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SILICON PRODUCTION IN AN AEROSOL REACTOR

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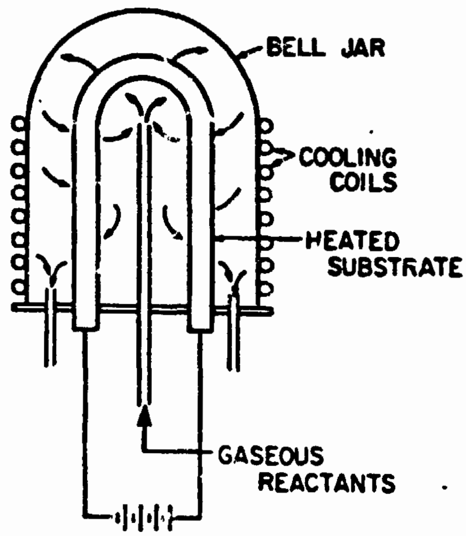
Siemens Process



Silane Pyrolysis

$$SiH_4 + M \xrightarrow{1} SiH_2 + H_2 + M$$

$$SiH_2 + SiH_4 \overset{2}{\rightleftharpoons} Si_2H_6 \xrightarrow{3} Si_2H_4 + H_2$$

$$SiH_2 + Si_2H_6 \overset{4}{\rightleftharpoons} Si_3H_8 \overset{5}{\rightleftharpoons} Si_2H_4 + SiH_4$$

$$SiH_2 \xrightarrow{6} surface - SiH_2$$

$$surface - SiH_2 + SiH_4 \xrightarrow{7} surface - SiH_3 + SiH_3$$

$$SiH_3 + SiH_3 \xrightarrow{8} Si_2H_6$$

Aerosol Reactor

- Efficiency - energy & reactant usage
- Product purity
- Continuous rather than batch process
- Product particle size $D > 10-50\ \mu m$ to facilitate separation and subsequent processing

Simultaneous Nucleation and Particle Growth

$$\rho_g \frac{\partial n(a,t)/\rho_g}{\partial t} + \rho_g \frac{\partial}{\partial a}[\dot{a} n(a,t)/\rho_g] = J_c \delta(a - a^*)$$

$$\rho_g \frac{\partial C_v/\rho_g}{\partial t} = -C_p \int_{a^*}^{\infty} 4\pi a^2 n(a,t) \dot{a}\, da - C_p \frac{4}{3}\pi a^{*3} J_c + R$$

Traditional approach:

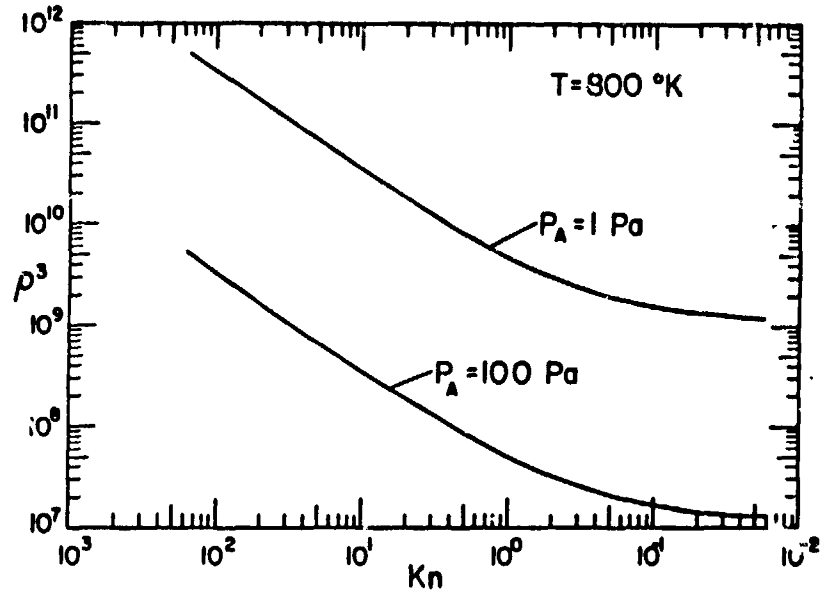
$$J_c = J(\overline{c_v})$$

Clearance Volume approach:

$$J_c = \begin{cases} J(c_{v\infty}) \cdot (1-\Omega) & 0 \leq \Omega \leq 1 \\ 0 & \Omega > 1 \end{cases}$$

