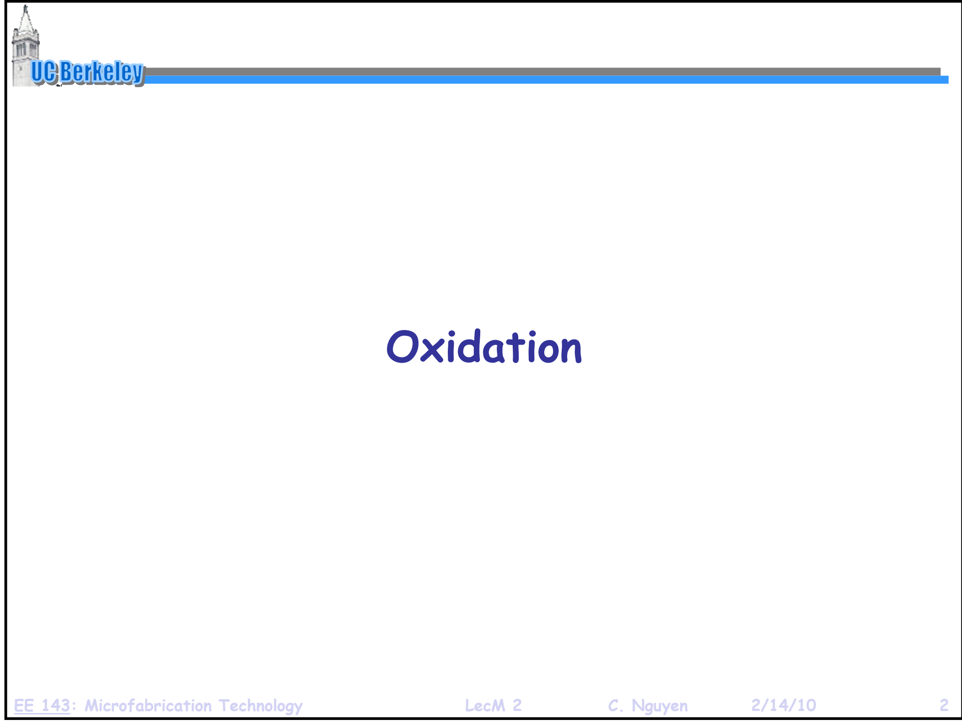

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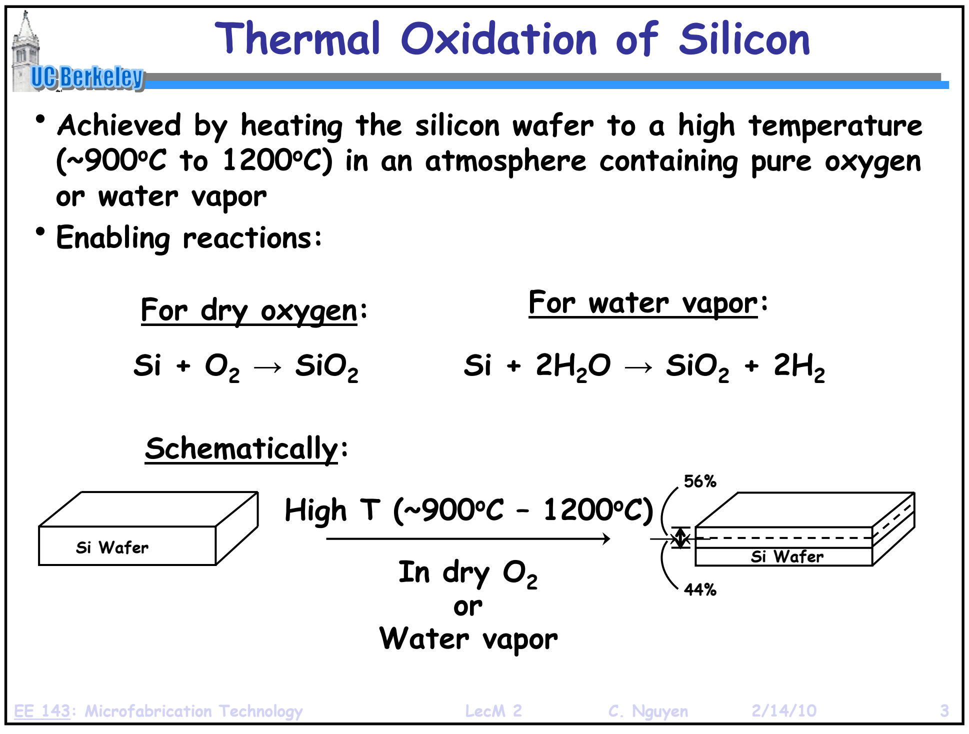

