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The evolution of structure and defects in the implanted Si surface: Inspecting by reflective second harmonic generation

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ABSTRACT

Detailed information about the recrystallization and formation of defects in the ultra-shallow junction of implanted Si is a key for semiconductor fabrication below 20 nm regime. The surface quality of highly doped Si via annealing treatment would influence the fabrication and yield. Here, we employ nonlinear optics to study the correlated physical phenomena and underlying evolution of restructure of P^+ ion implanted Si. Reflective second harmonic generation (RSHG) results reveal the restructure of the implanted Si layer that involves recrystallization, dopant activation and dopant diffusion in correlation with annealing temperature. In the implanted Si layer, defects cause inactivity in electrical properties and generate isotropic dipole contribution to the RSHG pattern. The trend of isotropic dipole contribution is consistent with the sheet resistance measurement that presents more information about the evolution of the restructure. At lower annealing temperatures, the precipitation and the interstitialcy pairs form due to the effect of transient enhanced diffusion, and then the isotropic contribution of the RSHG pattern and sheet resistance sharply increases because of aggregation of the dopants. The isotropic contribution of RSHG is an index of the transformation of the electrical property as well as estimate recrystallization during rapid thermal annealing.

1. Introduction

Doing technology is getting more important in next generation of Si based devices [1], such as power devices, memory large scale integration (LSI) and system LSIs devices [2,3]. Ion implantation technology with precise and accurate characteristics can achieve the device miniaturization and device demand damage control. As scaling of semiconductor devices, the merit of the ion implantation technology can also apply to improve the resistivity of source/drain region in metal-oxide-semiconductor field-effect-transistors (MOSFETs) [4]. Ultra shallow junction (USJ) and low resistance extension region are fabricated by low energy and high dose ion implantation, combined with a short duration of annealing treatment. Thermal processing is a most important key to enable the manufacturing devices to follow the performance of ion implantation processes [5]. Except the choice of the proper annealing method, annealing temperature and time are the core and critical factor to control the thermal budget which involves recrystallization, dopant activation and dopant diffusion depth [6]. It is a complicated phenomenon in the ultra-shallow junction during annealing since the amount and timing of the thermal budget usually influence the thermodynamics and kinetics of the implanted Si materials, such as recovery of the amorphous layer, annihilating defects (interstitial atoms and vacancies) and clustering of point defects [1]. Under the condition of heavier doping associated with thinner depletion layers, more recombination centers result in increased leakage current despite the absence or even without lattice damage [7]. The electrical properties are the main basis to determine appropriate implantation and thermal treatment in ultra-large-scale integration (ULSI) fabrication.

To diagnose the electrical properties and recrystallization of USJ after annealing treatment is a perplexed problem below 20 nm scale. The traditional electrical and composition measurements to analyze the electrical activation and dopant diffusion are performed by four-point probe (4PP) and secondary ion mass spectroscopy (SIMS) [8]. However, 4PP usually penetrate into the USJ and yield inaccurate sheet resistance due to the leakage current in the penetrated region beneath the USJ [8]. SIMS provides the depth analysis of dopant diffusion but it is not able to provide any information about the recrystallization. Besides, the destructive methods, such as transmission electron microscopy (TEM), the contact-probe method, such as current–voltage (I–V) and capacitance–voltage (C–V) measurements, deep-level transient spectroscopy (DLTS) need complicated sample preparation

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and doubts of penetration usually obstruct the analyses in the sequential evolution of annealed USJ, and cause unreliable electrical measurements. More and further analyses tools should be developed for accurate inspection of the variation of defects and structure below 20 nm. Recently, Yoshimoto et al., reported photoluminescence and ultraviolet Raman spectroscopy analysis on annealed USJ [9]. They found defect formation and annihilation in the USJ with PL intensity, which identifies the defects formed in the depletion layer. UV Raman spectroscopy reveals the variation between the amorphous phase and recrystallized phase. Optical method helps to analyze the evolution of the restructure via annealing. If the additional information correlated to the electrical properties is obtained by the non-destructive way, it will be valuable in further application and inspection. An effective measurement of dopant activity and recrystallization should be developed to face the further challenge of the 20 nm fabrication.

Optical reflected second harmonic generation (RSHG) has been proven to be a sensitive tool for obtaining information regarding the structure of semiconductor surfaces and interfaces [10,11]. Second harmonic generation has also been used to investigate the interface of native oxide and Si(1 1 1) with/without doping [12], doped or compositionally graded SeGe films [13] and titanium oxide [14]. Rotational anisotropy RSHG (RA-RSHG) is used to analyze the structural symmetry of crystals, especially the surface region of centrosymmetric materials [10,15]. More surface characteristics (trends in dopant diffusion and reconstruction of its step structure) of implanted vicinal Si(1 1 1) after rapid thermal annealing (RTA) are found by analysis of the parameters in RSHG patterns [10]. P precipitation occurs on the surface when the RTA temperature is not sufficiently high at high-influent conditions. These results were verified by reflectance spectroscopy [16]. P precipitation and interstitialcy pair, which are types of defects, diminish the degree of recrystallization and the electrical properties of Si during RTA. Be worthy to expect, an index should be generated from the parameters of RA-RSHG that correspond to the existence of defects and the related electrical properties of the implanted Si.

