

Mole fraction of DCS

$$y_{DCS} = \frac{Q_{DCS}}{Q_{NH_3} + Q_{DCS}} = \frac{70 \text{ sccm}}{200 \text{ sccm} + 70 \text{ sccm}}$$

$$y_{DCS} = 0.2593$$

Concentration of DCS

$$780 \times 10^{-3} \text{ Torr} \times \frac{133.322 \text{ Pa}}{1 \text{ Torr}} = 100 \text{ Pa}$$

$$\frac{n}{V} = \frac{P}{RT} = \frac{(0.2593)(100 \text{ Pa})}{(8.314 \text{ J/(K.mol)})(270+273) \text{ K}}$$

$$C_{DCS} = 9.97 \times 10^{-4} \text{ mol/m}^3$$

Kinetic Eq'n

$$J = k_0 \exp\left[\frac{-E_a}{RT}\right] C_{DCS}^{0.49}$$

$$= 82300 \text{ s}^{-1} \exp\left[\frac{-(169.4 \times 10^3 \text{ J/mol})}{(8.314 \text{ J/(K.mol)})(270+273) \text{ K}}\right] (9.97 \times 10^{-4} \text{ mol/m}^3)^{0.49}$$

$$= 9.14 \times 10^{-6} \text{ mol/(cm}^2.\text{s}) \quad \text{rate of change of } C_{DCS}$$

Deposition rate

Stoichiometric coefficient $\text{SiCl}_2\text{H}_2 : \text{Si}_3\text{N}_4 = 3 : 1$

approximate deposition rate $\approx \frac{1}{3} (9.14 \times 10^{-6} \text{ mol/(cm}^2.\text{s})) \approx 3.05 \times 10^{-6} \text{ mol/(cm}^2.\text{s})$
by neglecting surface kinetics.

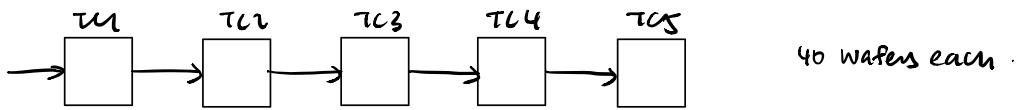
$$\text{MW}_{\text{Si}_3\text{N}_4} = 140.28 \text{ g/mol}$$

$$\rho_{\text{Si}_3\text{N}_4} = 3000 \text{ kg/m}^3$$

$$\frac{3.05 \times 10^{-6} \text{ mol}}{\text{m}^2 \cdot \text{s}} \times \frac{140.28 \text{ g}}{\text{mol}} \times \frac{\text{m}^3}{3000 \times 10^3 \text{ g}} = 1.43 \times 10^{-10} \text{ m/s}$$

$$\boxed{\text{deposition rate} = 1.43 \text{ \AA/s} = 85.8 \text{ \AA/min}}$$

$$\frac{2000 \text{ \AA}}{85.8 \text{ \AA/min}} = 23.31 \text{ mm/s} \approx 25 \text{ mm/s}$$



$$\text{Volume of } \text{Si}_3\text{N}_4 = (\nu)(200)(\pi)(0.15m)^2(1000 \times 10^{-6} m) \\ = 2.83 \times 10^{-6} \text{ m}^3$$

$$n_{\text{Si}_3\text{N}_4} = (2.83 \times 10^{-6} \text{ m}^3) \left(\frac{3000 \text{ kg}}{\text{m}^3} \right) \left(\frac{1 \text{ mol}}{0.14 \text{ kg}} \right)$$

$$n_{\text{Si}_3\text{N}_4} = 0.061 \text{ mol} \quad \text{which is} \quad n_{\text{DCS}} = 0.183 \text{ mol}$$

0.0813 mol Si_3N_4 for 20 sccm DCS flow
200 sccm NH_3 flow

which is 0.244 mol of DCS

material balance on DCS

$$in - out + gen - loss = \cancel{out}$$

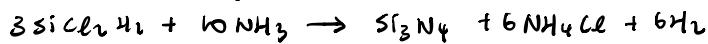
	$n \text{ (mol)}$
Si_3N_4	0.0813
SiCl_2H_2	0.2439
NH_3	0.813

$$in - out - loss = 0$$

$$0.244 \text{ mol} - out - \left(\frac{0.183 \text{ mol}}{200} \right) (40) = 0$$

$$out = 0.2074 \text{ mol} \quad in$$

Overall chem eq'n



At the end of TCI

	I	C	F
SiCl_2H_2	0.244	-0.0366	0.2074
NH_3	0.813	-0.122	0.691
H_2	0	+0.296	0.296

$$y_{\text{DCS}, \text{TCI}} = \frac{0.2074}{0.2074 + 0.691 + 0.296}$$

$$y_{\text{DCS}, \text{TCI}} = 0.1855$$

concentration of DCS exiting TCI / entering TCl

$$\frac{n}{V} = \frac{P_A}{RT}$$

concentration of DCS

$$C_{\text{DCS}, \text{TCl}} = \frac{(0.1855)(33.33 \text{ Pa})}{(8.314 \text{ J/(K.mol)}) (T_2)}$$

$$C_{\text{DCS}, \text{TCl}} = \frac{0.7437 \text{ K}}{T_2}$$

Kinetic Eq'n \Rightarrow we want the same deposition rate for each temp. zone.

