Extremely Sharp Phosphorus Turn-Off Slope and Effect of Hydrogen on Phosphorus Surface Segregation in Epitaxially-Grown Relxed $Si_{0.7}Ge_{0.3}$ by RTCVD

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I. Introduction

Si quantum dots formed in a Si/SiGe two-dimensional gas (2DEG) are a promising candidate for the realization of solid-state quantum computation. To achieve effective Schottky gating for charge manipulation in the normal structures (Fig. 1a), a sharp phosphorus turn-off is required. We investigated phosphorus surface segregation in relaxed $Si_{0.7}Ge_{0.3}$ epitaxially grown by rapid thermal chemical vapor deposition (RTCVD) and report a record sharp turn-off slope of phosphorus of 6 nm/dec. The hydrogen surface coverage, which increases at low temperature, is a key mechanism for such sharp slopes. We demonstrated the sharp phosphorus turn-off enables a high quality inverted 2DEG of high mobiltiy and low electron density.

II. Experiment

We have found that the slope of P turn-off is far worse in relaxed SiGe than in strained SiGe. Thus, in this work, we performed a detailed study on P segregation in relaxed SiGe. The samples were epitaxially grown by RTCVD in a hydrogen carrier at 6 torr with gas precursors of SiH_4, GeH_4, and PH_3. The growth temperature of the $Si_{0.7}Ge_{0.3}$ was varied from 500 ^oC to 600^oC with the growth rate of 0.1 ~ 30 nm/min to investigate the impacts of temperature and growth rate on P segregation. The peak phosphorus doping level is controlled between 10^{18} to 10^{19} cm^{-3}. A schematic representation of test structures in shown in Fig. 1. Phosphorus profiles were measured by secondary ion mass spectroscopy (SIMS).

III. Results

According to simple adsorpotion-incorporation-desorption model [1], phosphorus surface segregation becomes worse as growth temperature decreases. However, its inability to explain the opposite trend at lower temperatures made the two-state model (TSM) popular [2]. This intuitive apporach describes phosphorus segregation as a two-particle exchange process between surface layer and sub-surface layer beneath (Fig. 2). By including hydrogen as surface blocking sites for potential P segregation (Fig. 3), the P turn-off slope (nm/decade) from TSM can be modified as

$$x_0 = \frac{a_0 \ln 10}{4} \frac{1}{\ln\left(1+\frac{e^{-\frac{\Delta E}{kT}}}{1-\Theta}\right) - \ln\left\{1-e^{-[r_{12}(1-\Theta)+r_{21}]\frac{a_0}{4GR}}\right\}}, \quad (1)$$

where r_{12} and r_{21} are jumping rates of phosphorus atoms from layer 1 to 2 and 2 to 1, n_1 and n_2 are normalized phosphorus surface concentrations of layer 1 and 2, Θ is the hydrogen surface coverage of layer 2. Fig. 4a shows the data of the growth dependence of phosphorus turn-off slope at various temperatures without consideration of hydrogen coverage ($\Theta = 0$). There is a large discrepancy between experimental data and theoretical curves which cannot be resolved by adjusting parameters. Since the CVD process involves hydrogen, by considering H surface coverage ($\Theta \neq 0$) [3], better matches between experimental data and theoretical calculations based on eq. (1) are obtained (Fig. 4b). Without any growth interruption or ex-situ cleaning steps [4], record sharp phosphorus turn-off slope of 6 nm/decade is obtained at 500^{o}C of growth rate ~ 0.1 nm/min (Fig. 5).

For some Si-based quantum computing approaches, such as those with a bi-layer 2DEG, an inverted 2DEG with the phosphorus-doped layer below the Si 2DEG layer is desired (Fig. 1b). This structure is traditionally limited by phosphorus segregation into the Si 2DEG region. By epitaxially growing these structures at low temperature to reduce the phosphorus segregation, we demonstrated high quality inverted modulation-doped 2DEG with the distance from the surface to 2DEG layer less than 50 nm. The electron mobility is 60,000 cm^2/V-s and the density is 1.8 x 10^{11} cm^{-2} at 4K.

IV. Summary

An ultra-sharp phosphorus turn-off slope in $Si_{0.7}Ge_{0.3}$ (6 nm/dec) was achieved at low growth temperature (500^{o}C) by RTCVD. We proposed a modified two-state model including hydrogen surface coverage to explain P segregation behavior. The results enable an inverted 2DEG of high mobility up to 60,000 cm^2/V-s and charge density 1.8 x 10^{11} cm^{-2}.

