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The impact of platelet oxygen precipitates in silicon on the junction leakage current and the interstitial oxygen loss

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Abstract

The impact of oxide precipitates (OPs) on the p-n junction leakage current density for reverse voltage is studied for the case of oxygen precipitation in silicon in the form of oxide platelets, typical for 650–1000 °C treatment. A method is proposed which takes into account the precipitate morphology and the oxide stoichiometry for the extraction of leakage densities related to various parts of the defect structure, namely to: (i) the platelet planes, (ii) the sidewalls of platelets, and (iii) the dislocations formed as secondary defects. It is also shown that the impact of platelet OPs on junction leakage is expected to be dependent on the isolation scheme used for junction manufacturing.

1. Introduction

Czochralski (Cz) silicon is the semiconductor most widely used for integrated circuit (IC) fabrication. The morphology of thermally induced (amorphous) oxide precipitate (OP) in Cz silicon depends on the treatment temperature [1, 2], and corresponds to spheres (600-750 °C), platelets (650-950 °C [1], 700-1000 °C [2]), and polyhedra (950-1200 °C). The presence of OPs in the Cz silicon bulk has an impact on the leakage current of p–n junctions. This current determines the power consumption of ICs and also e.g. the retention time of dynamic random-access memories (DRAMs). Due to the formation of OPs the internal gettering (IG) process is possible but, conversely, the presence of a layer of OPs results in an increase of the diffusion current component of the junction leakage [3]. Moreover, the density of OPs within the denuded zone is lowered, but they can be still observed [4]. When OPs are considered to be distributed within the bulk silicon, the morphology of OPs must be accounted for.

2. Interstitial oxygen loss

The loss of the interstitial oxygen (ΔO_i) due to the thermal treatment, determined by the FTIR method, can be related to the average OP radius R_{op} by $\Delta O_i = (4/3)\pi C_p N_{op} R_{op}^3$ [5–7], where

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 N_{op} is the precipitate density and C_p is the atomic density of oxygen inside precipitates (about (4.2–4.6)×10²² cm⁻³ for SiO₂ [6–10]). However, for the square-shaped OP platelets, which have {100}-type habit planes and are the most common OPs in lightly doped Cz silicon [11], the $\Delta O_i = d^2 t C_p N_{\text{op}}/2$ relationship can be used instead [8], where *t* is the platelet thickness, and *d* is the precipitate size defined as the diagonal length of the platelet, which can be determined from electron microscopy. In this case a ΔO_i value can be estimated equal to 2.34×10^{18} cm⁻³ for SiO₂ precipitates, larger than the initial oxygen concentration prior to annealing, as discussed in [8]. However, the analysis of the OP stoichiometry in silicon often shows for SiO_x the stoichiometric value $x \approx 1$ for platelets [10, 12, 13]. In this case the oxygen density $C_p \approx 2.9 \times 10^{22}$ cm⁻³ [10], and ΔO_i drops to 1.47×10^{18} cm⁻³, a realistic value for Cz silicon. This C_p -value should also be taken to determine the average diagonal size, using the previously determined ΔO_i (by the FTIR method) and the precipitate density N_{op} . Several regularities can occur for oxide platelets, depending on the annealing temperature and the type of silicon substrate [12], namely:

- (i) the constant thickness t (often found close to $t \approx 5-6$ nm [9, 14]), and
- (ii) the constant thickness-to-diagonal-size ratio $\beta = t/d$ (found e.g. close to 0.01 [15]).

The correlation between values of t and d in platelet OPs can be found as $d = (2 \Delta O_i/t C_p N_{op})^{1/2}$, which for the above-mentioned cases (i) and (ii) leads to the relationships: $d \approx 0.115 (\Delta O_i/N_{op})^{1/2}$ nm for the case of constant thickness (with t = 5 nm here), and $d \approx 1.9 (\Delta O_i/N_{op})^{1/3}$ nm for the case of constant ratio β (with $\beta = 0.01$), assuming $C_p = 2.9 \times 10^{22}$ cm⁻³ as for SiO. The assumption that the OP stoichiometry is close to SiO₂ instead to SiO leads to about 55% overestimation of ΔO_i calculated from microscopic results, and to 20% or 10% underestimation of d calculated from FTIR results for the above cases (i) and (ii), respectively.

