CHE323/CHE384
Chemical Processes for Micro- and Nanofabrication

Formulas
Lectures 38-60

Chris A. Mack
Adjunct Associate Professor

http://www.lithoguru.com/scientist/CHE323/

Misc. Formulae

$$resist\ thickness \propto \frac{1}{\sqrt{spin\ speed}}$$

Proximity Printing Resolution ∝ $\sqrt{\lambda g}$ g = Mask-wafer gap

$NA = n\ sin\alpha$, α = maximum half-angle, n = refractive index

For a phase-shift mask (t = shifter thickness, n = refractive index):

Phase shift caused by optical path difference: $\Delta\phi = 2\pi t(n-1)/\lambda$

To get 180º (π) phase shift: $t = \lambda / 2(n-1)$

Fourier Transform

Diffraction Pattern ↓ ↙ Mask Transmittance

$$T_m(f_x, f_y) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} t_m(x,y)\exp\left(-2\pi i(f_x x + f_y y)\right)dx\,dy$$

$$f_x = \frac{x'}{\lambda z} = \frac{\sin\theta_x}{\lambda} \qquad f_y = \frac{y'}{\lambda z} = \frac{\sin\theta_y}{\lambda}$$

Bragg's Condition: $p\sin\theta_n = n\lambda$

Isolated space

$$T_m(f_x) = \mathcal{F}\{t_m(x)\} = \frac{\sin(\pi w f_x)}{\pi f_x}$$

Repeating lines and spaces

$$T_m(f_x) = \frac{1}{p}\sum_{n=-\infty}^{\infty}\frac{\sin(\pi w f_x)}{\pi f_x}\delta\left(f_x - \frac{n}{p}\right)$$

Fourier Transform Properties

$$\mathcal{F}\{g(x,y)\} = G(f_x, f_y)$$

Linearity: $\mathcal{F}\{af(x,y) + bg(x,y)\} = aF(f_x,f_y) + bG(f_x,f_y)$

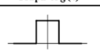
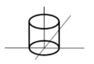
Shift Theorem: $\mathcal{F}\{g(x-a, y-b)\} = G(f_x,f_y)e^{-i2\pi(f_x a + f_y b)}$

Similarity: $\mathcal{F}\{g(ax,by)\} = \frac{1}{|ab|}G\left(\frac{f_x}{a}, \frac{f_y}{b}\right)$

Convolution: $\mathcal{F}\left\{\int_{-\infty}^{\infty}\int g(\xi,\eta)h(x-\xi, y-\eta)d\xi\,d\eta\right\} = G(f_x,f_y)H(f_x,f_y)$

Fourier Transform Examples

$$\mathcal{F}\{g(x)\} = G(f_x)$$

$g(x)$	Graph of $g(x)$	$G(f_x)$
$rect(x) = \begin{cases}1, & \lvert x\rvert < 0.5 \\ 0, & \lvert x\rvert > 0.5\end{cases}$		$\frac{\sin(\pi f_x)}{\pi f_x}$
$step(x) = \begin{cases}1, & x > 0 \\ 0, & x < 0\end{cases}$		$\frac{1}{2}\delta(f_x) - \frac{i}{2\pi f_x}$
Delta function $\delta(x)$		1
$comb(x) = \sum_{j=-\infty}^{\infty}\delta(x-j)$		$\sum_{j=-\infty}^{\infty}\delta(f_x - j)$
$\cos(\pi x)$		$\frac{1}{2}\delta\left(f_x + \frac{1}{2}\right) + \frac{1}{2}\delta\left(f_x - \frac{1}{2}\right)$
$\sin(\pi x)$		$\frac{i}{2}\delta\left(f_x + \frac{1}{2}\right) - \frac{i}{2}\delta\left(f_x - \frac{1}{2}\right)$
Gaussian $e^{-\pi x^2}$		$e^{-\pi f_x^2}$
$circ(r) = \begin{cases}1, & \lvert r\rvert < 1 \\ 0, & \lvert r\rvert > 1\end{cases}$ $r = \sqrt{x^2 + y^2}$		$\frac{J_1(2\pi\rho)}{\pi\rho}$ $\rho = \sqrt{f_x^2 + f_y^2}$