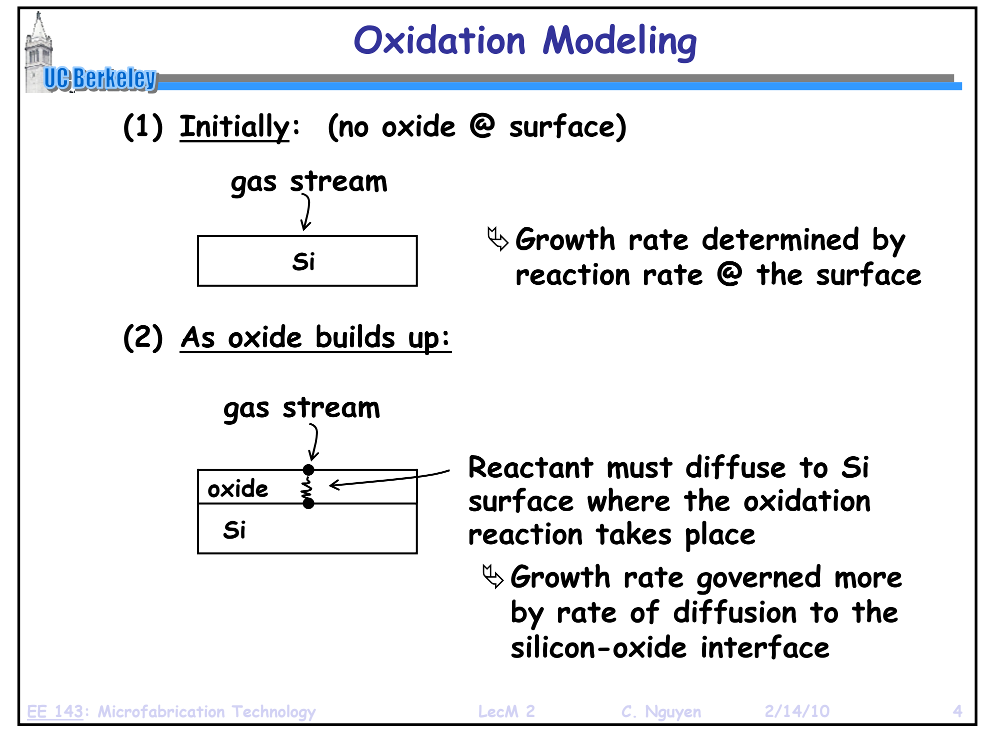

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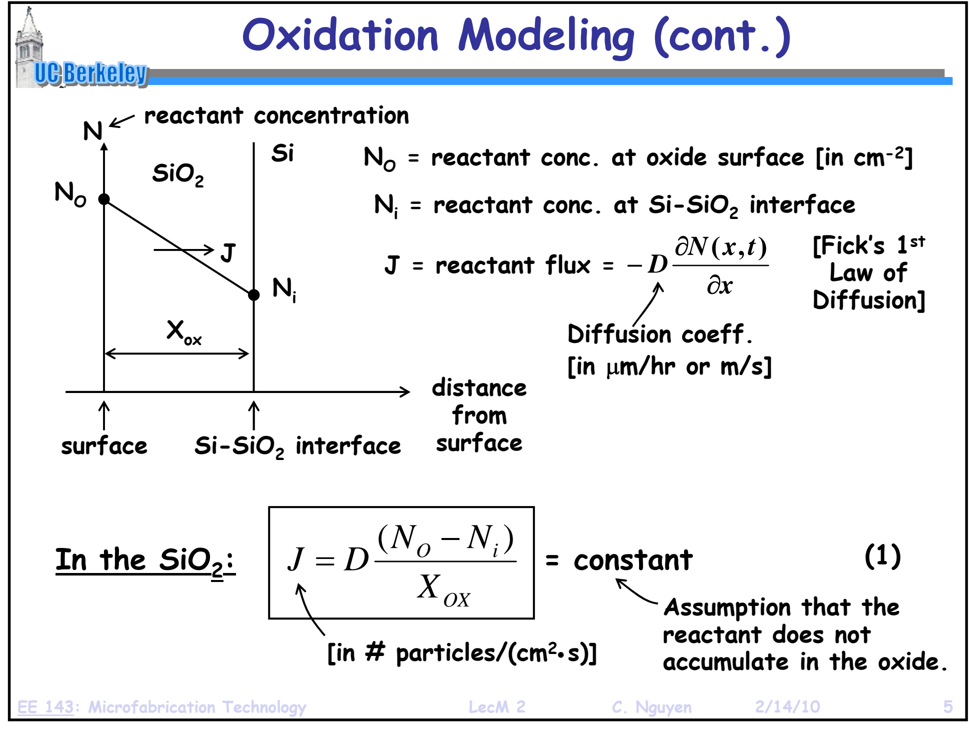