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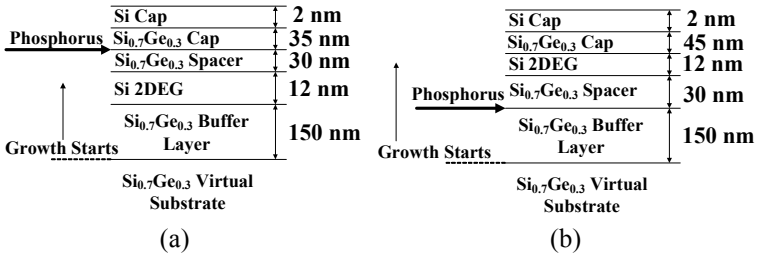


Fig. 1 Schematics of test structure: (a) normal 2DEG; (b) inverted 2DEG

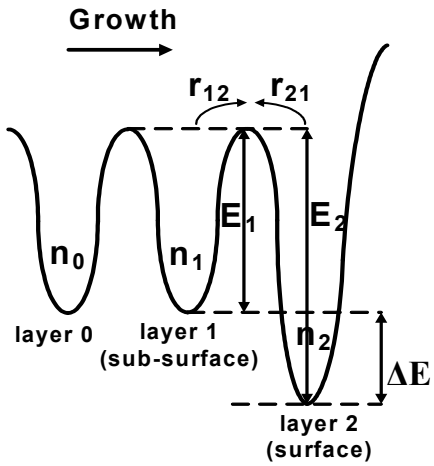


Fig. 2 Two-state model [2]

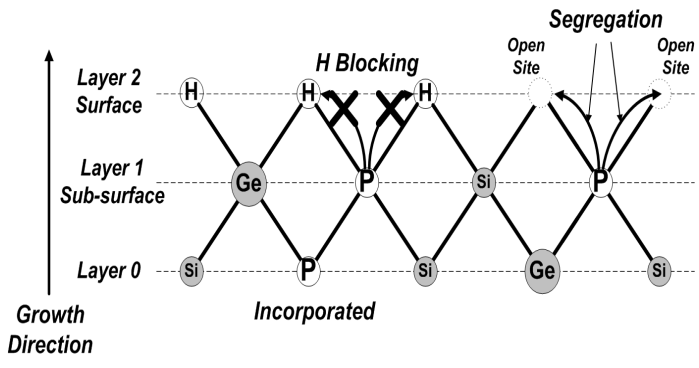
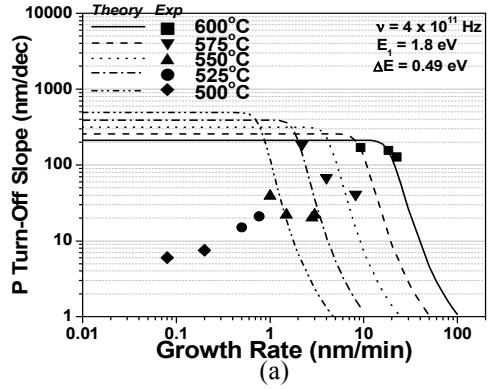


Fig. 3 Blocking effect of hydrogen on P segregation



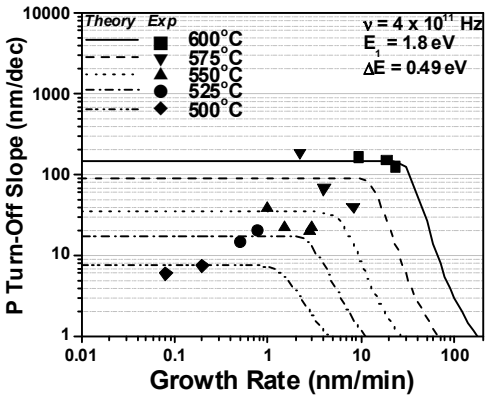


Fig. 4 Data (points) of P turn-off slope vs. growth rate with models (line) of (a) H coverage = 0; (b) H coverage ≠ 0.

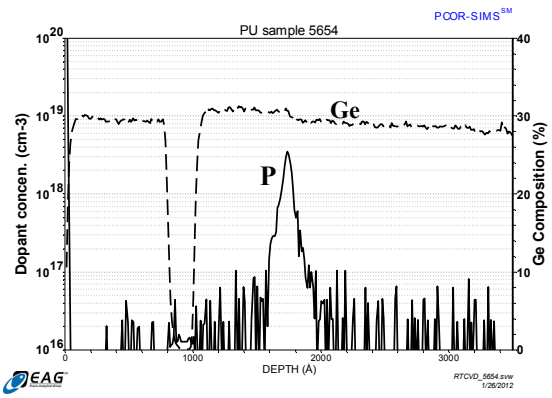


Fig. 5 SIMS profile of P segregation at 500°C with P turn-off slope of 6 nm/dec.