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Formation and annealing behavior of prominent point defects in MeV ion implanted n-type epitaxial Si

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ABSTRACT

Samples of epitaxially grown n-type Si have been implanted with low doses ($<1\times10^9$ cm^{-2}) of He, C, Si, and I ions using energies from 2.75 to 48 MeV. Deep level transient spectroscopy (DLTS) analysis of the implanted samples reveals a stronger signal for the signature of the singly negative charge state of the divacancy ($V_2(-/0)$) as compared to that of the doubly negative charge state of the divacancy ($V_2(=/-)$). Isochronal annealing for 20 min ranging from 150 to 400 °C results in a gradual decrease in the DLTS peak amplitude of the $V_2(-/0)$ signature, accompanied by an increase in the peak amplitudes of both the vacancy oxygen pair (VO) and the $V_2(=/-)$ levels, as well as an increase in the carrier capture rates for the levels. A model based on local compensation of charge carriers from individual ion tracks is proposed in order to explain the results, involving two fractions of V_2: (1) V_2 centers localized in regions with high defect density around the ion track (V_2^{dense}) and (2) V_2 centers located in regions with a low defect density (V_2^{dilute}).

1. Introduction

Understanding of ion implantation induced defect generation and ion track formation mechanisms in semiconductors is important because of fundamental interests in ion–matter interactions and applications in electronic device technology. It is well established that MeV electron irradiation and ion implantation of silicon give rise to similar kind of point defects when the ion dose is kept sufficiently low [1]. The dominant irradiation induced vacancy related defects are the vacancy oxygen pair (VO), associated with an acceptor level at E_c −0.18 eV [2], and the divacancy center (V_2), providing two electronic states in the upper part of the bandgap located at E_c −0.23 and E_c −0.43 eV and associated with doubly ($V_2(=/-)$) and singly ($V_2(-/0)$) negatively charged divacancy [3,4], respectively (E_c is the conduction band edge). Interestingly, when monitoring the V_2 center in electron irradiated and heavy ion implanted samples by deep level transient spectroscopy (DLTS), a different behavior is observed for the relative intensity of the $V_2(=/-)$ and $V_2(-/0)$ signals. In electron-irradiated samples, a close one-to-one proportionality holds between the DLTS amplitudes of the $V_2(=/-)$ and $V_2(-/0)$ states. However, in heavy ion implanted samples, the $V_2(=/-)$ peak intensity is reduced compared to that of $V_2(-/0)$. This observation, referred to as the ion mass effect, has lead to a long lasting discussion involving different and contradictory interpretations. Three proposed models to explain the ion mass effect are: (i) crystal strain induced by the heavy ion collision cascades prevents motional averaging of the V_2 state at low temperatures favoring $V_2(-/0)$ over $V_2(=/-)$ [1,5], (ii) additional electrically active levels, e.g., large vacancy clusters (V_n, $n>2$), contribute to the DLTS intensity of the peak E_c −0.43 eV artificially enhancing the "$V_2(-/0)$" signal [6], and (iii) incomplete occupation of the shallower $V_2(=/-)$ state occurs due to local charge carrier compensation around the ion trajectory [7,8]. There is still no consensus in the literature on the importance of the different models, and more investigations are needed. In particular, the annealing behavior of defects in heavily damaged regions is not well documented for impurity (C, O, H, etc.) lean material, and can reveal additional arguments supporting or excluding the mechanisms (i)–(iii). In particular, the V_2 centers in Si are known to form both by pairing of two migrating monovacancies [9] and when two nearest neighbor Si atoms are displaced by an impinging ion or recoiling atoms [3] in a violent collision. The density of V_2 centers is therefore non-uniformly distributed around the ion trajectory. The VO center, on the other hand, are formed through the capturing of migrating monovacancies by interstitial oxygen atoms (O_i). Especially, in samples with low oxygen concentration, one would therefore expect a wider spatial distribution of the VO centers than that of V_2 centers and less influenced by effects related to strong localization, such as the carrier compensation proposed in model (iii).

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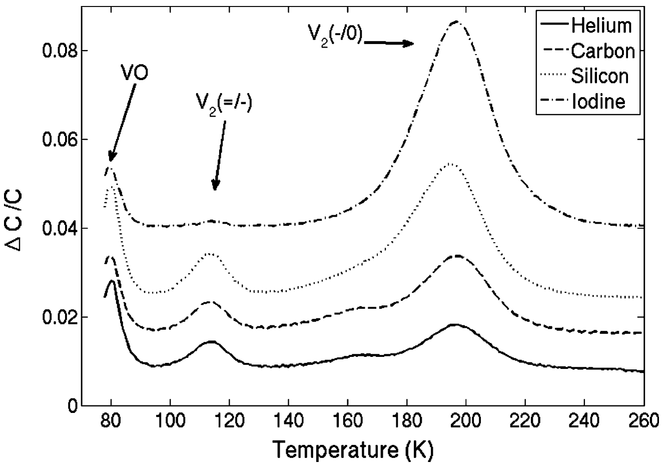

Fig. 1. DLTS spectra of epi-Si after implantation at RT with different kinds of ions. Offsets have been applied to separate the lines for clarity. $\Delta C/C$ is the DLTS signal (ΔC) divided by the reverse bias capacitance (C).

