Numerical Modeling of Oxygen Precipitation Behaviors in Semiconductor Silicon Wafer

Ping Xin and Toshio Abe

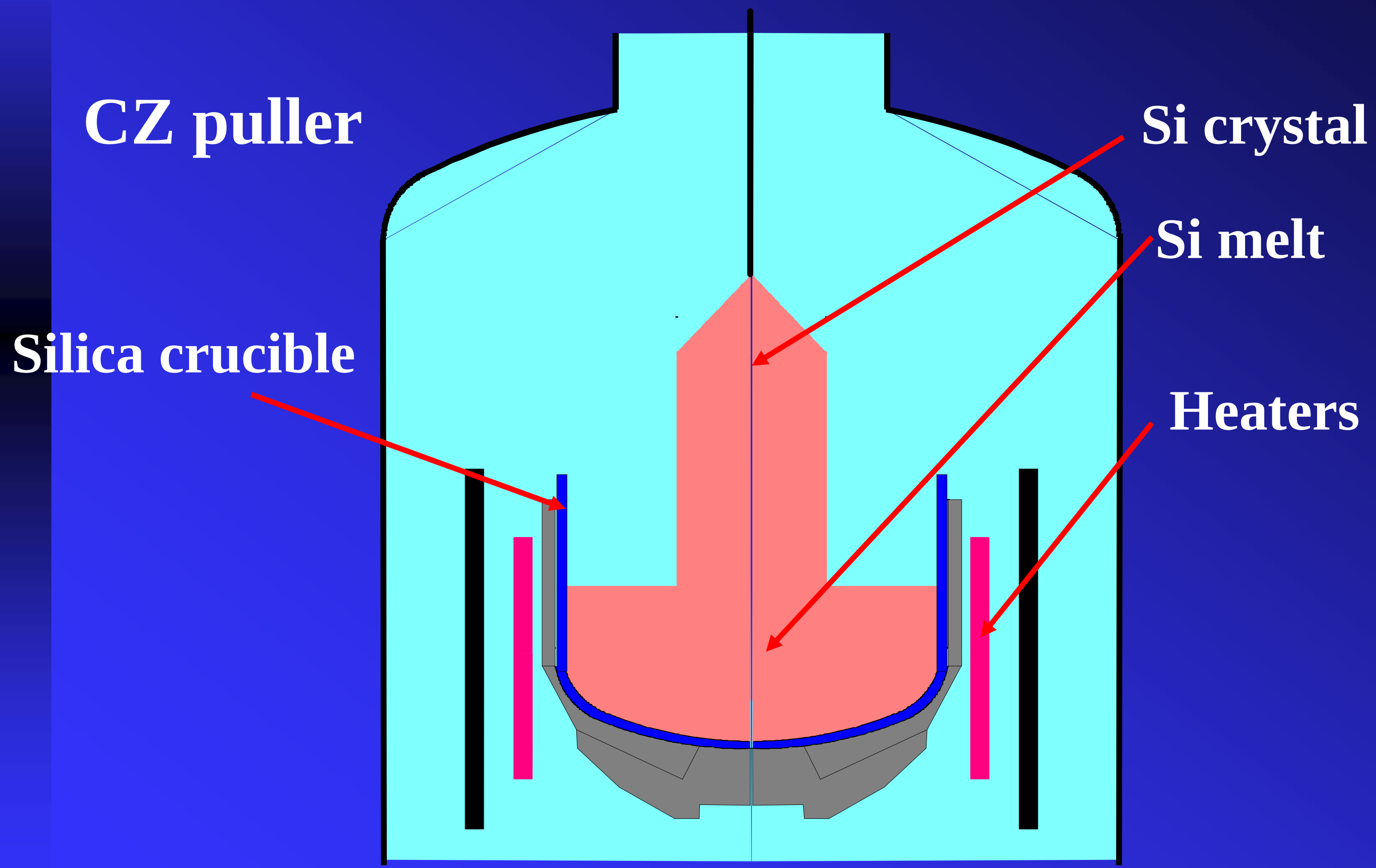
Toshiba Ceramics Co., Ltd.

Outline

- Background
- Wafer annealing process
- Modeling for oxygen precipitation
- Numerical analyses
- Summary