3. p-n junction leakage current

The deep levels related to the presence of OPs have been attributed to the interface states at the OP surface [5, 7], to the dislocation loops and point defect clouds [6, 14, 16–18], and to the oxidation-induced stacking faults [17]. For OPs with spherical form and a radius R_{op} , the carrier lifetime can be described by $\tau = (4\pi N_{op}R_{op}^2s_{ef})^{-1}$ [5–7], where s_{ef} is the effective surface recombination velocity [5]. Also the generation lifetime, related to the trap concentration, energy levels, and capture cross-sections, can be considered in the same way. When the real shape of platelets is taken, then a $\tau = [2L(L + 2t)N_{op}s_{ef}]^{-1}$ relationship results, where L is the platelet side. But the carrier generation or recombination parameters are different in various parts of the platelet, and a mechanical stress narrows the silicon energy band gap by 0.14 meV MPa⁻¹ [19], increasing the current. The stress reaches a maximum at the edge of platelets, where also the generation of dislocations is observed [11], as confirmed by the correlation between the platelet edge length and the dislocation size [9]. Thus, the components of the generation leakage I_{gen} of a p–n junction have been usually attributed to the OP interface for $I_{gen} \propto d^2$ and to dislocations for $I_{gen} \propto d$ [9, 20].

4. Extraction of current components related to various parts of the defect structure

A new method is proposed for extraction of the current components related to three parts of the defect structure, namely to: (i) the platelet planes, (ii) the sidewalls of platelets, and (iii) the dislocations. To illustrate the method, the results given in [20] were processed as the raw data



Figure 1. The extraction of the current density $J_{\text{gen},A}$, corresponding to the surface generation at platelet planes. The dependence of the $I_{\text{gen},OP}/A$ ratio on the P/A ratio is plotted, where $I_{\text{gen},OP}$ is the leakage current per platelet, A is the area of its planes, and P is its edge length. The extrapolation of this plot gives the $J_{\text{gen},A}$ -value at P/A = 0. The set of experimental results given in [20] was used as the raw data, to illustrate the application of the method and the impediments to its use, which can be avoided by the proper design of the experiment, as discussed in the main text.

with the use of our method. For the average diagonal sizes *d* equal to 82, 250, and 1000 nm, the average generation currents $I_{\text{gen,OP}}$ per platelet were respectively 0.494, 2.01, and 10.9 fA [20]. For the new method the current $I_{\text{gen,OP}}$ can be described as follows:

$$I_{\text{gen,OP}} = A J_{\text{gen,A}} + P J_{\text{gen,P}} \tag{1}$$

where $J_{\text{gen},A}$ and $J_{\text{gen},P}$ are respectively the current densities per planar area A of platelet and per edge length P = 4L. The linear extrapolation of the $I_{\text{gen},OP}/A$ plot to ratio P/A = 0gives the $J_{\text{gen},A}$ -value (figure 1). This value is constant if $J_{\text{gen},A}$ and $J_{\text{gen},P}$ are independent of the P/A ratio, and when they depend on the platelet size, a narrower range of sizes close to a chosen size (d_0) can be considered. This value of $J_{\text{gen},A}(d_0)$ can be used for the determination of the surface generation velocity s, defined by the general relationship $J = qn_is$, where J is a current density, q is the electron charge, and n_i is the intrinsic carrier density. When the Shockley–Read–Hall model describes the current generation, then also the concentration of interface traps N_{it} can be estimated in this way [21]. But when other carrier generation mechanisms, such as tunnelling, contribute to the current generation, this N_{it} extracted from $J_{\text{gen},A}$ is overestimated. A constant value of the activation energy ($E_{a,\text{gen}}$), determined from $J_{\text{gen},A}$ measured at different temperatures, is a criterion for constant conditions of the current generation, as they may depend on the platelet size, e.g. due to electric field enhancement and/or mechanical stress [22]. Similarly, constant activation energy of the diffusion current for various platelet sizes can be used as the criterion for conditions constant mechanical stress.

The knowledge of $J_{\text{gen},A}$ determined according to the above-described procedure allows one to extract the current density $J_{\text{gen},P}$, which corresponds to the platelet edge length P. This $J_{\text{gen},P}$ can be considered the sum of the components $J_{\text{gen},P,\text{sw}}$ and $J_{\text{gen},P,d}$, related respectively to the carrier surface generation at platelet sidewalls and to the current generation at dislocations: $J_{\text{gen},P} = J_{\text{gen},P,\text{sw}} + J_{\text{gen},P,d}$, in contrast with the usual identification of $J_{\text{gen},P}$ only with the current generation at dislocations, as is done in [9, 20]. The component $J_{\text{gen},P,\text{sw}}$ generated at platelet sidewalls is controlled there by the interface states and by the bulk traps residing in the near-surface depletion region. Although the area of sidewalls is many times smaller



Figure 2. The extraction of current components proportional to the leakage current densities $J_{\text{gen},P,\text{sw}}$ and $J_{\text{gen},P,\text{d}}$, corresponding to the carrier generation at platelet sidewalls and at dislocations respectively. A different dependence of the current density $J_{\text{gen},P}$ on the platelet size *d* for the platelets with sizes either smaller or larger than the critical size d_{crit} is used in this process, where $J_{\text{gen},P}$ is the current related to the platelet edge length *P*.