Delta Function:

$$\delta(x) = 0 \quad when \quad x \neq 0$$

$$\int_{-\infty}^{\infty}\delta(x)\,dx = 1$$

$$\int_{-\infty}^{\infty} f(x)\delta(x - x_o)dx = f(x_o)$$

Fourier Optics

- Pupil function, $P(f_x,f_y)$

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

- Diffraction pattern is T_m , the electric field of the image is E, image intensity is I

$$E(x,y) = \mathcal{F}^{-1}\{PT_m\} \qquad I(x,y) = |E(x,y)|^2$$

Image Example: equal lines and spaces

$$T_m(f_x)=\sum_{n=-\infty}^{\infty} a_n\delta\left(f_x-\frac{n}{p}\right), \qquad a_n=\frac{\sin(n\pi/2)}{n\pi}$$

For case of three diffraction orders going through the lens,

$$P(f_x)T_m(f_x)=\frac{1}{\pi}\delta\left(f_x+\frac{1}{p}\right)+\frac{1}{2}\delta(f_x)+\frac{1}{\pi}\delta\left(f_x-\frac{1}{p}\right)$$

$$E(x)=F^{-1}\{PT_m\}=\frac{1}{\pi}e^{-i2\pi x/p}+\frac{1}{2}+\frac{1}{\pi}e^{i2\pi x/p}=\frac{1}{2}+\frac{2}{\pi}\cos(2\pi x/p)$$

With defocus: $\Delta\Phi=2\pi(OPD)/\lambda=2\pi\delta(1-\cos\theta)/\lambda$

$$E(x)=\frac{1}{2}+\frac{2}{\pi}e^{i\Delta\Phi}\cos(2\pi x/p)$$

$$I(x)=\frac{1}{4}+\frac{2}{\pi}\cos(\Delta\Phi)\cos(2\pi x/p)+\frac{2}{\pi^2}\left[1+\cos(4\pi x/p)\right]$$

Traditional Limits of Lithography Resolution

- Generalized Rayleigh Resolution: $R=k_1\frac{\lambda}{NA}$
- For 3-beam imaging, $k_1\geq 0.5$
- For 2-beam imaging, $k_1\geq 0.25$

Partial Coherence Factor (for circular source shape):

$$\sigma=\frac{diameter\ of\ illumination\ spot}{diameter\ of\ objective\ lens\ entrance\ pupil}=\frac{\sin(\theta'_{\max})}{NA_o}$$

Rayleigh Depth of Focus

- Three-beam imaging: lines and spaces where only the 0th and ±1st orders are used
- Feature is at the resolution limit
- k_2 is unknown (but it must be < 1)
- For low numerical apertures (< 0.5): $DOF=k_2\frac{\lambda}{NA^2}$
- For any numerical aperture: $DOF=\frac{k_2}{2}\frac{\lambda}{n(1-\cos\theta)}$

$$\frac{DOF(immersion)}{DOF(dry)}=\frac{1-\sqrt{1-(\lambda/p)^2}}{n-\sqrt{n^2-(\lambda/p)^2}}$$

Standing Wave Expression

Average Intensity — Amplitude — Period = $\lambda/2n_2$

$$I\sim e^{-\alpha z}+Re^{-\alpha(2D-z)}-\left(2\sqrt{R}e^{-\alpha D}\right)\cos(4\pi n_2(D-z)/\lambda+\phi_{23})$$

where $R=|\rho_{23}|^2$ = reflectivity of the substrate

α = resist absorption coefficient

D = resist thickness

n_2 = resist index of refraction (real part)