Background

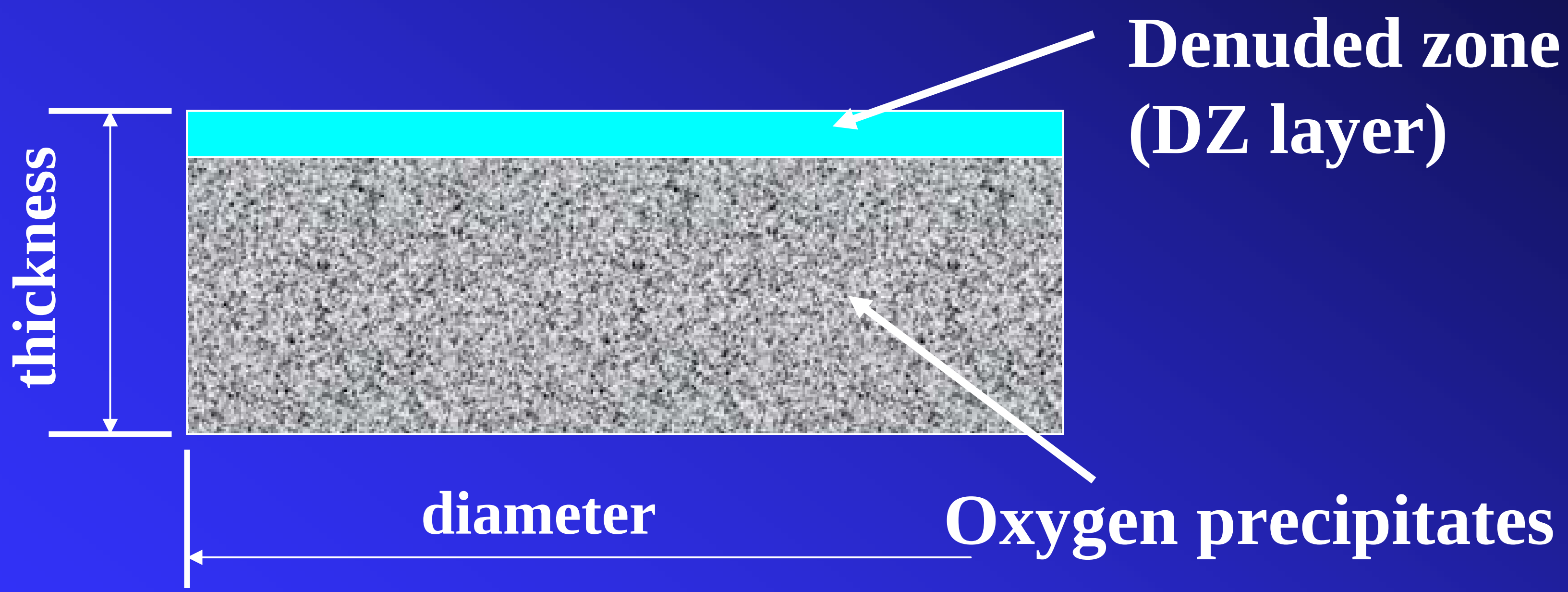
- LSI industry needs Czochralski Silicon crystal