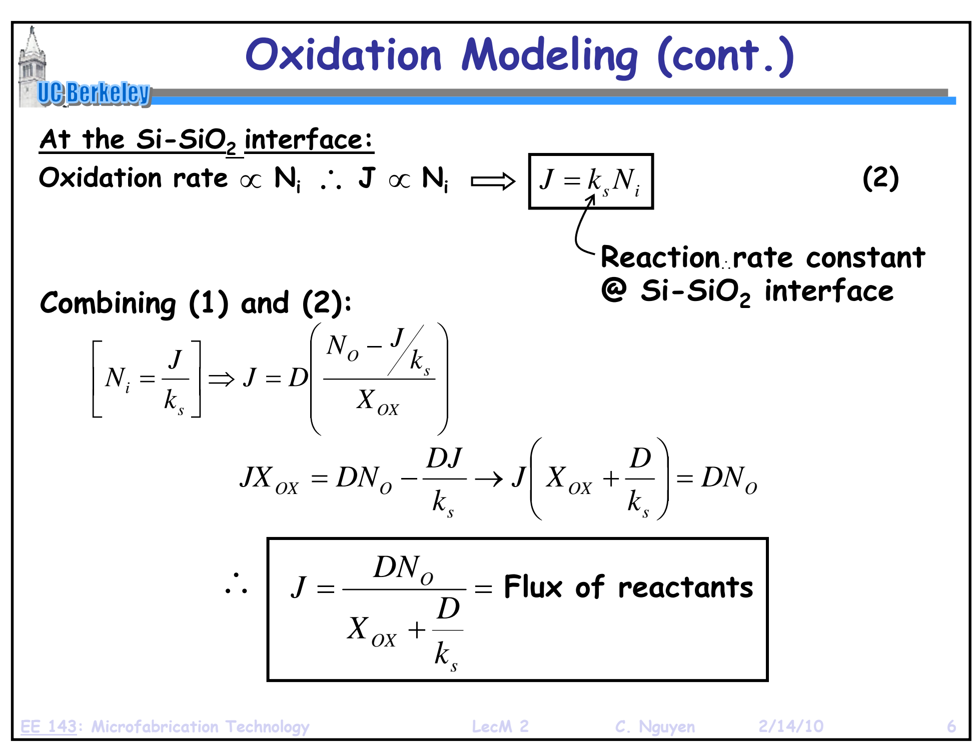

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Oxidation Modeling (cont.)

