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Inherent point defects in thermal biaxially tensile strained-(1 0 0)Si/SiO_2 probed by electron spin resonance

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Abstract

Electron spin resonance studies are reported on (1 0 0)Si/SiO_2 entities grown by thermal oxidation of biaxial tensile strained-(1 0 0)Si layers epitaxially grown on relaxed virtual substrates, with main focus on P_b-type interface defects, in particular the electrically detrimental P_{b0} variant. In the as-grown state a significant decrease (>50%) in interface defect density compared to the standard (1 0 0)Si/SiO_2 interface was observed. As compared to the latter, this inherent decrease in electrically active interface trap density establishes strained Si/SiO_2 as a superior device entity for all electrical properties in which (near) interface traps may play a detrimental role. For one, it may be an additional reason for the commonly reported mobility enhancement in strained silicon inversion layers and the reduction in 1/*f* noise. The data also confirm the admitted relationship between inherent incorporation of the P_b related interface defects and the Si/SiO_2 interface mismatch.

Keywords: Strained silicon; Interface defects; Electron paramagnetic resonance; Thermal oxidation; Paramagnetic point defects

1. Introduction

For decades the scaling of the metal oxide semiconductor field effect transistor (MOSFET) – the key component of integrated circuits (ICs) – has enabled for tremendous improvements in the performance of semiconductor-based devices. However, this trend has progressed that far that scaling of the conventional Si-based MOSFET will face its limits in the coming years [1,2]. In order to maintain the trends in improvements some drastic change in the conventional MOSFET structure will be needed. One way to further boost the device performance is the use of high mobility substrates, e.g. germanium and strained silicon (sSi) [3,4].

Strained silicon is preferred because of its easy integration in the existing production lines. Strained silicon layers may be obtained by pseudomorphically growing Si on a lattice of larger unit cell dimensions such as a strain relaxed $Si_{1-x}Ge_x$ buffer layer, mostly with $0.2 < x < 0.4$. The difference in lattice constant between Si and the $Si_{1-x}Ge_x$ buffer gives rise to an in-plane biaxial tensile strain in the Si. As presently understood this strain will improve the electron mobility (μ) through the reduction of intervalley scattering and carrier effective mass as a result of lifting of the six-fold degeneracy of the Si conduction band minima [5]. However, there appears to be some shortcomings in the quantitative theoretical understanding of the enhanced mobility, at least in some cases, suggesting an additional effect. Surprisingly, it was indicated [6] that state-of-the-art theoretical calculations of μ may (only) account for the experimental data [6,7] if introducing the ad hoc assumption of substantial reduction of carrier scattering with interfacial roughness, i.e. reduction of average sSi/SiO_2 interface roughness at larger values of strain. Yet, it was considered rather unrealistic as there appears to be no obvious physical justification for this assumption.

A prominent aspect related to interface scattering concerns interface traps, because of the drastic influence of these point imperfections on μ. As well known, the elimination of these traps, or at least reduction to strict sub-critical limits, is a prerequisite for functional devices. Over the decades electron spin resonance (ESR), in conjunction with electrical diagnosis, has appeared a most adequate tool to characterize and identify these interface traps to atomic scale, i.e. unveil the atomic nature [8]. As known [9], interface defects are inherently generated at the Si/SiO_2 interface during thermal oxidation, termed P_b-type centers in ESR terminology. Specifically, in (1 0 0)Si/SiO_2 the dominant paramagnetic interface defects are P_{b0} (assigned to $Si_3{\equiv}Si^{\bullet}$) and P_{b1} (likely an approximately $\langle 2\,1\,1\rangle$-oriented unpaired Si hybrid at a strained $Si_3{\equiv}Si^{\bullet}$ entity) with naturally occurring site densities of [P_{b0}], [P_{b1}] $\sim 1\times10^{12}\,cm^{-2}$ for conventional

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oxidation temperatures (∼850–950 °C) and oxide thicknesses. Admittedly, the dominant cause of interface defect formation is intrinsic interface strain resulting from the difference in molar volume of both solids confronted at a single Si/SiO_2 interface, i.e. the difference in bond length, angles and bond density. This would suggest that applying in plane pre-tensile stress to Si could result in a lower density of ESR active interface defects. Results into this direction have already been reported [10] by ESR measurements of the dangling bond related P_b defect in thermal (1 1 1)Si/SiO_2 structures that were in situ mechanically stressed during oxidation. For the maximum strain applied, these authors found a reduction of P_b density (∼30%) for tensile-strained silicon, while for compressive strain the P_b density had increased.

The current work intends to extend the work to the case of strained Si. It deals with a true comparison of the inherent quality of Si/SiO_2 interfaces formed by thermal oxidation of the biaxial tensile strained Si and the unstrained Si in terms of occurring (paramagnetic) point defects. Four slightly different as-grown (1 0 0)sSi/SiO_2 structures were analyzed by electron spin resonance. Compared to unstrained silicon, a significant decrease in paramagnetic centers located at the (1 0 0)sSi/SiO_2 interface is observed, implying, among others the detrimental P_{b0} traps. This decrease in inherent density of interface traps constitutes a much desirable bonus for the sSi/SiO_2 entity when it comes to improving electrical properties of Si-based devices, such as enhancement of carrier mobility, reduction of traps, suppression of noise, and more generally, enhance device reliability and stability.