Background

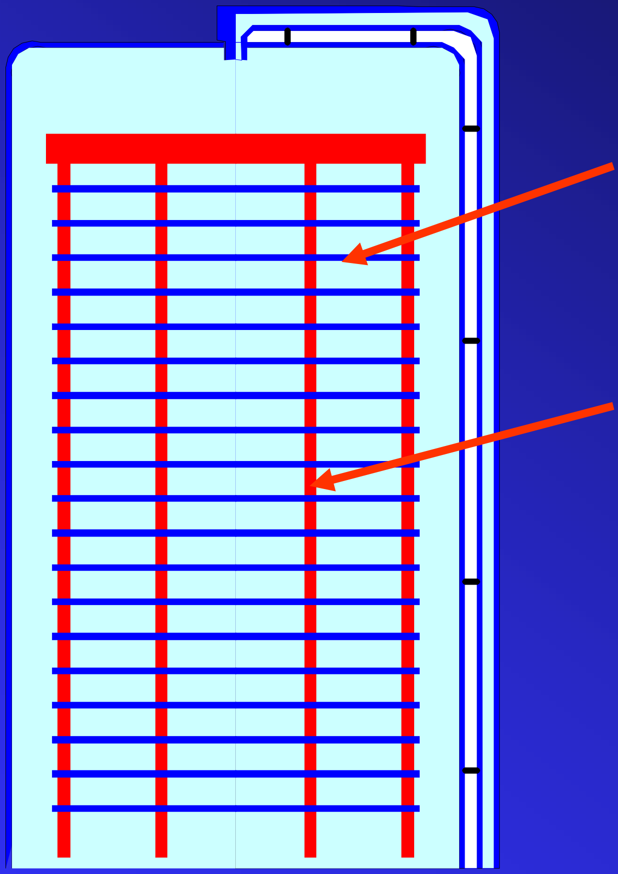
- **Needs for a silicon wafer**

Cross section of silicon wafer



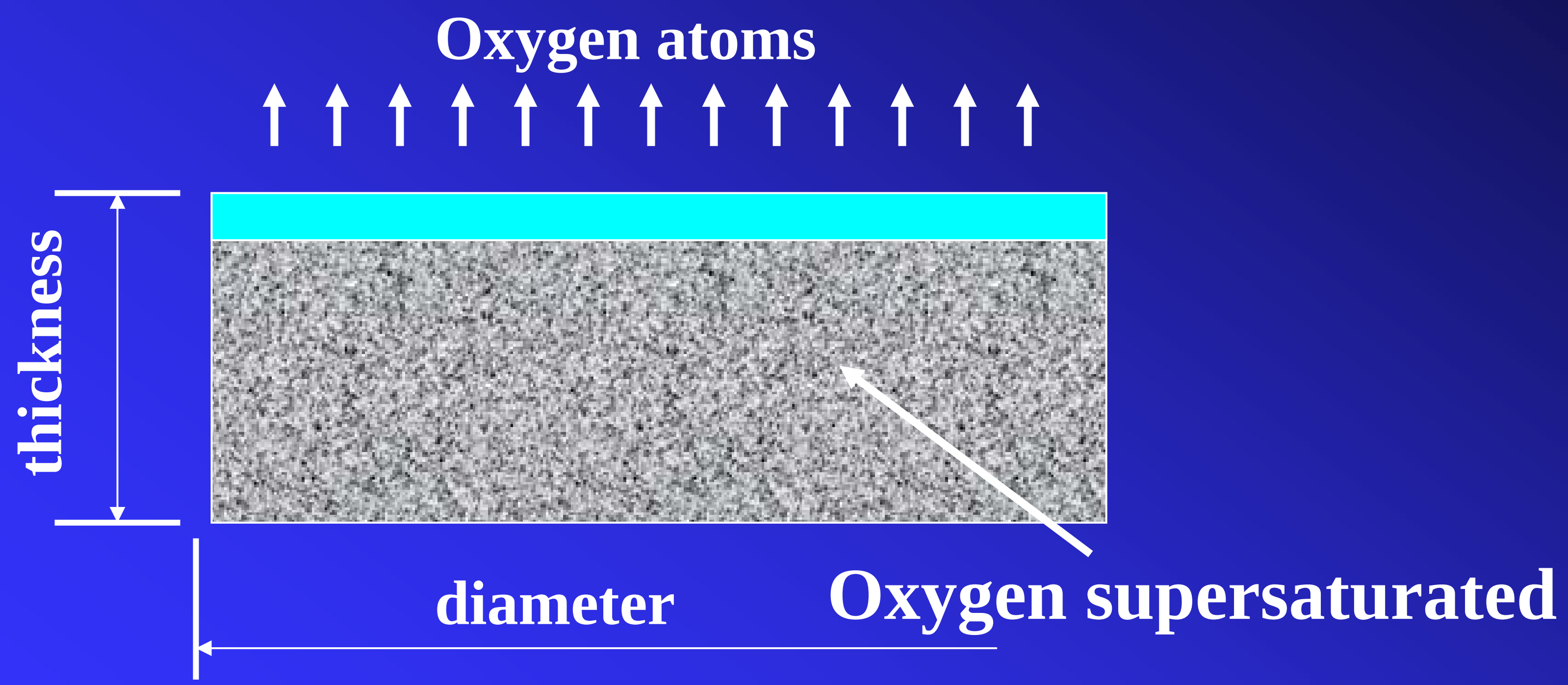
Wafer Annealing Process

Cross section of an annealing furnace



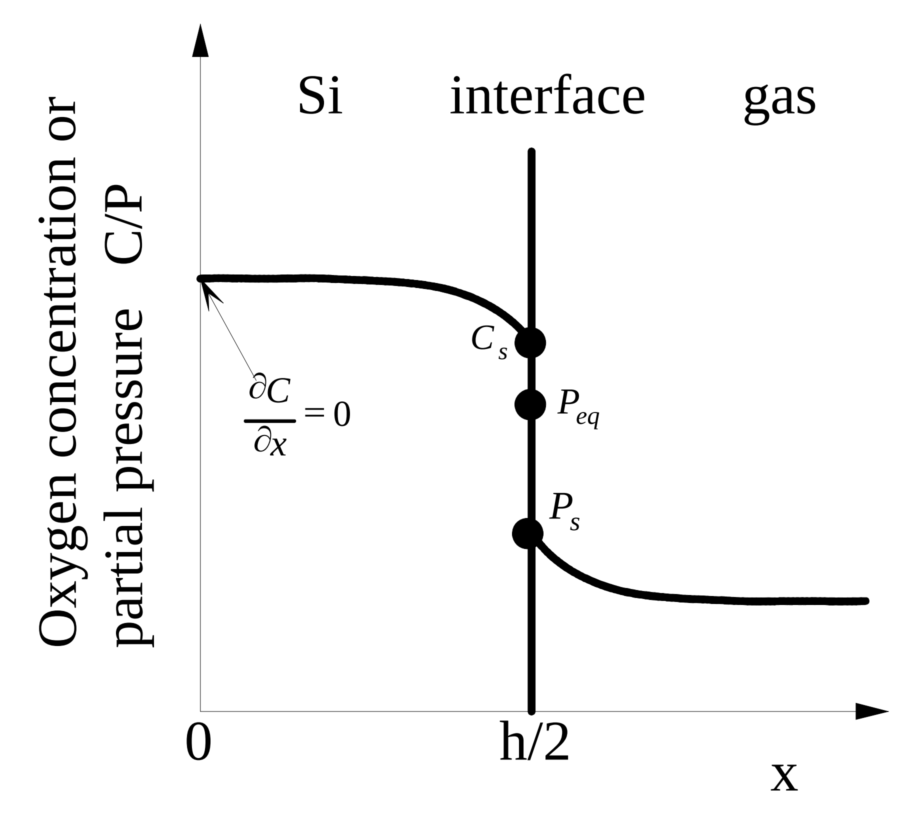
Wafer Annealing Process

- **Out-diffusion of oxygen from wafer surface**
- **Precipitation of resolved oxygen in bulk wafer**



