pole with respect to the center of the lens that gives optimum DOF is \( \sqrt{2} \lambda / (2pNA) \). Note that this positioning of the quadrupoles gives the same horizontal and vertical spacing between poles as in the dipole case, but places them closer to the edge of the lens aperture.

While the quadrupole shape provides optimum performance for vertical and horizontal lines, other orientations (such as a line/space array oriented at 45°) will not be optimum. For any orientation of lines, the optimum dipole for that pattern will be spread in a direction perpendicular to the line orientation, and can be shifted parallel to the lines in any amount that keeps the dipoles within the lens. If the mask will contain arbitrary orientations of lines, many rotations of the dipoles will produce an annulus of illumination. The optimum center of the annular ring is the same as the optimum dipole position.

For each illumination shape discussed—dipole, quadrupole, and annular illumination—there is one size that maximizes the depth of focus for a given pitch. While pitches close to this optimum will get most of the benefit of the off-axis illumination, pitches sufficiently far away from the optimum will receive little or no benefit. In fact, the worst-case pitch for any given off-axis configuration would put one of the diffracted orders dead center in the lens, the situation that off-axis illumination is designed to avoid. This worst-case pitch occurs at exactly twice the pitch for which the illumination was optimized. Since this pitch receives none of the focus-enhancing benefits of the off-axis illumination, it is sometimes called a “forbidden” pitch, indicating the lithographer’s desire that this pitch be avoided during circuit design.
Lithography Simulation

In the 30+ years since optical lithography modeling was first introduced to the semiconductor industry, it has gone from a research curiosity to an indispensable tool for research, development, and manufacturing. There are four major uses for lithography simulation: 1) as a research tool, performing experiments that would be difficult or impossible to do any other way, 2) as a development tool, quickly evaluating options, optimizing processes, or saving time and money by reducing the number of experiments in the fab, 3) as a manufacturing tool, for troubleshooting process problems and determining optimum process settings, and 4) as a learning tool, to help provide a fundamental understanding of all aspects of the lithography process.

Some of the most common-use cases for lithography simulation are:

- Film stack optimization (including BARC)
- Process window prediction
- NA/σ optimization
- Overall process optimization and specification
- Troubleshooting/root cause analysis
- OPC and OPC verification
- RET design and development
- NGL evaluation and projection

Today, commercial lithography simulation tools such as PROLITH are ubiquitous throughout the industry.
Moore's Law

In 1965, Gordon Moore observed that since the first planar transistor was built in 1959, the number of components per chip was doubling every year. Extrapolating this trend for a decade, Moore predicted that chips with 65,000 components would be available by 1975.

In 1975 Moore revisited his 1965 prediction and divided the advances in circuit complexity among its three principle components: increasing chip area, decreasing feature size, and improved device and circuit designs. Minimum feature sizes were decreasing by about 10% per year, chip area was increasing by about 20% each year, and design cleverness made up the rest of the improvement (about 33%).

Moore also extrapolated each individual trend into the future and predicted an end to design cleverness improvements, and thus a change in the slope of his overall trend from doubling every year to doubling every two years. However, Moore’s prediction of a slowdown was too pessimistic. The industry followed a “new” Moore’s Law trend of doubling of transistor counts per chip every eighteen months or so throughout the 1980s and early 1990s.

By the mid-1990s Moore’s Law had become a self-fulfilling prophesy, now enshrined as the International Technology Roadmap for Semiconductors (ITRS), which continues to be updated every two years or so.
Next-Generation Lithography (NGL)

Since the mid-1970s, nearly all semiconductor manufacturing has used projection optical lithography due to its good resolution and low cost. There have been many lithography approaches with much higher resolution (such as electron beam direct-write and x-ray proximity lithographies) that are not used for manufacturing due to cost rather than technical capability. Immersion lithography at 193-nm wavelength is expected to allow printing of pitches down to 80 nm or so, but it is not clear if continued evolutionary improvements of this technology beyond this regime is practical. As a result, several next-generation lithography (NGL) technologies are being developed.

While direct-write electron-beam lithography is too slow to be practical, projection e-beam might overcome this throughput hurdle. Drawbacks include the need for stencil masks and Coulomb-Coulomb interactions within the e-beam optics that limits current and thus throughput.

