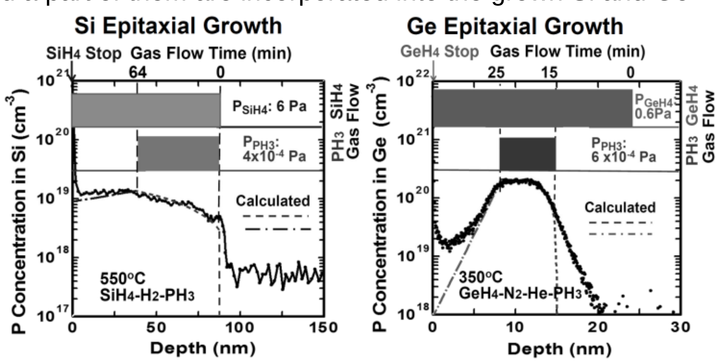
ATOMICALLY CONTROLLED PROCESSING FOR DOPANT SEGREGATION IN CVD SILICON AND GERMANIUM EPITAXIAL GROWTH

Junichi Murota, Tohoku Univ
murota@riec.tohoku.ac.jp
Yuji Yamamoto, IHP/ Ioan Costina, IHP/ Bernd Tillack, IHP and TU Berlin
Vinh Le Thanh, Aix Marseille Univ./ Roger Loo, imec / Matty Caymax, imec

Key Words: Atomically controlled processing, group IV semiconductor, CVD, Si, Ge.

Atomically controlled processing has become indispensable for the fabrication of Si-based ultra-small devices and heterodevices for ultra-large scale integration. This is because high performance devices require atomic-order abrupt heterostructures and doping profiles as well as strain engineering which is obtained by the introduction of Ge into Si. Our concept of atomically controlled processing is based on atomic-order surface reaction control in Si and Ge-based CVD growth [1-4]. The fabrication of atomic-level steep doping profiles requires the suppression of dopant segregation during epitaxial growth [5,6]. In this work, P and B impurity segregation during in-situ doping in Si and Ge CVD epitaxial growth is reviewed.

The epitaxial growth of undoped Si/in-situ doped Si film with a Si buffer layer grown at 750 ºC on Si(100) was performed at 550 ºC using SiH_4-dopant (PH_3 or B_2H_6)-H_2-He gas mixtures. Undoped Ge/in-situ doped Ge/ undoped Ge on a few nm-thick $Si_{0.5}Ge_{0.5}$/Si(100) was performed at 350 ºC using GeH_4-dopant (PH_3 or B_2H_6) - N_2-He-H_2 gas mixtures. The doping profile in the films and the segregated dopant atomic amount on the surface of the in-situ doped films were measured by SIMS and XPS, respectively. In case of P doping, the P atoms segregate to the growing Si and the Ge surfaces and a part of them are incorporated into the grown Si and Ge top layers. The P segregation during Si growth is larger than that during Ge growth (Fig.1). In the case of B doping, the B atoms scarcely segregate to the growing Si and Ge surface. Based on these results, the in-situ doping processes are explained by a modified Langmuir-type model (Table I (7)). Using the model, we estimated the incorporation rate of dopant atoms into Si or Ge from the surface and the surface adsorption rate of dopant species from the SIMS data. From these parameters, the amount of dopant segregation at the surface is calculated. The calculated value is in good agreement with the values obtained from XPS measurements. These results demonstrate the capability of atomically controlled processing for group IV semiconductors.This work is partially supported by the JSPS Core-to-Core Program, "International Collaborative Research Center on Atomically Controlled Processing for Ultralarge Scale Integration".



Fitting Parameters for Calculation
k_P = 9 min^{-1}Pa^{-1}, k_{-P} = 0 min^{-1}
$k_{INC\text{-}P}$ = 0.007min^{-1}
$Q_D(0) = 3.5 \times 10^{13}$ cm^{-2} on buffer layer

Fitting Parameters for Calculation
k_P = 36 min^{-1}Pa^{-1}, k_{-P} = 0 min^{-1}
$k_{INC\text{-}P}$ = 0.46 min^{-1}

Figure 1 – In-situ doping of P for Si and Ge epitaxial

Table I – Equations in the modified Langmuir-type model for formulating in-situ doping in Si and Ge epitaxial

Site density where dopant molecules are occupied at the surface during in-situ doping (Dopant : P or B=D)

$$Q_D(t) = \frac{k_D P_D n_0}{k_D P_D + k_{-D} + k_{INC\text{-}D}}\{1-\exp[-(k_D P_D + k_{-D} + k_{INC\text{-}D})t]\} + Q(0), \quad (1)$$

k_D : adsorption rate constant of dopant species at M surface site, k_{-D} : desorption rate constant of dopant species at M surface site, $k_{INC\text{-}D}$: incorporation rate of dopant atoms into M epitaxial layer from the surface dopant atoms, P_D : partial pressure of dopant gas. n_0 : total adsorption site density.

After switching off the dopant gas supply,

$$Q_D(t) = Q_D(t_D)\exp[-(k_{-D}+k_{INC\text{-}D})(t-t_D)], \quad (2)$$

t_D is the time of dopant gas supply.

SiH_4 and GeH_4 (MH_4;M=Si, Ge) reaction rates

$$R_M(t) = \frac{k_1 P_{MH4} n_0}{1+(k_1/k_M)P_{MH4}}\left(1-\frac{Q_D(t)}{n_o}\right), \quad (3)$$

k_1 : adsorption rate constant of MH_4, k_M : reaction rate constant of MH_4, P_{MH4} : partial pressure of MH_4.

Dopant concentration in epitaxial Si or Ge

$$C_D(t) = \frac{k_{INC\text{-}D} Q_D(t)}{R_M(t)}. \quad (4)$$

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