Modeling for Oxygen Precipitation

- **Out-diffusion of oxygen from wafer surface**



$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2}$$

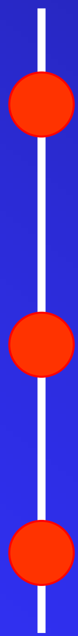
Modeling for Oxygen Precipitation

- **Out-diffusion of oxygen from wafer surface**

Wafer surface

$$-D\frac{\partial C}{\partial x}\Big|_{x=h/2} = k(P_{eq} - P_s)$$

Oxygen con-Centration Cs



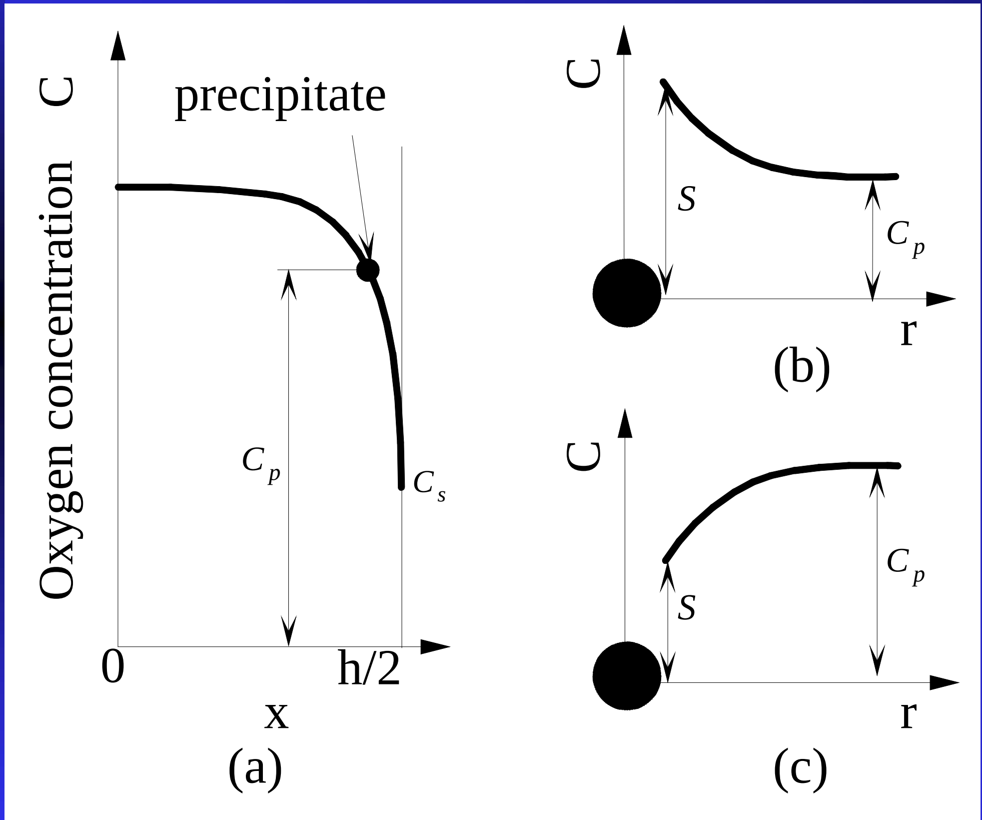
Equilibrium vapor phase pressure Peq

Si wafer

Real partial pressure of oxygen Ps

Modeling for Oxygen Precipitation

- **Oxygen precipitation**



dissolution process

Growth process

Modeling for Oxygen Precipitation

- **Oxygen precipitation**

$$\frac{\partial^2 C}{\partial r^2} + \frac{2}{r}\frac{\partial C}{\partial r} = 0$$

Solution of the equation

$$C = (S - C_p)\frac{r_0}{r} + C_p$$

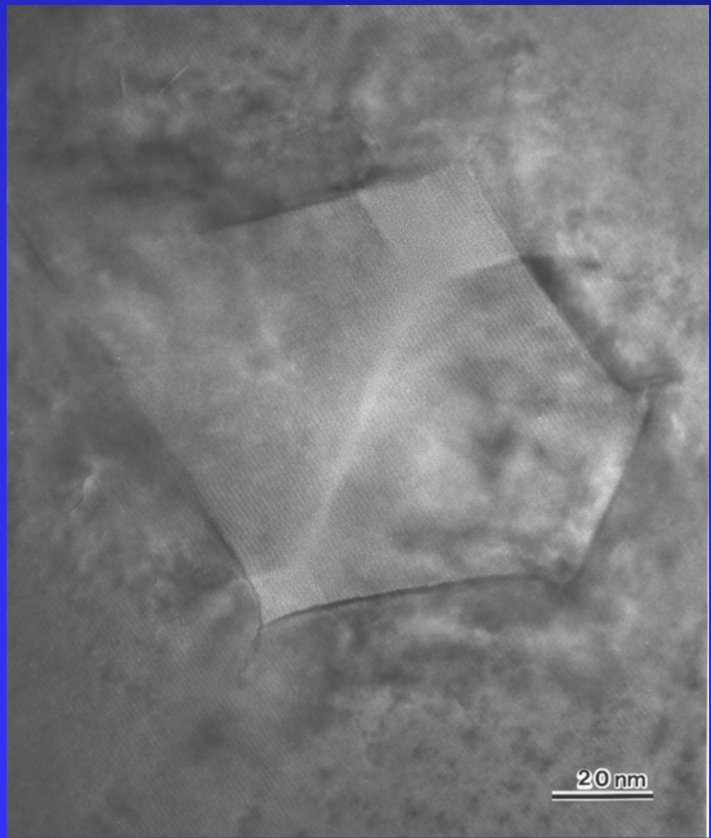
Variation rate of the precipitate

$$\frac{\partial r_0}{\partial t} = \Omega_p D(S - C_p) / r_0$$

S: Solubility of O in Si
Cp: O concentration at precipitate site
D: Diffusivity of O in Si
Ω: molecular volume of precipitate

