DESIGN OF MOCVD FILM GROWTH IN A HOT WALL TUBULAR REACTOR

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The deposition kinetics for MOCVD film growth was investigated in a range of common process parameters during laminar flow in horizontal hot wall tubular reactor. Particular attention was paid to the relationship between growth rate and reactor dimensions as well as process temperature. The development of the modeling procedure permited to predict growth rates and precursor concentrations at different experimental conditions. The starting point was the official modeling procedure of members of CVD project of Society of Chemical Engineers of Japan (1), (see Table 1). On the other hand, details of experimental verification were given for low pressure MOCVD deposition of TiO_2 and Al_2O_3 films (2-4), (see example on Figure 1).

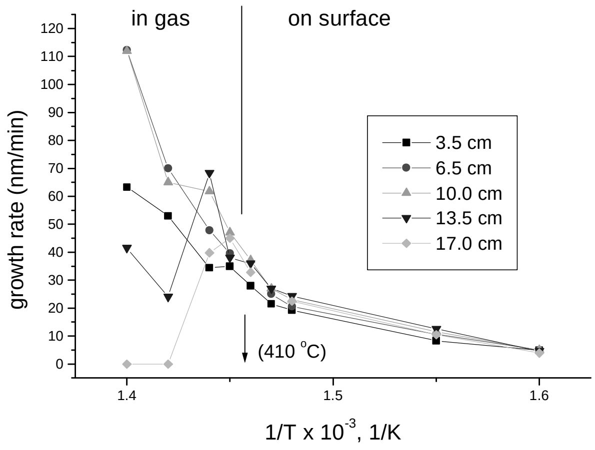

Figure 1. Temperature dependence of overall rate constant for TiO_2 film deposition

We suggested the relation:

$$\mathbf{[C_{s(x)}/C_{(x=0)}] = [\exp(-K\xi)]/[1 + z_{(x)}]}$$

or

$$\mathbf{[r_{s(x)}/r_{(x=0)}] = (k_{s(x)} / \Sigma k_{(x=0)})[\exp(-K\xi)]/[1 + z_{(x)}]}$$

where: $C_{(x)}$: concentration at x position; $C_{(x = 0)}$: concentration at inlet,$C_{s(x)}$: surface concentration at x position, $r = d\delta/dt$ (nm/min): deposition rate, $\Sigma k_{(x=0)} = [(k_g\ k_{s(x=0)}\ k_{d(x=0)})/(k_g + k_{s(x=0)} + k_{d(x=0)})]$: overall transport cofficient., $[C_{s(x)}/C_{(x=0)}]$: relative surface concentration; $[r_{s(x)}/r_{(x=0)}]$: relative deposition rate; $K = (k_g x_{ref}/u)$: dimensionless gas rate group; $\xi = x/x_{ref}$: normalized position; $z_{(x)} = (k_{s(x)}/k_{d(x)})$ or in simplified form: $z = (k_s/k_d)$, when k_s and k_d are constant values at any x position (for characteristic values see Table 2.).

So, we have the possibility to take into account the influence of k_g, k_s (or $k_{s(x)}$) and k_d (or $k_{d(x)}$) on overall deposition process. Also, we are in position to explane the exact deposition rate at any position, see the example on Figure 2.

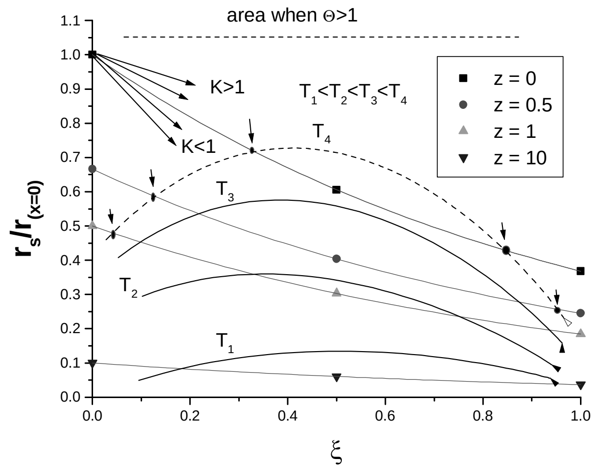

Figure 2. Relative deposition rate vs normalized reactor x-coordinate for z = 0; 0.5; 1 and 10 (k_s and k_d : constant values at any x position; ($\Theta = k_{s(x)} / \Sigma k_{(x=0)}) \approx 1$; K = 1 ; $T = T_4$ = const) compared with possible experimental data at different temperatures. Areas for K<1 and K>1 are indicated but only for z = 0. Area when $\Theta = k_{s(x)} / \Sigma k_{(x=0)}$) >1 is above the straight doted line.

Table 1. Dependences on temperature and reactor diameter for k_g, k_s, and k_d (1)

Constant	Dependence on Temperature	Dependence on Reactor diameter
k_g (gas-phase reaction rate)	Arrhenius type	-
k_s (surface reaction rate)	Arrhenius type	1/d
k_d (diffusion rate)	$T^{3/2}$	$1/d^2$

Table 2. Characteristic relationships when $z_{(x)}$ or z = 0; = 1; > 1.(in all cases $(k_{s(x)} / \Sigma k_{(x=0)}) \approx 1$)

$z_{(x)} = 0$ $z = 0$	$k_{s(x)} << k_{d(x)}$ $k_s << k_d$	$C_{s(x)} = C_{(x)}$ or $r_{s(x)} = r_{(x)}$ $C_s = C_{(x)}$ or $r_s = r_{(x)}$
$z_{(x)} = 1$ $z = 1$	$k_{s(x)} = k_{d(x)}$ $k_s = k_d$	$C_{s(x)} = 0.5C_{(x)}$ or $r_{s(x)} = 0.5r_{(x)}$ $C_s = 0.5C_{(x)}$ or $r_s = 0.5r_{(x)}$
$z_{(x)} > 1$ $z > 1$	$k_{s(x)} > k_{d(x)}$ $k_s > k_d$	$C_{s(x)} < 0.5C_{(x)}$ or $r_{s(x)} < 0.5r_{(x)}$ $C_s < 0.5C_{(x)}$ or $r_s < 0.5r_{(x)}$

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