Extreme Ultraviolet (EUV) lithography uses light at a wavelength near 13 nm. At this “soft x-ray” wavelength, multilayer mirrors can be made with about 70% reflectivity (refractive lenses are not possible). Thus, using mirrored imaging tools with numerical apertures up to 0.3, pitches down to 40 nm can be printed. Several technical roadblocks remain, however. Because of the low mirror efficiency, much light is lost and bright sources are not yet available. At 13 nm, making mirrors with sufficient smoothness (as a fraction of the wavelength) is very hard, and current systems suffer from high flare levels. Resists with sufficient sensitivity and low line edge roughness have yet to be developed. Finally, defect levels on photomasks are several orders of magnitude too high to be practical as of yet.

Imprint lithography uses the seemingly low-tech process of embossing to print ultrafine patterns (below 20 nm). While very low cost, it uses 1 × templates that are hard to make and requires direct contact with the wafer, with unknown defect consequences.
Equation Summary

Maxwell's Equations (in CGS):
\[
\vec{\nabla} \times \vec{H} - \frac{1}{c} \frac{\partial \vec{D}}{\partial t} = \frac{4\pi}{c} \vec{J}
\]
\[
\vec{\nabla} \times \vec{E} + \frac{1}{c} \frac{\partial \vec{B}}{\partial t} = 0
\]
\[
\vec{\nabla} \cdot \vec{B} = 0
\]
\[
\vec{\nabla} \cdot \vec{D} = \frac{4\pi}{c} \rho
\]

Material Equations:
\[
\vec{J} = \sigma \vec{E}, \quad \vec{D} = \varepsilon \vec{E}, \quad \vec{B} = \mu \vec{H}
\]

Plane wave traveling along +z:
\[
E(P, t) = A \cos(\omega t - kz)
\]

Phasor representation of \( E(P, t) \):
\[
U(P) = A(P)e^{-i\phi(P)}, \quad E(P, t) = \text{Re}\{U(P)e^{-i\omega t}\}
\]

Fourier transform of 1D mask pattern:
Isolated space:
\[
T_m(f_x) = \frac{\sin(\pi w f_x)}{\pi f_x}
\]
Dense space:
\[
T_m(f_x) = \sum_{n=-\infty}^{\infty} \frac{\sin(\pi w f_x)}{\pi f_x} \delta\left( f_x - \frac{n}{p} \right)
\]

Pupil function of ideal lens:
\[
P(f_x, f_y) = \begin{cases} 
1, & \sqrt{f_x^2 + f_y^2} < NA/\lambda \\
0, & \sqrt{f_x^2 + f_y^2} > NA/\lambda 
\end{cases}
\]

Electric field image at the wafer:
\[
E(x, y) = F^{-1}\{T_m(f_x, f_y)P(f_x, f_y)\}
\]

Zernike formulae for aberrations:
X Tilt: \( R \cos \theta \)
Y Tilt: \( R \sin \theta \)
Power (focus): \( 2R^2 - 1 \)
3rd-Order Astigmatism: \( R^2 \cos 2\theta \)

3rd-Order 45° Astigmatism: \( R^2 \sin 2\theta \)

3rd-Order X Coma: \((3R^2 - 2)R \cos \theta \)

3rd-Order Y Coma: \((3R^2 - 2)R \sin \theta \)

3rd-Order Spherical: \(6R^4 - 6R^2 + 1 \)

3rd-Order Trefoil: \( R^3 \cos 3\theta \)

45° Trefoil: \( R^3 \sin 3\theta \)

5th-Order Astigmatism: \((4R^2 - 3)R^2 \cos 2\theta \)

Pupil phase error due to 3rd-order astigmatism:

\[
\text{phase error} = 2\pi Z_{\text{astig}} R^2 \cos 2\theta
\]

Optical path difference due to defocus:

\[
OPD = \delta (1 - \cos \theta) \approx \frac{1}{2} \delta \sin^2 \theta
\]

Pupil phase error due to defocus:

\[
\text{phase error} \approx \frac{\pi \delta NA^2}{\lambda} R^2
\]

Horizontal-vertical bias:

\[
H-V \text{ bias} \approx \frac{8a \delta Z_{\text{astig}} \lambda}{NA^2}
\]

Flare measurement:

\[
Flare = \frac{E_0}{E_{0\text{-island}}}
\]

Magnification and the Lagrange (optical) Invariant:

\[
m = \frac{n_o \sin \theta_o}{n_i \sin \theta_i}
\]
Equation Summary (cont’d)

Reflection and transmission coefficients (between layers \(i\) and \(j\)), normal incidence:

\[
\rho_{ij} = \frac{n_i - n_j}{n_i + n_j}, \quad \tau_{ij} = \frac{2n_i}{n_i + n_j}
\]

Internal transmittance of a resist:

\[
\tau_D = e^{-i2\pi n_i D/\lambda}
\]