Find an expression for $X_{OX}(t)$:

oxidizing flux

Rate of change of oxide layer thickness w/time } $= \frac{dX_{OX}}{dt} = \frac{J}{M} = \frac{DN_O/M}{X_{OX} + D/k_s}$ (3)

# of molecules of oxidizing species incorporated into a unit volume of oxide } $= 2.2\times10^{22} cm^{-3}$ for O_2; $= 4.4\times10^{22} cm^{-3}$ for H_2O

Solve (3) for $X_{OX}(t)$: [Initial condition $X_{OX}(t=0) = X_i$]

$$\frac{dX_{OX}}{dt} = \frac{DN_O/M}{X_{OX} + D/k_s} \quad ☞ \quad \int_{X_i}^{X_{OX}} \left(X_{OX} + \tfrac{D}{k_s}\right) dX_{OX} = \int_0^t \frac{DN_O}{M} dt$$

Oxide Thickness Versus Time

Result:

additional time required to go from $X_i \rightarrow X_{OX}$

time required to grow X_i [X_i = initial oxide thickness]

$$X_{OX}(t) = \frac{A}{2}\left\{\left[1 + \frac{4B}{A^2}(t+\tau)\right]^{1/2} - 1\right\}$$

where $A = \frac{2D}{k_s}$ $\qquad \tau = \frac{X_i^2}{B} + \frac{X_i}{(B/A)}$

$B = \frac{2DN_O}{M}$ $\qquad D = D_O \exp\left(-\frac{E_A}{kT}\right)$

i.e., D governed by an Arrhenius relationship → temperature dependent

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Oxidation Modeling (cont.)

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For shorter times:

$$\left[(t+\tau) << \frac{A^2}{4B}\right] \Rightarrow X_{OX}(t) = \left(\frac{B}{A}\right)(t+\tau) \Rightarrow$$

oxide growth limited by reaction at the Si-SiO_2 interface

Taylor expansion (first term after 1's cancel)

B/A: linear growth rate constant

For long oxidation times: oxide growth diffusion-limited

$$\left[(t+\tau) >> \frac{A^2}{4B}\right] \Rightarrow X_{OX}(t) = \sqrt{B(t+\tau)} \approx \sqrt{\mathrm{Bt}}$$

$t >> \tau$

B: Parabolic rate constant

Oxidation Rate Constants

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Table 6–2 Rate constants describing (111) silicon oxidation kinetics at 1 Atm total pressure. For the corresponding values for (100) silicon, all C_2 values should be divided by 1.68.

Ambient	B	B/A
Dry O_2	$C_1 = 7.72 \times 10^2\ \mu m^2\ hr^{-1}$	$C_2 = 6.23 \times 10^6\ \mu m\ hr^{-1}$
	$E_1 = 1.23$ eV	$E_2 = 2.0$ eV
Wet O_2	$C_1 = 2.14 \times 10^2\ \mu m^2\ hr^{-1}$	$C_2 = 8.95 \times 10^7\ \mu m\ hr^{-1}$
	$E_1 = 0.71$ eV	$E_2 = 2.05$ eV
H_2O	$C_1 = 3.86 \times 10^2\ \mu m^2\ hr^{-1}$	$C_2 = 1.63 \times 10^8\ \mu m\ hr^{-1}$
	$E_1 = 0.78$ eV	$E_2 = 2.05$ eV

- Above theory is great … but usually, the equations are not used in practice, since measured data is available
  - ↳ Rather, oxidation growth charts are used