Modeling for Oxygen Precipitation

- **Morphology of oxide precipitates**



TEM image of oxide precipitate

Octahedral shape

↓

Assumption in model:
Spherical shape

Numerical Analyses

- **Diffusivity and Solubility of O in Si**

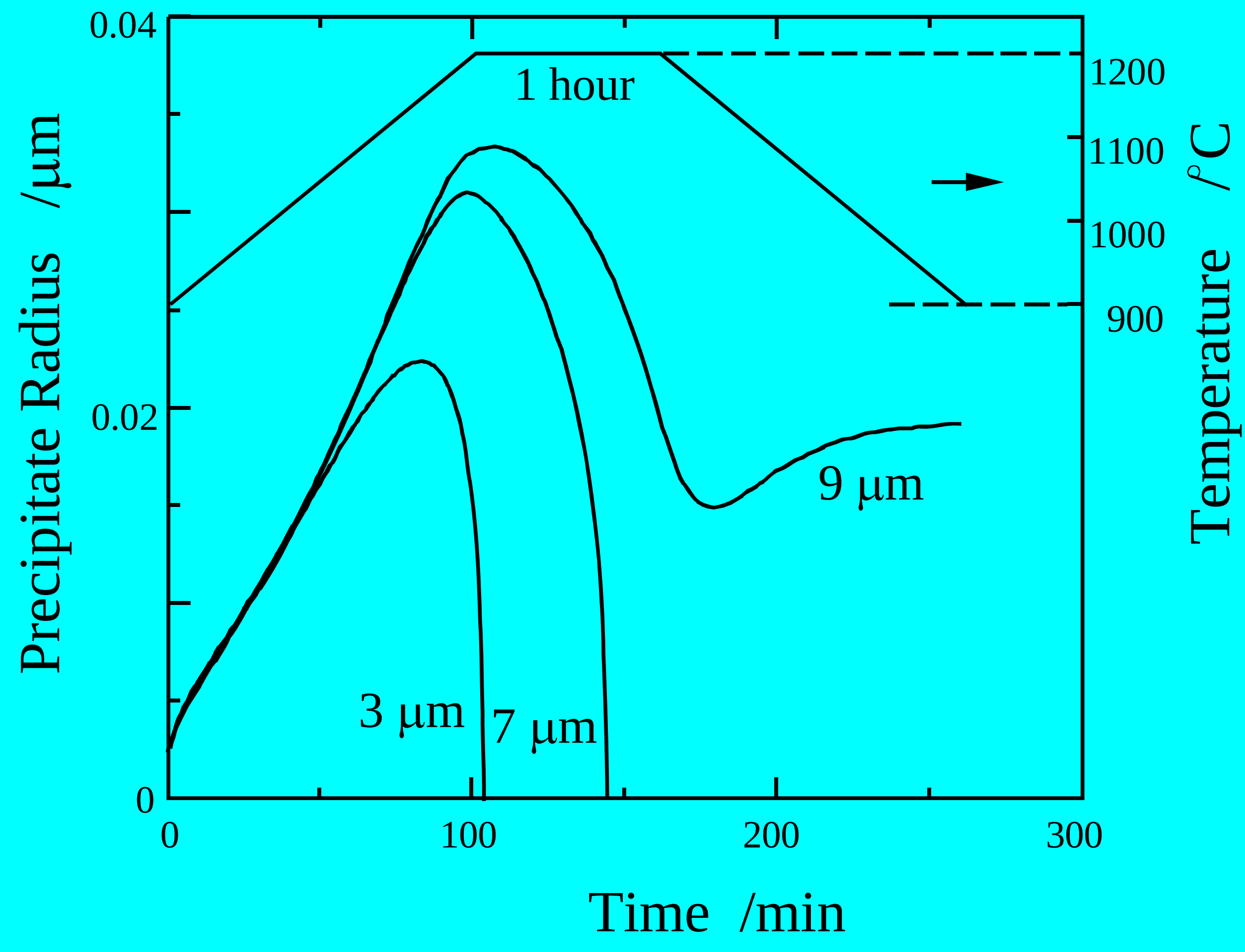
$$D = 0.13\exp\left(-58.4kcal/mol \Big/ RT\right) \quad \mathrm{cm^2/s}$$

$$S = 9.0\times10^{22}\exp\left(-35.1kcal/mol \Big/ RT\right) \quad \mathrm{atom/cm^3}$$