2. Experimental

Strained Si layers with a thickness of 12 nm (samples A1, A2, A3) or 30 nm (sample B) were epitaxially grown on a 200-nm thick strain relaxed (virtual substrate layer) $Si_{0.8}Ge_{0.2}$ buffer, in turn grown on a strain relaxed $Si_{0.78}Ge_{0.22}$ buffer layer. Starting from four-200 mm diameter (1 0 0)Si wafers as substrates, the epitaxial layers were grown by an ASM2000 epsilon reactor, as described elsewhere [11]. Samples A1, A2, A3 are nominally identical samples, slightly differing in measured strain (within 6%) of the top strained Si layer. After appropriate wet chemical cleaning, terminated by a dip in aqueous HF, pieces of wafers were thermally oxidized at T_{ox} = 800 °C (1.1 atm O_2), for such times resulting in an oxide thickness of $d_{ox} = 3.5 \pm 3$ nm on co-processed standard unstrained Si, as measured ellipsometrically. The latter served as reference sample. According to the literature the SiO_2 thickness grown on strained Si substrates will be comparable [12,13]. We refer to future work for more details. At this T_{ox}, no relaxation of the sSi layer should occur [13,14]. An unstrained Si sample was oxidized under the same conditions to serve as reference sample.

Conventional absorption derivative *K*-band (∼20.5 GHz) dP_μ/dB spectra, where P_μ is the incident microwave power and *B* the magnetic field, were measured at 4.2 K in the adiabatic mode. Defect densities and *g*-values where determined relative to that of a comounted Si:P reference sample. The attained absolute and relative accuracies are estimated at 20% and ≤10%, respectively.

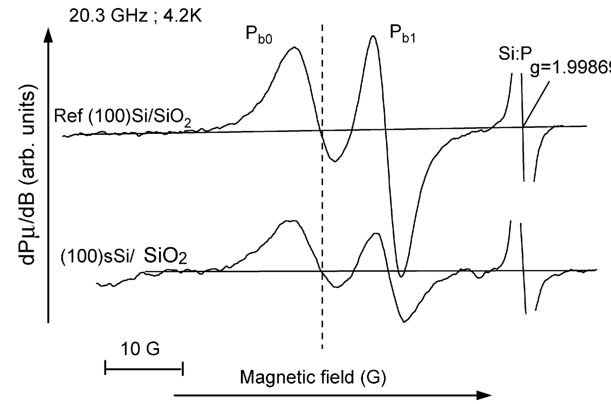

Fig. 1. Comparison of *K*-band ESR spectra (*B*//*n*) observed at 4.2 K on thermal unstrained (1 0 0)Si/SiO_2 and an (1 0 0)sSi/SiO_2 sample. The two spectra are scaled to equal scanned interface area and Si:P reference signal ($g = 1.99869 \pm 0.00002$) intensity. The applied microwave power and modulation field amplitude was ∼0.3 nW and ∼1 G, respectively.

3. Results and discussion

Fig. 1 shows representative ESR spectra of the as-grown (1 0 0)sSi/SiO_2 structure for ***B*//*n***, the (1 0 0) surface normal, and the reference sample. The spectral intensities are normalized to equal scanned interface area and Si:P reference signal intensity. The two types of signals observed in the as-grown (1 0 0)sSi/SiO_2 correspond to the two known anisotropic interface defects P_{b0} and P_{b1}.This assignment is inferred from angular dependent measurements where the single line observed for each type of defect for the ***B*//*n*** case is seen to split, generally, into a characteristic three-line spectrum (***B*** rotating in the (0 $\bar{1}$ 1) plane): As to P_{b0} the ESR characteristic properties, like line shape and *g*-value of the signal imputed to P_{b0} centers in (1 0 0)sSi/SiO_2 ($g_\perp = 2.0080 \pm 0.0001$ and $g_\parallel = 2.002 \pm 0.0001$) are close to those encountered in standard [9] (1 0 0)Si/SiO_2. For the P_{b1} signal the *g*-value of $g_c = 2.0036 \pm 0.0001$ was found for ***B*//*n*** which is identical to that found in standard [9] (1 0 0)Si/SiO_2. Double integration of the simulations of the different defects resulted in the bar map of the P_{b0} and P_{b1} densities for the four samples shown in Fig. 2. Within experimental error,

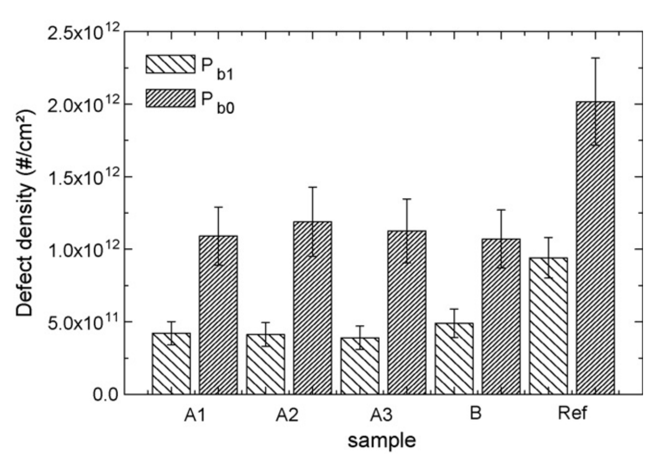

Fig. 2. The measured defect densities for the different samples of as-grown (1 0 0)sSi/SiO_2 together with a reference standard thermal (1 0 0)Si/SiO_2.