## Boron diffusion and activation in polycrystalline Si<sub>1-x</sub>Ge<sub>x</sub> films for CMOS gate electrodes

T. Sulima, J. Schulze, U. Abelein, A. Ludsteck, I. Eisele Institute of Physics (EIT 9.2)

University of the German Federal Armed Forces Munich Werner-Heisenberg-Weg 39, D-85577 Neubiberg, Germany

#### **INTRODUCTION**

We have studied the B diffusion process in polycrystalline  $Si_{1-x}Ge_x$  films fabricated by means of molecular beam epitaxy (MBE) on top of thermally grown SiO<sub>2</sub> dielectric films. The diffusion parameters: diffusion length  $L(T_A, t_A)$ , diffusion coefficient D(T), diffusion constant  $D_0$ , and activation energy  $W_A$  were investigated as functions of Ge mole fraction *x* in the grown films and of MBE deposition temperature  $T_D$  for achieving different poly grain sizes. The stochiometry of the grown polycrystalline Si<sub>1-x</sub>Ge<sub>x</sub> films was determined by Rutherford-backscattering spectrometry (RBS).

For an accurate determination of  $L(T_A, \tau)$  for different annealing temperatures  $T_A$  and annealing process times  $\tau$ we used the delta doping technique to obtain a well defined initial B depth and concentration profile  $c_B(z, T_A = 0, \tau = 0)$  in the fabricated Si<sub>1-x</sub>Ge<sub>x</sub> films. The annealing process time  $\tau$  consists of the temperature ramping time  $t_R$  and the annealing time  $t_A$  at  $T_A$ . Rapid thermal annealing (RTA) was used to minimize B diffusion during ramping times  $t_R$ . The B and the Si<sub>1-x</sub>Ge<sub>x</sub> concentration profiles were measured by means of secondary ion mass spectrometry (SIMS).

# SAMPLE PREPARATION

By using MBE an undoped homogeneous Si<sub>1-x</sub>Ge<sub>x</sub> film  $(0 \le x \le 1)$  with a thickness of 150nm was grown at a temperature  $T_D$  ( $T_D = 200/500/700^{\circ}C$ ) on top of a 10nm thermally grown SiO<sub>2</sub> film. In a second step pure B with a dose of  $\varphi_0 = 5e12cm^{-2}$  was deposited at  $T_D = 200^{\circ}C$ . Finally an undoped 50nm Si cap was deposited also at  $T_D = 200^{\circ}C$ . This cap is needed to form an ultra-sharp and well defined buried B delta doping spike with a thickness smaller 3nm [1] and for an accurate SIMS analysis.

After MBE pieces of a grown sample were annealed by means of RTA each at an individual annealing time  $t_A$  and temperature  $T_A$  ( $T_A = 750/800/850/900/950/1050^{\circ}C$ ). To determine the influence of the RTA ramping phases pieces were annealed at the chosen annealing temperatures  $T_A$  for  $t_A = 0$ . The resulting diffusion profiles  $c_B(z, T_A, \tau)$  were measured by SIMS.

#### **DIFFUSION MODELLING**

Time and temperature dependent impurity diffusion processes are described by the second Fick's law:

$$d/dt[c(z, T, t)] = D(T)^{*}d^{2}/dz^{2}[c(z, T, t)].$$
 [1]

For an initial ultra-sharp impurity concentration  $c(z = 0, T < T_{crit}, t = 0) = \varphi_0$  the solution of eq.1 is given by:

$$c(z, T, t) = 2^* \varphi_0 / (\pi^{0.5} L(T, t)) \exp(-z^2 / L(T, t)^2).$$
[2]

Below the critical temperature  $T_{crit}$  diffusion is negligible. The diffusion length L(T, t) is given by :

$$L(T, t) = 2^* (D(T)^* t)^{0.5}.$$
 [3]

The diffusion coefficient D(T) is given by :

$$D(T) = D_0 * exp(-W_A / (k_B * T)).$$
[4]

#### RESULTS

To calculate the diffusion coefficient  $D(T_A)$  as function of Ge mole fraction *x*, MBE deposition temperature  $T_D$ , and annealing temperature  $T_A$  the diffusion length  $L(T_A, \tau = t_A)$  was calculated by:

$$L(T_{A}, \tau = t_{A}) = L(T_{A}, \tau = t_{R} + t_{A}) - L(T_{A}, \tau = t_{R}).$$
 [5]

The diffusion lengthes  $L(T_A, \tau = t_R + t_A)$  and  $L(T_A, \tau = t_R)$  were extracted from the individual SIMS profiles (see fig.1).



**Fig.1:**  $ln[c(z, T_A, \tau)]$  vs.  $z^2$  for Ge mole fraction x = 0.2and  $T_D = 500^{\circ}C$ 

The individual activation energy  $W_A$  and diffusion constant  $D_0$  as functions of Ge mole fraction x and MBE deposition temperature  $T_D$  were extracted from an Arrhenius plot  $ln[D(T_A)]$  vs.  $1/T_A$  (see fig.2).



**Fig.2:** Arrhenius plot  $ln[D(T_A)]$  vs.  $l/T_A$  for Ge mole fraction x = 0.2 and  $T_D = 500^{\circ}$ C

As known from literature the activation energy  $W_A$  of B in Si is  $W_A = 3.46 \ eV$ . This is in accordance to our experimental results for polycrystalline Si. With increasing Ge mole fraction x the B activation energy decreases. This allows a lower thermal budget for CMOS processing. Experimental results of the whole process parameter matrix given by deposition temperature  $T_D$ , Ge mole fraction x, annealing temperatures  $T_A$ , and annealing times  $t_A$  are presented. In addition the poly grain size dependence will be discussed.

## REFERENCES

[1] Zeindl, Wegehaupt, Eisele, Oppolzer, Reisinger, Tempel, Koch, Appl. Phys. Lett. 50 (1987) 1165