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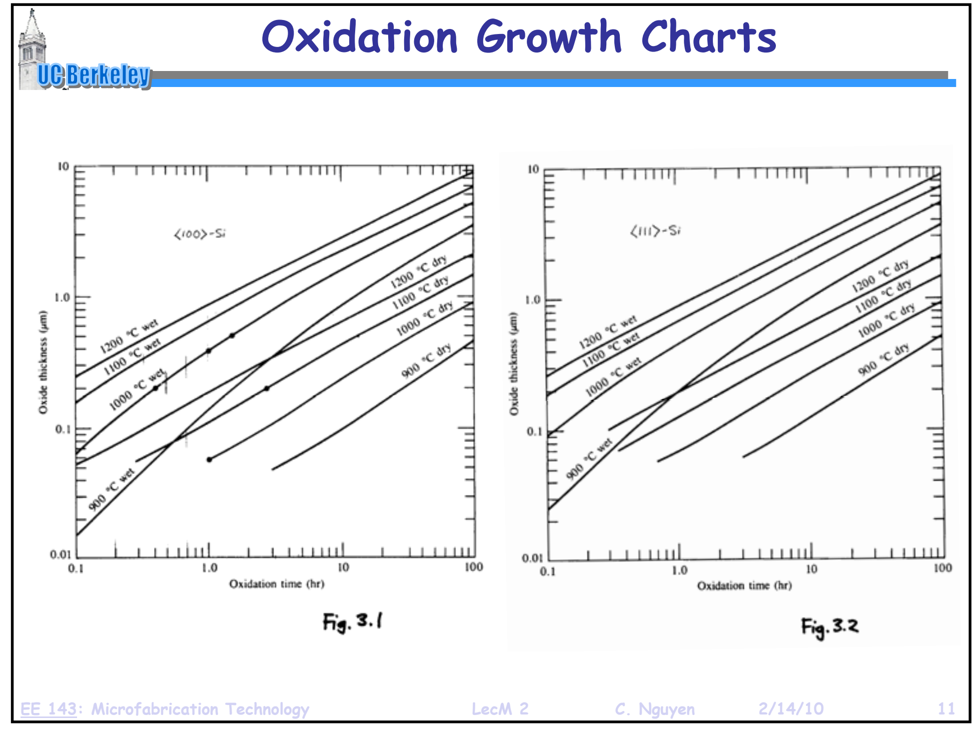

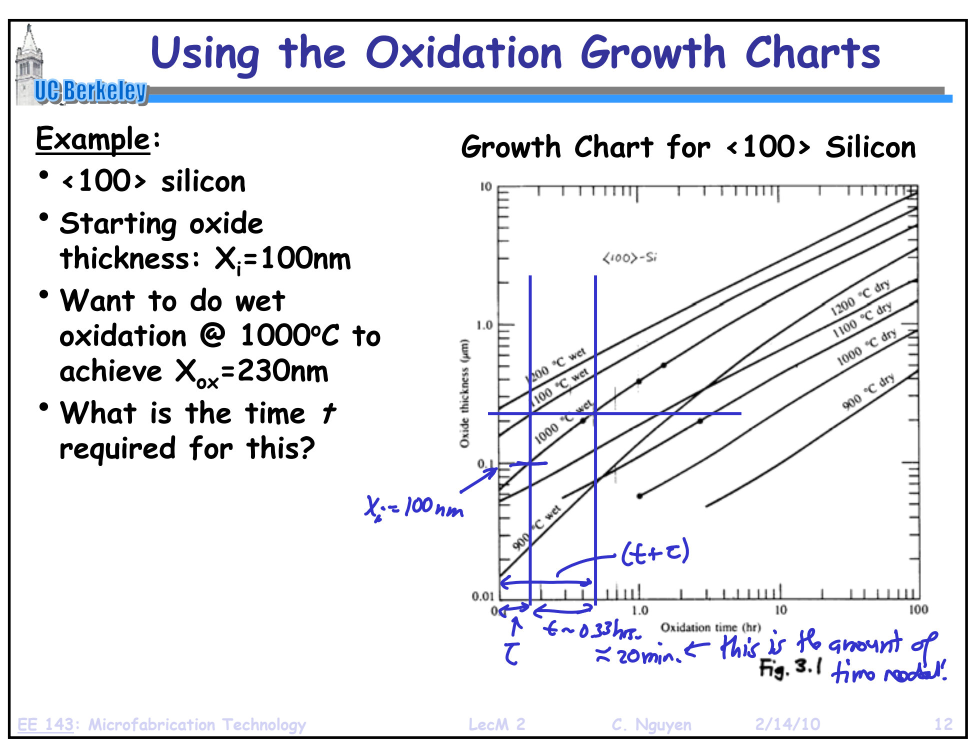

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Factors Affecting Oxidation

- In summary, oxide thickness is dependent upon:
  1. Time of oxidation
  2. Temperature of oxidation
  3. Partial pressure of oxidizing species ($\propto N_o$)
- Also dependent on:
  4. Reactant type:
     - Dry O_2
     - Water vapor ⇨ faster oxidation, since water has a higher solubility (i.e., D) in SiO_2 than O_2
  5. Crystal orientation:
     - <111> ← faster, because there are more bonds available at the Si-surface
     - <100> ← fewer interface traps; smaller # of unsatisfied Si-bonds at the Si-SiO_2 interface