J. C. Mikkelsen, Jr., MRS, Pittburger, 1986, 19.

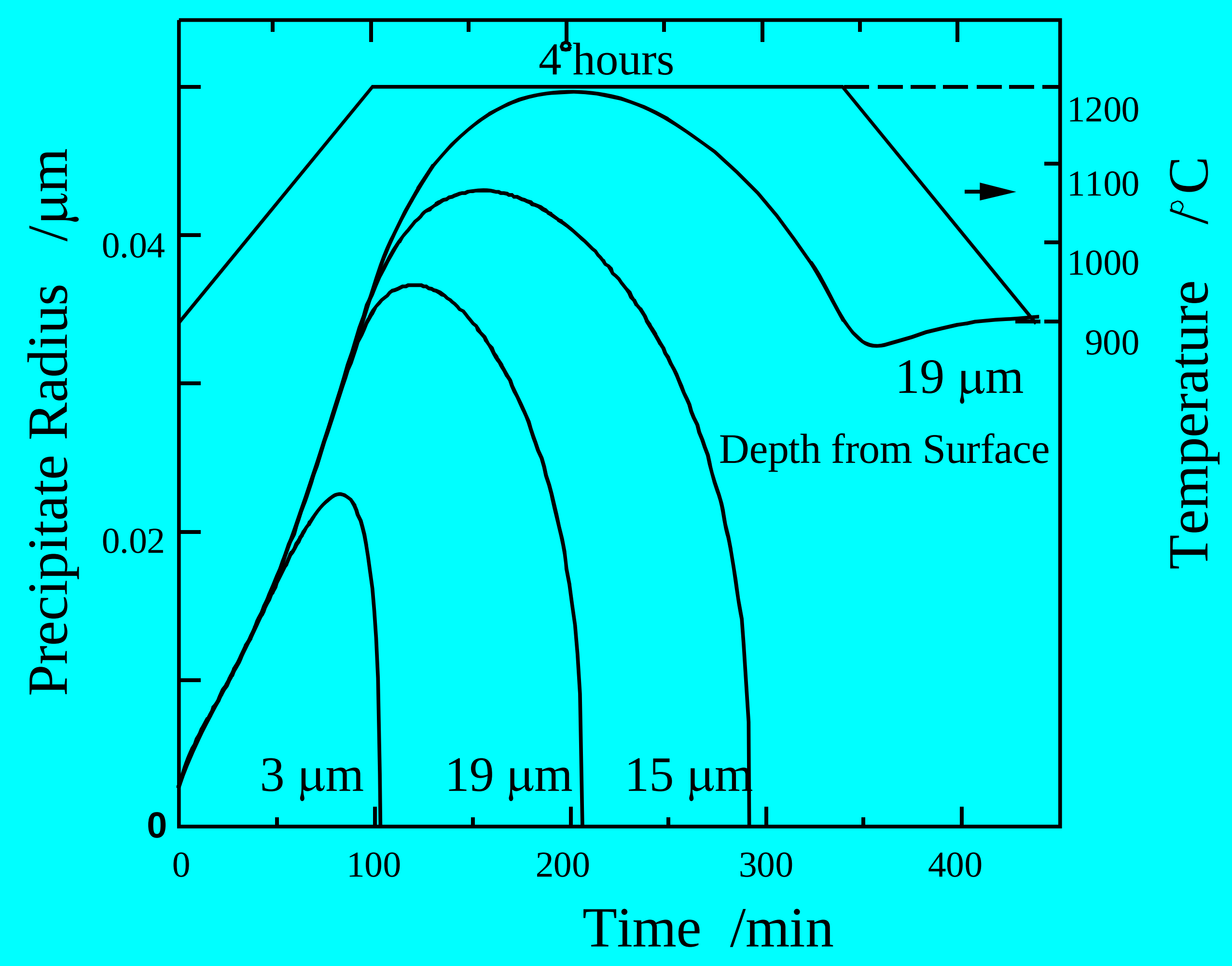
Numerical Analyses

- **Behaviors of precipitates different depth**



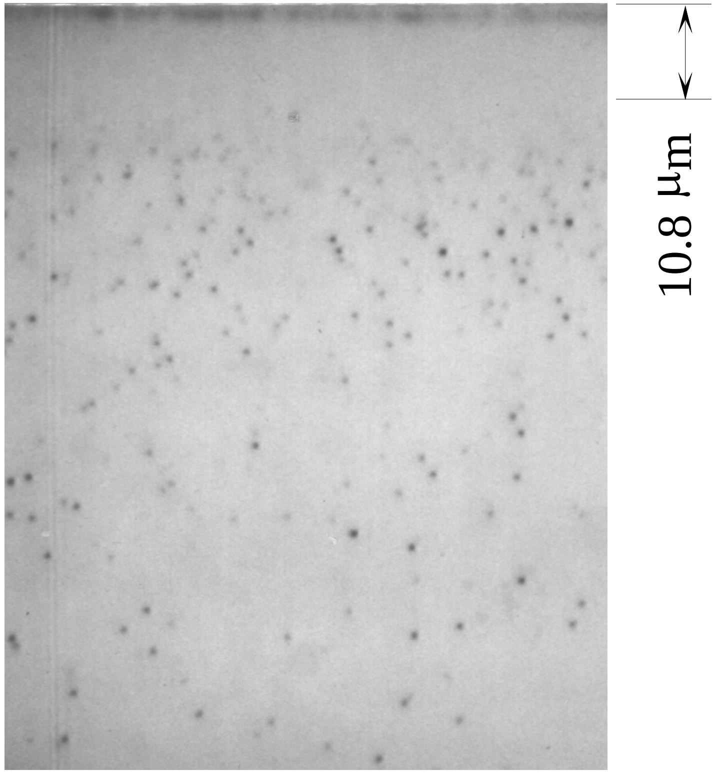
Numerical Analyses

- **Effect of annealing time on precipitates**

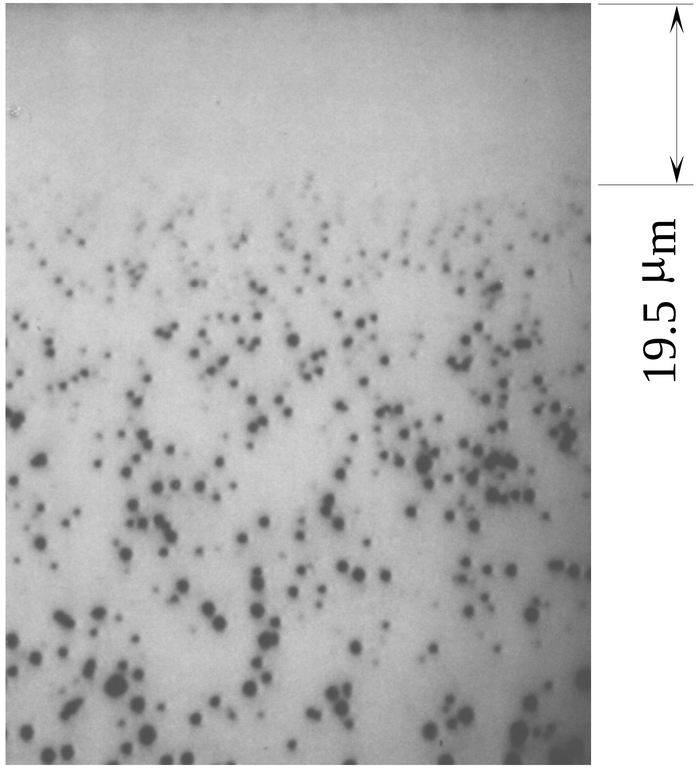


Numerical Analyses

- **Infrared tomography images of silicon wafers**