where

$$\Omega = \int_0^{\infty} \frac{4}{3} \pi a^3 \rho^3 n(a,t)\, da$$



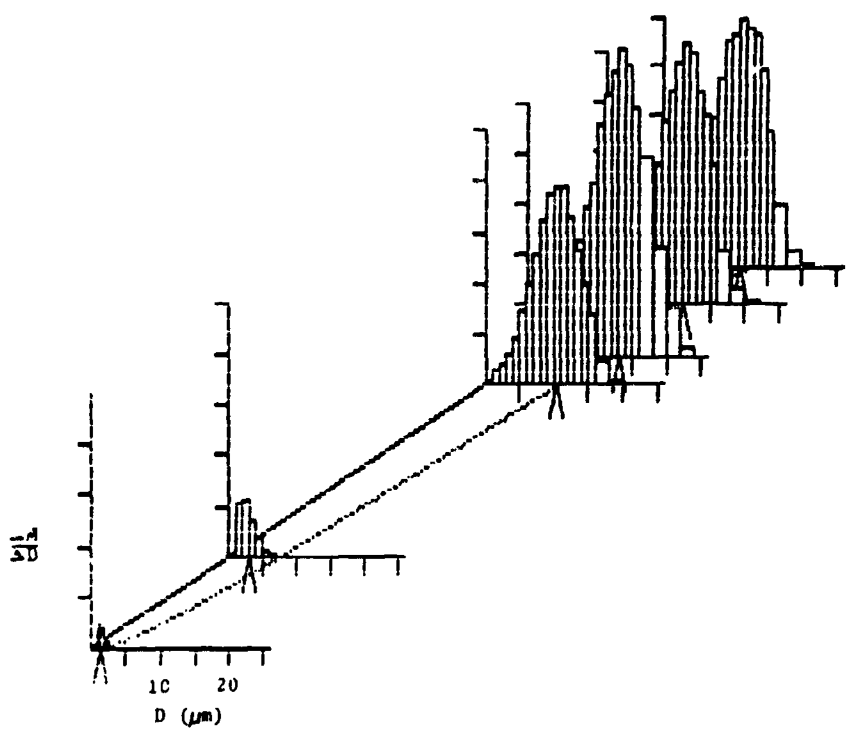
Aerosol Reactor for Growth of Large Siiicon Particles by Silane Pyrolysis

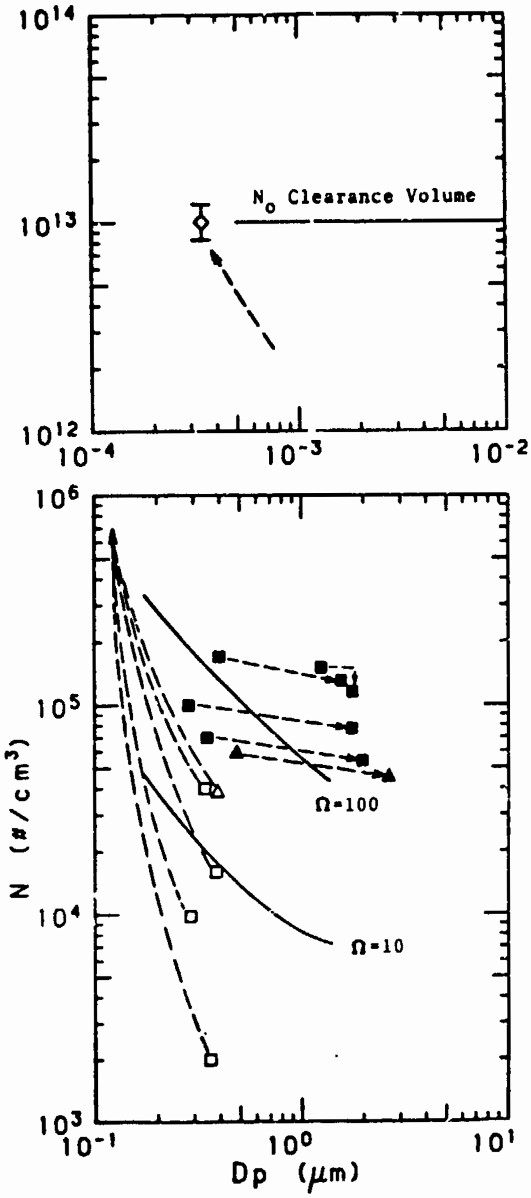
1. Generate seed particles by pyrolysis of a small amount of silane.
2. Mix seed aerosol with primary silane flow, limiting number concentration such that the amount of silane is sufficient to grow the desired size of particles from the seed.
3. React the silane at a rate which is controlled such that the seed particles scavenge the condensible vapors rapidly enough to inhibit further nucleation.

Reactor Optimization

- Control rate of condensible vapor production by limiting rate of temperature increase.
- Maintain $\Omega > \Omega^*$ to prevent nucleation.
- Ω depends on particle size and concentration so the growth history is important.
- Integrate rate equations to evaluate $\Omega(t)$. Adjust $T(t)$ to satisfy $\Omega_{min} > \Omega^*$ at all times.
- Use high temperature burn-off to guarantee complete reaction.

WHAT IS THE APPROPRIATE VALUE FOR Ω^*?




10^14
10^13
10^12
N_o Clearance Volume
10^-4
10^-3
10^-2
10^6
10^5
10^4
10^3
N (#/cm^3)
Ω=100
Ω=10
10^-1
10^0
10^1
Dp (μm)

Conclusions

- Particles of low volatility materials can be grown to large size in aerosol reactors by controlling the reaction rates to minimize nucleation.
- The clearance volume model provides reasonable estimates of suitable operating conditions.
- The "total clearance volume fraction" must be large (order 20-40) to quench nucleation.
- Nucleation quenching by a growing aerosol is extremely sensitive to seed particle size.