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Electrical characterization of Si(100) surface at p-Si/SiGe/Si structure using low temperature Hall measurement analysis

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ABSTRACT

The pinning position of Fermi level and surface charge density at Si(100) surface of epitaxially grown p-Si/SiGe/Si structure has been evaluated via low temperature Hall experiment analysis. It is explained how the density of two-dimensional hole gas (2DHG) formed in the SiGe quantum well is affected by structural parameters, and proximity of Si surface charges and 2DHG. This approach is based on static charge transfer and Mid-gap Pinning Model (MPM). Finally, the passivation of Si surface by diluted HF etchant has been discussed.

1. Introduction

Semiconductor surfaces are of great interest from physical study and device applications point of views [1,2]. For instance, bare or covered Si surfaces are integral parts of silicon microelectronics device technology including field effect transistors (FETs) and solar cells (SC) [3]. Performance of such devices is fundamentally limited by the large number of defect levels within the band gap resulting from dangling bonds on the silicon surface. In crystalline silicon (c-Si), for instance, the surface defects increase substantially the recombination of minority carriers, undesirably bend the band and reduce the solar cell efficiency [4,5], therefore, surface characterization is essential in designing of such devices. This has been carried out via scanning surface voltage, surface photovoltage [6–8], X-ray excited photoelectron spectroscopy (XPS) [9], capacitance–voltage and current–voltage methods [10]. Moreover, the low temperature carrier transport analysis in quantum well heterostructures has been employed for this study too [1]. Here, we used inverted remote (modulation) doped p-Si/$Si_{1-x}Ge_x$/Si structure, where a two-dimensional hole gas (2DHG) is formed in the SiGe quantum well buried beneath the final Si (cap layer) thin film. We demonstrated before that the sheet density of 2DHG confined in this structure depends on the vicinity of SiGe layer and bare Si surface [11], consequently, the electrical properties of 2DHG depends on Si cap layer thickness. Thus, it has been implemented in density dependence studies of transport properties of 2DHG in Si/SiGe/Si quantum wells [12]. This behavior is attributed to the existence of donor surface states that trap holes from SiGe quantum well to some extent. In this paper, the position of Fermi level pinning and surface charges density on the epitaxially grown Si surface of Si/SiGe/Si structure are evaluated via low temperature Hall measurement analysis in the Mid-gap Pinning Model (MPM) [13].

2. Theoretical considerations

It is well established that one kind of point defect on the semiconductor surfaces known as the C-defects, occupies an area of two neighboring dimers from the same dimer row. On the clean Si(100) surface, they are the only abundant native point defects which introduce local metallic (amphoteric in the bulk properties terminology) electronic states [14] and can trap electron or holes from interior. In the case of a buried SiGe quantum well adjacent to the Si surface, this phenomenon leads to significant changes in the electrical properties of 2DHG confined in the SiGe channel resulted for example via remote doping, thus the sheet density of 2DHG can be a measure of electrical characterization of Si surface.

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Fig. 1(a) depicts layer sequence of p-Si/$Si_{1-x}Ge_x$/Si inverted modulation doped (IMD) structure under study. As the SiGe alloy layer thickness (20 nm) is less than Matthews/Blakeslee limit critical thickness [15], the lattice matched (pseudomorphic) growth occurs, therefore, the lattice constant of the alloy in the growth plan is the same as Si under layer and as a consequence, the SiGe is compressively strained while the Si cap is not. In this case, theory and experiment reveal that there is a valance band offset at Si/SiGe/Si interfaces [16], thus, a quantum well is formed in the compressively strained SiGe alloy layer. The valance band edge profile across the structure has been shown in Fig. 1(b). This quantum well can accommodate heavy holes produced by adjacent Si–B doped layer, as a result, the 2DHG is formed. The low temperature charge distribution in this structure has been shown in Fig. 1(b). As seen, the 2DHG located near the lower (inverted) interface of Si/SiGe/Si quantum well, while positive surface charges (induced by surface donor states) are accommodated on the Si cap surface. Ignoring the background ionized impurities in the epitaxially grown cap layer, the charge neutrality law implies that the area density of ionized Boron atoms in the depleted region (L_d) of Si–B doped layer counterbalances the 2DHG sheet density n_h, and surface charge density n_{sur}:

$$L_d N_A = n_h + n_{sur} \tag{1}$$

where N_A is B impurity concentration at doped layer (the excess holes in the rest of doped layer have been frozen at low temperature). At electrostatic equilibrium, the Fermi level must be coincident through the structure so, for the lower side of SiGe quantum well one finds out:

$$\Delta E_V = E_b + E_0 + E_F + e\Delta V_{spac} + e\Delta V_B \tag{2}$$

where ΔE_v is the valance band offset at the Si/SiGe interfaces (which is proportional to the Ge content x in the SiGe alloy), E_b, E_0