Fresnel reflection and transmission coefficients:

\[
\rho_{12\perp} = \frac{n_1 \cos(\theta_i) - n_2 \cos(\theta_t)}{n_1 \cos(\theta_i) + n_2 \cos(\theta_t)} \quad \tau_{12\perp} = \frac{2n_1 \cos(\theta_i)}{n_1 \cos(\theta_i) + n_2 \cos(\theta_t)}
\]

\[
\rho_{12\parallel} = \frac{n_1 \cos(\theta_i) - n_2 \cos(\theta_t)}{n_1 \cos(\theta_i) + n_2 \cos(\theta_t)} \quad \tau_{12\parallel} = \frac{2n_1 \cos(\theta_i)}{n_1 \cos(\theta_i) + n_2 \cos(\theta_t)}
\]

Lambert law of absorption:

\[
\frac{dI}{dz} = -\alpha I, \quad I(z) = I_0 e^{-\alpha z}
\]

Beer’s law:

\[
\alpha_{solution} = ac
\]

Dill ABC parameters taken from photoresist transmittance curve:

\[
A = \frac{1}{D} \ln \left[ \frac{T(\infty)}{T(0)} \right], \quad B = -\frac{1}{D} \ln \left[ \frac{T(\infty)}{T_{12}} \right]
\]

\[
C = \frac{A + B}{AT(0)(1 - T(0))T_{12}} \frac{dT}{dE} \bigg|_{E=0}, \quad T_{12} = 1 - \left( \frac{n_{\text{resist}} - 1}{n_{\text{resist}} + 1} \right)^2
\]

Diffusion (1D):

\[
\frac{\partial H}{\partial t} = \frac{\partial}{\partial z} \left( D_H \frac{\partial H}{\partial z} \right), \quad D_H(T) = A_T e^{-E_c/RT}
\]

Mack 4-parameter dissolution rate model:

\[
r = r_{\max} \frac{(a + 1)(1 - m)^{a}}{a + (1 - m)^{a}} + r_{\min}, \quad a = \frac{(n + 1)}{(n - 1)}(1 - m_{TH})^{n}
\]
NILS and the lithographic imaging equation:

\[ NILS = w \frac{d \ln(I)}{dx} m(x, y, z) = e^{-CE_{r1}(x,y)} \]

\[ \frac{\partial m}{\partial x} = m \ln(m) \frac{\partial \ln I}{\partial x} \quad \frac{\partial m^*}{\partial x} \approx \frac{\partial m}{\partial x} e^{-\sigma^2 \pi^2 / 2L^2} \]

\[ \gamma \equiv \left. \frac{\partial \ln R}{\partial \ln E} \right|_{\text{max}} \quad \frac{\partial \ln R}{\partial x} = \gamma(E) \frac{\partial \ln I}{\partial x} \]

Critical dimension variational equation:

\[ \frac{\Delta CD}{CD} = \frac{\Delta v_1}{v_1} \frac{\partial \ln CD}{\partial \ln v_1} + \frac{\Delta v_2}{v_2} \frac{\partial \ln CD}{\partial \ln v_2} + \cdots \]

Rayleigh Criteria:

\[ R = k_1 \frac{\lambda}{NA} \quad DOF = 2\delta_{\text{max}} = k_2 \frac{\lambda}{\sin^2 \theta} = k_2 \frac{\lambda}{NA^2} \]

Immersion–High NA depth of focus Rayleigh criterion:

\[ DOF = k_2 \frac{\lambda}{2 n_{\text{fluid}}(1 - \cos \theta)} \]

Mask error enhancement factor:

\[ MEEF = \frac{\partial CD_{\text{resist}}}{\partial CD_{\text{mask}}} \]
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Chris A. Mack received Bachelor of Science degrees in physics, chemistry, electrical engineering, and chemical engineering from Rose-Hulman Institute of Technology in 1982, a Master of Science degree in electrical engineering from the University of Maryland in 1989, and a Ph.D. in chemical engineering from the University of Texas at Austin in 1998. Dr. Mack founded FINLE Technologies, the developer of the lithography simulation software PROLITH, in 1990, serving as President and Chief Technical Officer until the acquisition of FINLE by KLA-Tencor in 2000. For the next five years he served as Vice President of Lithography Technology for KLA-Tencor. In 2003 he received the SEMI Award for North America for his efforts in lithography simulation and education. He is also an adjunct faculty member at the University of Texas at Austin. Currently, he writes, teaches, and consults on the field of semiconductor microlithography in Austin, Texas, where he lives with his wife Susan and their daughter Sarah.