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C-6-5 Simulation and Modeling of Boron Diffusion in Silicon

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A computer simulation program for the diffusion of impurity ions in silicon incorporating the continuity and Poisson equations has been established. A diffusion model based on the vacancy-interstitialcy dual mechanism is used to express the boron diffusivity in silicon during both predeposition and drive-in processes. Deposition of boron atoms into silicon crystals using BN and BBr_3 sources and redistribution of deposited layers under dry nitrogen, dry oxygen, and water vapor have been investigated experimentally and mathematically.

High resistivity n-type silicon slices were used as starting materials. The sheet resistance was obtained using a four-point probe. The oxide thickness was measured by ellipsometry. The impurity profile of diffused layer was determined for some slices by using the incremental sheet conductance method. While some slices were analyzed using the spreading resistance measurement. By properly choosing the boundary conditions and diffusivity parameters, the impurity profile and sheet resistance as a function of time for various temperatures can be calculated.

Assuming that boron atoms are completely ionized at process temperature, the motion of acceptor ions in silicon can be described by[1] the continuity equation

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial y}\left(D\frac{\partial C}{\partial y} - DC\frac{\partial \psi}{\partial y}\right) \tag{1}$$

and the Poisson equation

$$\frac{\partial^2 \psi}{\partial y^2} = 2 \sinh \psi + C \tag{2}$$

where C is the boron concentration normalized to the intrinsic carrier concentration n_i, ψ is the space-charge potential normalized to the thermal potential kT/q, D is the diffusion coefficient normalized to the intrinsic diffusivity D_i, y is the distance normalized by a length $L=(\varepsilon_s \, kT/q^2 \, n_i)^{1/2}$, and t is the time normalized by a factor L^2/D_i.

During deposition process, a condition of constant surface concentration is assumed. For drive-in under inert ambient, a slight out-diffusion must be taken into account. Under oxidized ambient, boron is segregated into the growing oxide according to the interface condition[2]

$$D\frac{\partial C}{\partial y} = (k-m)\ C_{i+} \frac{dX_o}{dt} \tag{3}$$

where k is the segregation coefficient defined as the ratio of boron concentration in the oxide C_{i-} to that in silicon C_{i-} at the SiO_2-Si interface, m is the volumetric ratio for silicon converted to silicon dioxide, and dX_o/dt is the oxide growth rate given by

$$\frac{dX_o}{dt} = \frac{B}{2X_o+A} \quad (4)$$

In addition, during thermal oxidation, the moving boundary problem is solved with a moving coordinate system.

The parabolic rate constant B and the linear rate constant B/A depend not only on oxidation ambient but also on dopant concentration. Based on the vacancy statistics model, the oxidation rate constants can be expressed as[3]

$$B/A = (B/A)^i[1+\gamma\{f(\psi)/f(0)-1\}] \quad (5)$$

$$B = B^i[1+\delta\{f(\psi)/f(0)\}^\nu] \quad (6)$$

where $(B/A)^i$ and B^i are the intrinsic linear and parabolic rate constants, γ, δ and ν are the empirical parameters, and

$$f(\psi) = \beta^+e^{-\psi} + 1 + \beta^-e^{\psi} + \beta^=e^{2\psi} \quad (7)$$

with β^+, β^- and $\beta^=$ known as the vacancy statistics parameters[4].

From the study of high concentration and thermal oxidation enhanced diffusions of boron and phosphorus atoms in silicon, it is generally believed that a substitional impurity diffuses via a dual mechanism of vacancy and interstitialcy and the effective diffusivity may be related to the space-charge potential and thermal oxidation rate by[5]

$$D = \alpha f(\psi)/f(0) + \beta(dX_o/dt)^\eta \quad (8)$$

where α, β and η are the empirical parameters.

The vacancy and interstitialcy contribution parameters α, β and η have been determined for various diffusion conditions. The thermal oxidation rate parameter γ, δ and ν and the segregation coefficient k obtained in this work are in good agreement with those reported on the literatures[2,3,6].

References

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