Due to the very low thickness (below 20 nm) of the ultra-shallow junction, the measurement of the electrical properties by four point probe method is not accurate [17]. RA-SHG method can provide a reliable diagnosis to find out the defect generation and correlated electrical properties in agreement with four point probe measurement. Therefore, in order to build the correlation between the RA-SHG results and the electrical properties, the standard shallow junction should have enough thickness of the amorphous layer to avoid the probe penetration into the amorphous layer.

This study is conducted to determine the correlation among the electrical property, defects, and results of RA-SHG. In order to obtain accurate sheet resistance values, we used the high phosphorous dose of 1×10^{16}/cm^{-2} and the implantation energy of 20 keV to fabricate shallow junctions about 50 nm thick [10]. For realizing the thermal budget controlled by annealing temperature and time, we analyzed the restructure evolution after implantation with annealing temperature and then fixed annealing temperature to observe the influence of the annealing time. The variation in the sheet resistance clearly coincides with the isotropic contribution of RA-SHG. Furthermore, the occurrence of dopant precipitation and interstitialcy pair, which exist bondings (dipoles) in implanted Si, were well explained by RA-SHG analysis. This work presents a method in probing the effective electrical properties of ultra-shallow junctions by non-destructive RSHG.

2. Experimental

Vicinal Si(1 1 1) substrates with p-type Si wafers (10–20 Ω cm, B dopant) cut with a small offset angle α of 2.88° from [1 1 1] toward the [$\bar{2}$ 1 1] direction are used in this study [10]. Vicinal Si(1 1 1) is used in this work to confirm the restructure on the surface [10,15]. These vicinal Si(1 1 1) samples were implanted with P^+ ions with an energy of 20 keV and a dose of 1.0×10^{16} atoms/cm^2. The projected range of low-energy implantation was 28 nm. In the first experiment, the RTA temperature was varied from 700 °C to 950 °C with the step of 25 °C and RTA time was fixed at 30 s. Following the results of the first experiment, the RTA temperatures were set at 850 °C and 900 °C and RTA treatment was performed from 10 s to 40 s in the second experiment to observe the evolution of implanted Si with time. The details of RA-SHG experiment is described elsewhere [11]. The laser source used was a pulsed Q-switched Nd:YAG laser with a wavelength of 1064 nm, a pulse duration of 6 ns, and a repetition rate of 20 Hz. The laser spot was not tightly focused, and the pulse energy was well controlled to avoid the surface annealing effect.

2.1. The correlation between RA-SHG and sheet resistance

2.1.1. Parameters of RA-SHG

The symmetry group of the surface layer structure could be obtained by analyzing the Fourier transform of the RA-RSHG pattern. Typically, the *s*-wave polarized RSHG with the irradiation of *s*-wave polarized fundamental light (*ss*-RSHG) exhibits sensitivity to structural symmetry because the isotropic contribution is forbidden in *ss*-RSHG [11,15]. On the other hand, the *p*-wave polarized RSHG with the irradiation of *s*-wave polarized fundamental light (*sp*-RSHG) for vicinal Si(1 1 1) is expressed as [17,18]

$$I_{S,P}(2\omega) = \left| b_0 + b_1 e^{i\psi_1} \sin(\varphi) + b_3 \cos(3\varphi) \right|^2 \quad (1)$$

where, the rotation angle φ is defined as the angle between the plane of incidence and the projection of the crystallographic [0 0 1] axis on the surface. The coefficients b_0, b_1, and b_3 describe the polarization contributions with structural symmetries belonging to the isotropy, C_{1v}, and C_{3v}, respectively. The second-order nonlinear polarization has the formula $P_i(2\omega) = \chi^{(2)}_{ljk} : E_j(\omega)E_k(\omega)$, where $\chi^{(2)}_{ijk}$ denotes the second-order susceptibility tensor, and E_j and E_k represent the incident fundamental electric fields. The isotropic parameter b_0 is contributed from χ_{zxx} and χ_{zyy} with $\chi_{zxx} = \chi_{zyy}$, and the anisotropic parameter b_3 is contributed from the residual electric dipole ($\chi^{(2)}_{RD}$) and the bulk quadrupole from χ_{xxx}, χ_{xyy} and χ_{yxy} with $\chi_{xxx} = -\chi_{xyy} = -\chi_{yxy}$ [15], where the *z* axis is perpendicular to the sample surface. The contribution of b_1 originates from the step-induced dipoles in the vicinal Si(1 1 1). The phase ψ_1 denotes the phase difference between b_1 and b_3 [19]. The actual *sp*-RSHG field represents the superposition of these three components (b_0, b_1, and b_3); thus, the shape of the *sp*-RSHG pattern is influenced by the interference of these contributions with the phase difference. The phase ψ_1 and the parameter b_1 were discussed elsewhere [18] and have no clear correlation with defects. In this work, we focus on the evolution of defects in the implanted layer with RTA via RA-SHG analysis but do not discuss the variation of ψ_1 and b_1.

For *sp-SHG* mode, the output SHG light in the *z* direction is allowed and the SHG field contributed from χ_{zxx} and χ_{zyy} is acquired. The *z*-component of *sp*-RSHG cannot be canceled out and reveal the dipole contribution which is combined into b_0 and invariant under the azimuthal rotation [20]. Therefore, the isotropic contribution b_0 is generated by residual non-canceled isotropic dipoles in the normal direction (normal to surface). The components of b_0 include the contribution of Si(1 1 1) matrix and the defects generated from implanted Si via RTA process. The correlation between b_0, the electrical activation and the sheet resistance via varied annealing process is complicated but regular with the detailed analysis via annealing mechanism in the implanted Si.