than the area of big planes, the conditions at sidewalls may induce a larger current density than in the planar area, due to increased (i) density of interface states, (ii) electrical field, and (iii) mechanical stress. To extract the components $J_{\text{gen},P,\text{sw}}$ and $J_{\text{gen},P,\text{d}}$ with the new method, the existence of a critical platelet size d_{crit} is used, where d_{crit} is the minimal size of a platelet OP at which the dislocations are generated. This size, stated to be equal to 140 nm in [15, 23], depends on the OP density and growth temperature, and generally on the precipitation kinetics. Thus, for larger platelets, the sizes of the dislocation loops generated are related to the platelet diagonal size [9], while for platelets with size smaller than d_{crit} , the component $J_{\text{gen},P,\text{d}}$ corresponding to dislocations does not affect the leakage current $I_{\text{gen},OP}$ related to OPs. The $J_{\text{gen},P,\text{sw}}$, while the difference between the value of $J_{\text{gen},P}$ extracted in the $d > d_{\text{crit}}$ range and the value of $J_{\text{gen},P,\text{sw}}$ extrapolated from the $d < d_{\text{crit}}$ range to the $d > d_{\text{crit}}$ range can be attributed to the influence of dislocations, i.e. to the density $J_{\text{gen},P,\text{d}}$ (figure 2).

Figures 1 and 2 illustrate the method and also show the possible impediments to its accurate use, exploiting the fact that the limited set of available $I_{\text{gen},OP}$ -data from [20] violates some conditions necessary for the use. One impediment results from the small number of experimental points. Since only one point belongs to the $d < d_{\text{crit}}$ range, an extrapolation to the ratio P/A = 0 with the use of the experimental point at d = 82 nm must involve also a point from the $d > d_{\text{crit}}$ range, where dislocations already contribute to the current. The $J_{\text{gen},A}$ -value determined in this way is overestimated (the line a in figure 1). The real value of $J_{\text{gen},A}$ is also smaller than the value obtained for the $d > d_{\text{crit}}$ range (the line b in figure 1). That is, the activation energy $E_{a,\text{gen}}$ given in [20] for the platelet size d = 1000 nm is much lower than a typical value for smaller sizes, close to 0.7 eV. When a proper $J_{\text{gen},A}$ -value is extracted by the procedure shown in figure 1, then a proper value of $J_{\text{gen},P,\text{sw}}$ and $J_{\text{gen},P,\text{d}}$, as shown in figure 2. An auxiliary procedure seen in figure 2 can also be used to get the $I_{\text{gen},OP}(d = d_{\text{crit}})$ value extrapolated from the $d > d_{\text{crit}}$ range. This value of $I_{\text{gen},OP}(d_{\text{crit}})$ may serve as an additional point in the $d \leq d_{\text{crit}}$ range, where the leakage is attributed only

to the platelet sidewalls. When this leakage is extrapolated towards larger platelet sizes, and subtracted there from the real $I_{\text{gen,OP}}$ -values measured in the $d > d_{\text{crit}}$ range, then the current component related to dislocations is determined.

5. Platelet OP impact on the junction leakage dependent on the isolation scheme

The peripheral regions of p–n junctions are the dominant sources of the leakage current in ULSI circuits. If platelet OPs are encountered in these regions, then as in planar regions, platelets are lying on the (100) plane. Thus, for (100) silicon wafers typically used in CMOS IC production, they lie parallel to the silicon wafer surface. The direction of the electric field in these regions of junctions is very different to that in planar regions for local oxidation of silicon (LOCOS) isolation, while this is not the case for shallow trench isolation (STI) junctions. Thus, the electric field is always perpendicular to the platelet plane in STI junctions, while in LOCOS junctions this is true for planar regions, but in regions of junction edges and corners the electric field can even be parallel to the platelet plane. A large enhancement of the electric field, much stronger at small and sharp edges of the defect than at planar sides, occurs in the vicinity of defects encountered within the junction depletion width [22]. Thus, the different placement of oxide platelets according to the electric field direction in planar and in peripheral parts of LOCOS p–n junctions creates different conditions of carrier generation in these regions, while no such difference exists in STI junctions.

6. Summary

A method is given which takes into account the precipitate morphology and the oxide stoichiometry in order to extract the junction current leakage densities corresponding to various parts of the platelet OPs, namely to: (i) the platelet planes, (ii) the sidewalls of platelets, and (iii) the dislocations formed as the secondary defects, as well as to determine the oxygen-atom losses during annealing. The observation is also made that the impact of platelet OPs on junction leakage is expected to be dependent on the isolation scheme used.

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