$$\begin{aligned} J &= k_0 \exp \left[\frac{-E_A}{RT} \right] C_{\text{DOS}}^{0.49} \\ &= 82300 \text{ s}^{-1} \exp \left[\frac{-(169.4 \times 10^3 \text{ J/mol})}{(8.314 \text{ J/(K mol)}) (770 + 273) \text{ K}} \right] (9.97 \times 10^{-6} \text{ mol/m}^3)^{0.49} \\ &= 9.14 \times 10^{-6} \text{ mol/(m}^2 \cdot \text{s}) \quad \text{rate of change of } C_{\text{DOS}} \end{aligned}$$

$$9.14 \times 10^{-6} \text{ mol/(m}^2 \cdot \text{s}) = 82300 \text{ s}^{-1} \exp \left[\frac{-(169.4 \times 10^3 \text{ J/mol})}{(8.314 \text{ J/(K mol)}) (T_2)} \right] \left(\frac{0.7437 \text{ K}}{T_2} \right)^{0.49}$$

Trial and error

T_2	$J [\text{mol/(m}^2 \cdot \text{s})]$
$775^\circ\text{C} = 1048\text{K}$	8.49×10^{-6}
$780^\circ\text{C} = 1053\text{K}$	9.29×10^{-6}
$779^\circ\text{C} = 1052\text{K}$	9.12×10^{-6}

$$T_2 = 779^\circ\text{C}$$

At the end of T_{C2}

	I	C	F
SiCl ₄	0.1094	-0.0366	0.1708
NH ₃	0.691	-0.122	0.569
H ₂	0.296	+0.296	0.4392

$$\begin{aligned} y_{\text{DOS}, T_{C2}} &= \frac{0.1708}{0.1708 + 0.569 + 0.4392} \\ y_{\text{DOS}, T_{C2}} &= 0.1449 \end{aligned}$$

Concentration of DOS

$$C_{\text{DOS}, T_{C2}} = \frac{(0.1449)(23.33 \text{ Pa})}{(8.314 \text{ J/(K mol)}) (T_3)}$$

$$C_{\text{DOS}, T_{C2}} = \frac{0.5809 \text{ K}}{T_3}$$

Trial and error

(°C)	$J [\text{mol/(m}^2 \cdot \text{s})]$
787	9.32×10^{-6}
785	8.99×10^{-6}
790	9.83×10^{-6}

$$T_3 = 786^\circ\text{C}$$

At the end of TLC3

	I	C	P
SiCl ₂ H ₆	0.1708	-0.0366	0.1342
NH ₃	0.569	-0.122	0.447
H ₂	0.4392	+0.296	0.6588

$$y_{DCS,TCL} = \frac{0.1342}{0.1342 + 0.447 + 0.6588}$$

$$y_{DCS,TCL} = 0.1082$$

Concentration of DCS

$$C_{DCS,TCL} = \frac{(0.1082)(83.33 \text{ Pa})}{(8.3145 / (6.01)) (T_4)}$$

$$C_{DCS,TCL} = \frac{0.4338 \text{ K}}{T_4}$$

Trial and error

(°C)	J [mol / (m ³ ·s)]
793	8.975 × 10 ⁻⁶
795	9.294 × 10 ⁻⁶
794	9.133 × 10 ⁻⁶

$$T_4 = 794 \text{ °C}$$

At the end of TLC4

	I	C	P
SiCl ₂ H ₆	0.1342	-0.0366	0.0976
NH ₃	0.447	-0.122	0.325
H ₂	0.6588	+0.296	0.8784

$$y_{DCS,TCL} = \frac{0.0976}{0.0976 + 0.325 + 0.8784}$$

$$y_{DCS,TCL} = 0.07502$$

Concentration of DCS

$$C_{DCS,TCL} = \frac{(0.07502)(83.33 \text{ Pa})}{(8.3145 / (6.01)) (T_5)}$$

$$C_{DCS,TCL} = \frac{0.3007 \text{ K}}{T_5}$$

Trial and error

T [°C]	J [nmol / (nm² · s)]
805	9.22×10^{-6}
804	9.07×10^{-6}
803	8.92×10^{-6}
801	8.62×10^{-6}

$$T_5 = 805^{\circ}\text{C}$$

Final Temperature

zone	temperature (°c)
1	770
2	779
3	786
4	794
5	805

$\downarrow +9^{\circ}\text{C}$
 $\downarrow +7^{\circ}\text{C}$
 $\downarrow +8^{\circ}\text{C}$
 $\downarrow +11^{\circ}\text{C}$