λ = vacuum wavelength

ϕ_{23} = phase change of substrate reflectivity

Photoresist Exposure

First order exposure kinetics — It = exposure dose

relative sensitizer concentration $m=\frac{M}{M_o}=\exp(-CIt)$

M_O = initial (unexposed) sensitizer concentration

Lambert Law of Absorption $\frac{dI}{dz}=-\alpha I$

If α = constant, $I=I(z=0)e^{-\alpha z}$

Beer's Law of Absorption $\alpha=\sum a_i c_i$

a_i = molar absorptivity of i

c_i = concentration of i

Photoresist ABCs

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

M = Unexposed sensitizer concentration

P = Exposed sensitizer concentration

R = Resin concentration

S = Solvent concentration

$$\alpha=Am+B$$

$$A=(a_M-a_P)M_0 \qquad B=a_P M_0+a_R R+a_S S$$

A = bleachable absorption coefficient

B = non-bleachable absorption coefficient

m = relative sensitizer concentration

Measuring A, B, and C

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

$$C = \frac{A+B}{A}\left(\frac{1}{1-T(0)}\right)\left(\frac{1}{T(0)}\right)\left(\frac{1}{T_{12}}\right)\left.\frac{dT}{dE}\right|_{E=0}$$

where D = resist thickness
$T(0)$ = initial transmittance
$T(\infty)$ = final transmittance
T_{12} = air-resist interface transmittance $= 1 - \left(\frac{n_2 - n_1}{n_2 + n_1}\right)^2$
E = incident dose

Chemically Amplified Resist

First order exposure kinetics: $h = 1 - e^{-CIt}$

Approximation: if h is locally constant (ignoring diffusion),

First order amplification kinetics: $m = e^{-\alpha_f h}$

where K_{amp} = $G_o k_4$ = normalized rate constant
α_f = $K_{amp} t_{PEB}$ = amplification factor

$$h = \frac{H}{G_o} \qquad m = \frac{M}{M_o}$$

$$K_{amp} = A_r e^{-E_a/RT}$$

Photoresist Development

Mack kinetic model: $r = r_{max}\frac{(a+1)(1-m)^n}{a+(1-m)^n} + r_{min}$

where r_{max} = maximum development rate
r_{min} = minimum development rate
n = dissolution selectivity parameter
a = $[(n+1)/(n-1)](1-m_{th})^n$
m_{th} = threshold inhibitor concentration

Photoresist Contrast: $\gamma_{th} = \frac{d\ln r}{d\ln E} \qquad \frac{d\ln r}{dx} = \gamma_{th}\frac{d\ln I}{dx}$

Exposure Latitude and NILS

Nominal Feature Size

Normalized Image Log-Slope: $NILS = w\frac{\partial \ln I}{\partial x}$

CD sensitivity to exposure dose E:

Resist thickness

$$\frac{\partial \ln CD}{\partial \ln E} \approx \frac{2}{NILS}\left[1 + \frac{2}{\gamma\, NILS} + \gamma\, NILS\frac{D}{CD}e^{-\gamma\, NILS/4}\right]$$

Critical Dimension

Useful Constants

• Avogadro Constant	6.02204 X 10^{23} mole^{-1}
• Boltzmann Constant (k)	1.38066 X 10^{-23} J/K 8.617 X 10^{-5} eV/K 1.3626 X 10^{-22} atm-cm^3/K
• Gas Constant (R)	1.987 cal/mole/K
• Electric Charge (q)	1.60218 X 10^{-19} C
• Permittivity in vacuum (e_o)	8.854 X 10^{-14} F/cm
• Thermal voltage at 300 K (kT/q)	0.0259 V

- **Pressure**: 1 atm = 1.01325 ×10^5 Pa = 1.01325 bar = 760 torr = 14.696 psi (1 Pa = 1 kg/(m·s^2) = 1 N/m^2)
- **Energy**: 1 J = 1 kg m^2/s^2 = 9.4782 ×10^{-4} Btu = 6.2415 ×10^{16} eV = 0.23901 cal = 1 A V s
- **Capacitance**: 1 F = 1 A s/V = 1 C/V = 1 s/W