Factors Affecting Oxidation

6. Impurity doping:
   - P: increases linear rate const.
     no affect on parabolic rate constant
     faster initial growth → surface reaction rate limited
   - B: no effect on linear rate const.
     increases parabolic rate const.
     faster growth over an initial oxide → diffusion faster

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Dopant Redistribution During Oxidation

- This must be considered and designed for when generating any process flow, especially for transistor circuits, e.g., CMOS
- During oxidation, the impurity concentration at the Si-SiO_2. interface can increase (pile-up) or deplete, depending upon the dopant type
- Whether a particular impurity depletes or piles up @ the interface depends on:
  1. Diffusion coefficient, D (of the impurity in SiO_2)
  2. Segregation coefficient, m:

$$m = \frac{\text{impurity equil. conc. in Si}}{\text{impurity equil. conc. in SiO}_2}$$

Dopant Behavior During Oxidation

- Segregation coefficient (m) and diffusion constant (D) combine to determine dopant behavior during oxidation:

Impurity	m	D in SiO_2	Dopant Behavior During Oxidation
B	<0.3 (small)	Small	depl. f/Si surface, pile up in oxide
B (oxidation w/H_2)	<0.3 (small)	Large	depl. f/Si surface, depl. from oxide
P, Sn, As	~10 (large)	Small	pile up in Si, very little diff. into SiO_2
Ga	20 (large)	Large	depl. f/Si, depl. from oxide

e.g., wet oxidation where H_2 is present as a by-product.

So large that it depletes the dopant @ the Si surface despite

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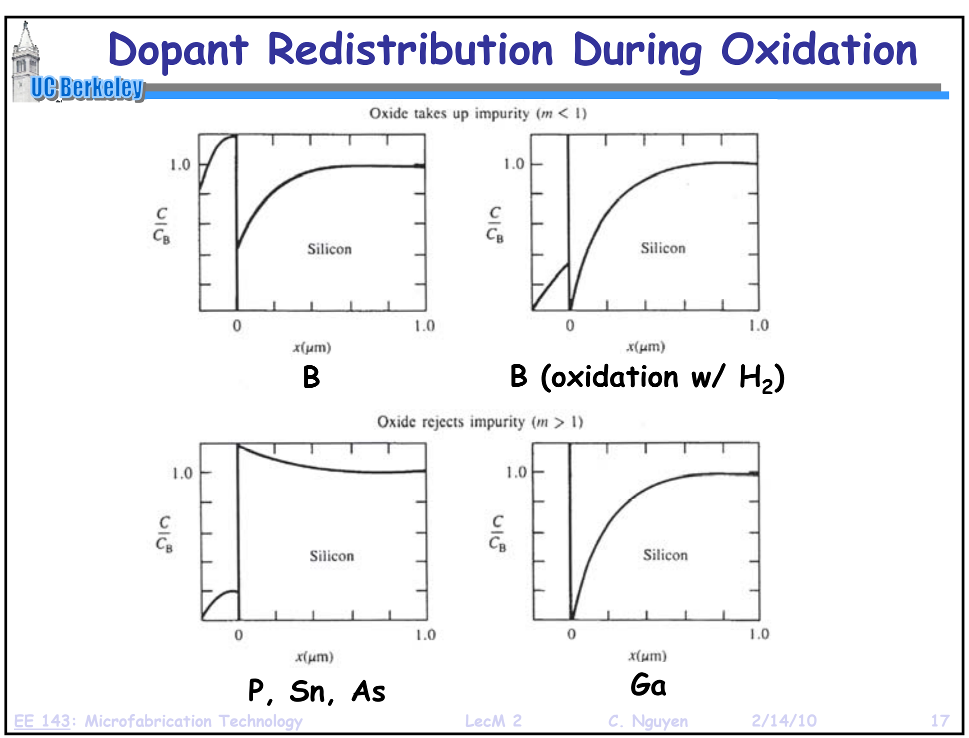

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