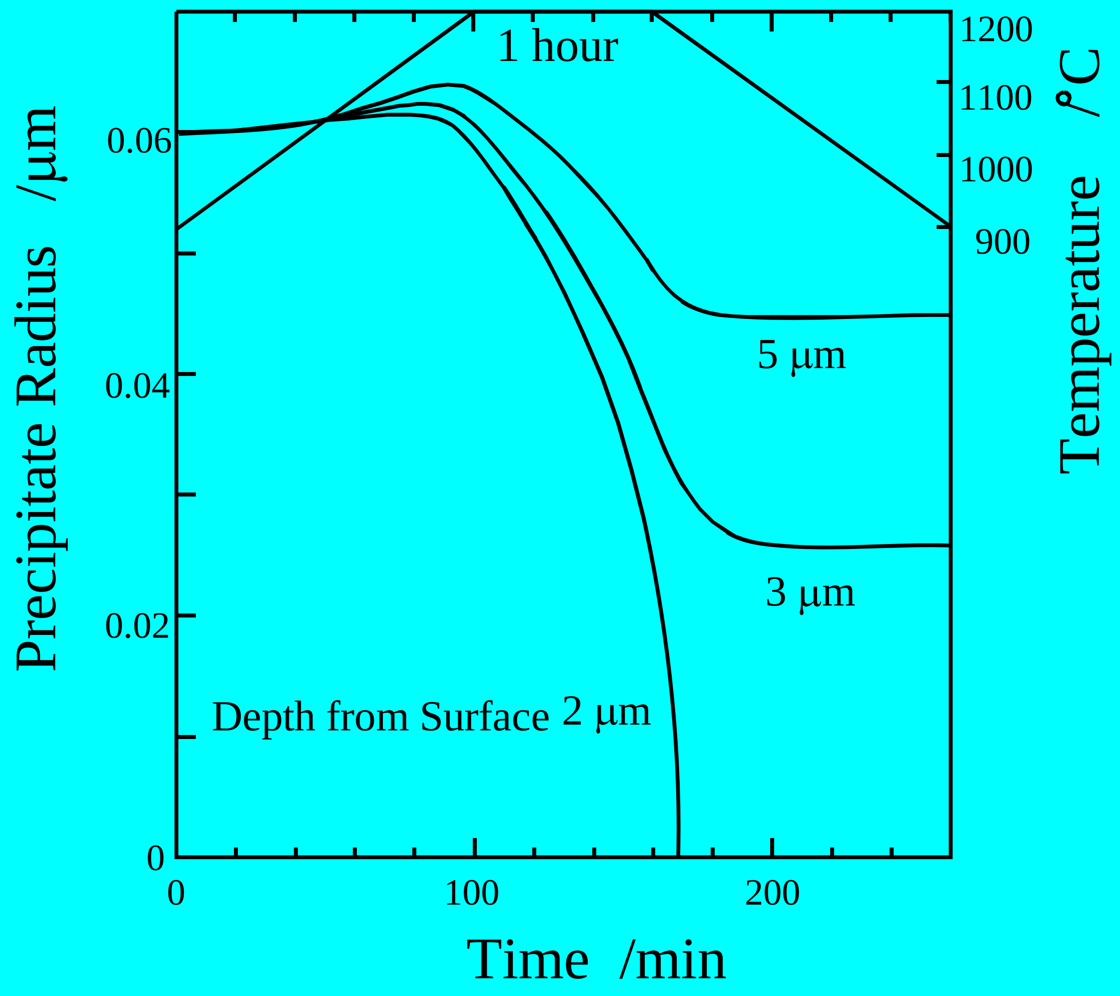
1 hour annealing



4 hours annealing

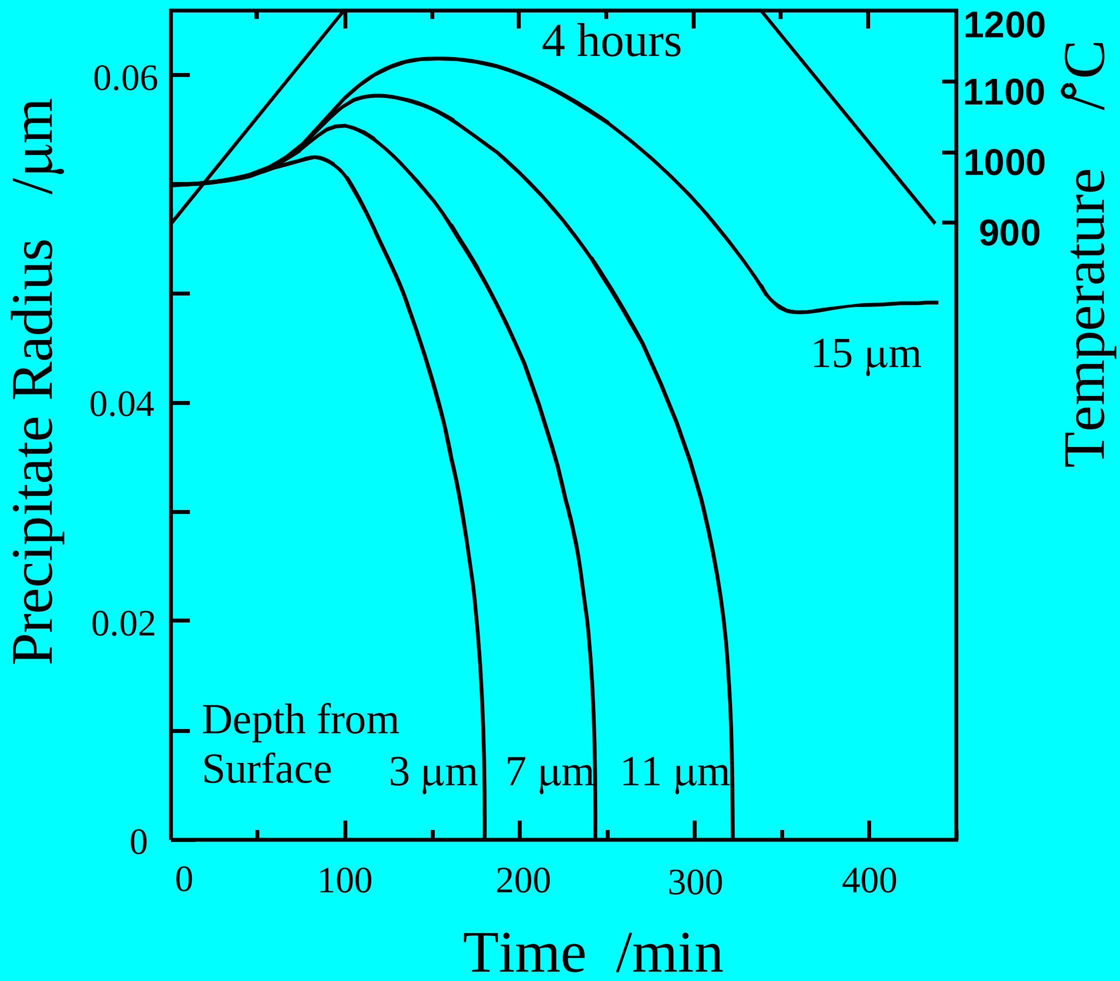
Numerical Analyses

- **Behaviors of inhomogeneous precipitates**



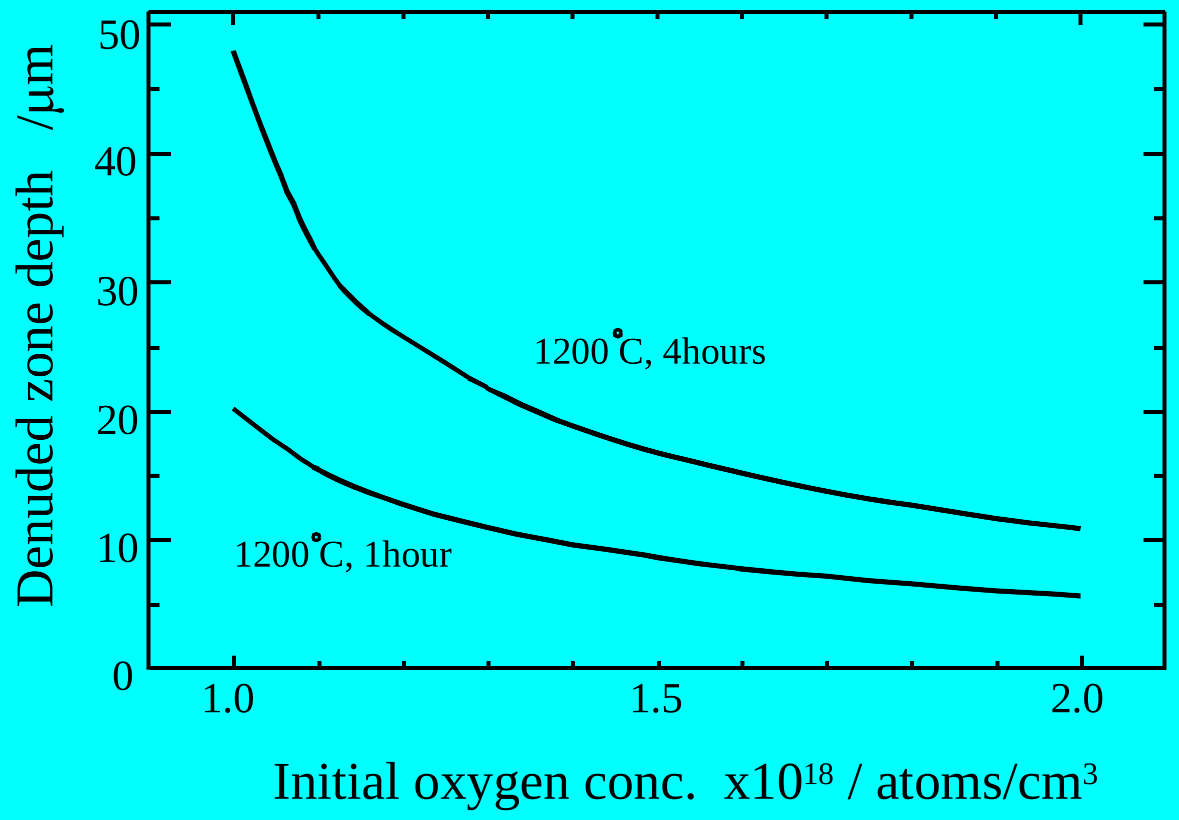
Numerical Analyses

- **Behaviors of inhomogeneous precipitates**



Numerical Analyses

- **Effect of initial oxygen concentration on DZ depth**



TOSHIBA

Summary

- A numerical model concerning behaviors of oxide precipitates in silicon crystal grown by Czhochralski technique has been established on the basis of diffusion theory.
- Simulation results of the annealing processes for silicon wafers with present model show good agreement with observations. Annealing processes can be designed with present model.