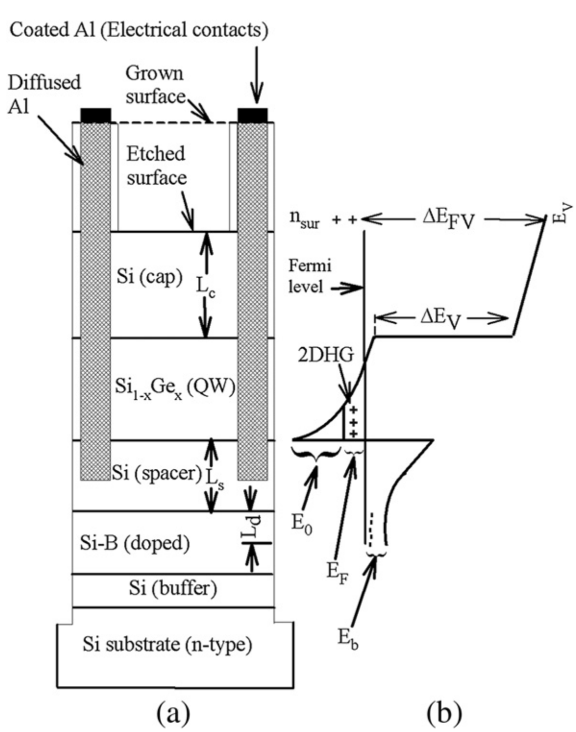

Fig. 1. Layers sequence (a), and valance band edge profile along the growth direction (b), of IMD structure under study.

are the Boron impurity binding energy and first subband heavy hole energy in the triangular quantum well respectively, e, is the electron charge, $e\Delta V_B$, $e\Delta V_{spac}$, are the valance band bending across the depleted region and spacer layer respectively, as follow:

$$e\Delta V_B = \frac{N_A L_d^2}{2\varepsilon\varepsilon_r} e^2 \tag{3}$$

$$e\Delta V_{spac} = \frac{N_A L_d L_s}{\varepsilon\varepsilon_r} e^2 \tag{4}$$

where ε is the permittivity of free space and ε_r is the dielectric constant of silicon semiconductor. The E_F is the position of the Fermi level respect to bottom of the parabolic heavy hole subband in the well as:

$$E_F = \frac{\pi \hbar^2}{m^*} n_h \tag{5}$$

where m^* is the heavy hole effective mass and $\hbar$ is the reduced Plank's constant.

The 2DHG in SiGe layer (confined in z direction), is a quantum mechanical problem, indeed, for thick enough alloy layer, it can be approximated by a triangular-shaped quantum well and the one-dimensional Schrödinger's equation must be solved. The corresponding eigenfunctions are Airy functions but for practical purposes it is more convenient to use a variational wave function which enables us to calculate various parameters. Here we use Fang and Haward trial envelope wave function [17]:

$$\chi(z) = \left(b^3/2\right)^{1/2} z e^{-bz/2} \tag{6}$$

where $z \geq 0$ and b is the variational parameter as:

$$b = \left\{ \frac{12 m^* e^2}{\hbar^2 \varepsilon\varepsilon_0} \left(n_h + \frac{11}{32} n_{sur} \right) \right\}^{1/3} \tag{7}$$

Thus, the first subband heavy hole energy in triangular quantum well can be calculated as:

$$E_0 = \left(\frac{\hbar^2}{2m^*}\right)^{1/3} \left[\frac{9}{8\varepsilon\varepsilon_r'} \pi e^2 (n_{sur} + n_h/2) \right]^{2/3} \tag{8}$$

where ε_r' is the dielectric constant of SiGe semiconductor. On the other hand, the Fermi level in the quantum well and Si cap should be coincident with that of surface, this implies pinning position of surface Fermi level respect to valance band edge ΔE_{FV} is as follow:

$$\Delta E_{FV} = e\Delta V_c + \Delta E_v + e\Delta V_w - (E_0 + E_F) \tag{9}$$

where $e\Delta V_c$ and $e\Delta V_w$ are the valance band bending across the cap layer and quantum well respectively, as:

$$e\Delta V_c = \frac{e^2 L_c}{\varepsilon\varepsilon_r} n_{sur} \tag{10}$$

$$e\Delta V_w = e^2 \int_0^{l_w} E_w(z) dz \cong \frac{e^2}{\varepsilon\varepsilon_r'} (L_w n_{sur} + Z_{av} n_h) \tag{11}$$

where Z_{av} ($=3/b$) is the average distance of 2DHG from inverted interface.