In this work we report on an annealing study of the V_2 and VO centers in epitaxially grown and impurity lean Si layers (epi-Si) implanted with low doses of heavy ions. The results are discussed in terms of the three models outlined above with a particular emphasis on local carrier compensation in regions subjected to violent collision cascades (model (iii)).

2. Experimental

$p^+n^-n^+$ diodes were fabricated from an epitaxial silicon structure grown by chemical vapor deposition (CVD) having a carrier concentration of $1 \times 10^{14}\,cm^{-3}$ in the n^- region. Front and backside Ohmic contacts to the p^+ and n^+ regions, respectively, were made by Al evaporation. The thickness of the epi n^- layer was $\sim$60 μm. Chemical profiling using secondary ion mass spectrometry revealed carbon and oxygen concentrations below 5×10^{16} and $2 \times 10^{17}\,cm^{-3}$ in the epi-layers, respectively. The fully processed diodes were then implanted at room temperature (RT) at the Tandem Laboratory, Uppsala University, with He, C, Si, and I ions using energies of 2.75, 11, 30, 46 MeV, respectively, and doses from 6×10^6 to $2 \times 10^8\,cm^{-2}$. These energies give approximately the same projected range, about 10 μm, for the different kinds of ions which were selected to span a large mass range in order to study the ion mass effect.

DLTS was carried out using a refined version of a setup described in detail elsewhere [10]. In short, the sample temperature was scanned between 77 and 300 K, where the capacitance transients were averaged within an interval of 1 K. The DLTS signal was extracted using a lock-in type of weighting function with six traditional rate windows from $(20\,ms)^{-1}$ to $(640\,ms)^{-1}$, applying a reverse bias of typically −10 V and a filling pulse of +10 V with a duration of 50 ms. The amplitudes of overlapping DLTS peaks have been resolved by curve fitting. The isochronal annealing was performed in 25 °C steps lasting 20 min ranging from 150 to 400 °C.

3. Results and discussion

DLTS spectra of the as implanted samples, Fig. 1, reveal three prominent electrons traps with energy levels at E_c −0.18, E_c −0.23, and E_c −0.43 eV, and they are assigned to VO, V_2(=/−), and V_2(−/0), respectively. In addition, one hole trap with an energy level E_v +0.35 eV is observed and attributed to the carbon-interstitial oxygen-interstitial pair (C_iO_i) [11] (E_v is the valence band edge). Fig. 2 shows results of isochronal heat treatments for 20 min in the range of 150–400 °C. In all the samples, the amplitude of the V_2(−/0) peak starts to decrease gradually above 150 °C and is below the detection limit after ∼325 °C. For all the samples, a shift in the peak position of the V_2(−/0) level, as well as in the position of the V_2(=/−) peak, occur at around 275 °C, where the V_2(=/−) level shifts to lower temperature, while V_2(−/0) shifts to higher temperatures. This shift has also been found in electron-irradiated samples and is attributed to a transition from V_2 to the divacancy-oxygen center (V_2O) [12–15]. The V_2O centers form by O_i atoms trapping migrating V_2 centers. The V_2O pair has a singly and doubly negative charge state at E_c −0.46 and E_c −0.20 eV, respectively, and in Fig. 2(a)–(d), the contributions from these two levels have been separated by fitting of the experimental DLTS data assuming that V_2 only is present for annealing temperatures <225 °C and V_2O only above 350 °C. In contrast to V_2(−/0), the amplitude of the V_2(=/−) peak is stable or even increases for annealing temperatures up to ∼250 °C (Fig. 2), before decreasing to the detection limit at ∼325 °C. The wide temperature range over which the amplitude of the V_2(−/0) level decreases and the simultaneous increase in the V_2(=/−) peak indicate that V_2 exhibits a complex annealing kinetics. The annealing of V_2 is, however, correlated with the rise of V_2O, which increases in amplitude from ∼275 to 325 °C, before it anneals out around 350–375 °C. The E_c −0.46 eV level persists to somewhat higher temperatures than the E_c −0.20 eV level; this has also been observed in electron-irradiated samples and after some detailed investigations ascribed to an additional level overlapping with the V_2O(−/0) signal [12,16,17]. Interestingly, the VO peak displays a similar increasing trend as the V_2(=/−) peak in the Si and I implanted samples and the trend persists up to ∼300 °C. Above 350 °C, the VO peak starts to decrease rapidly and is below the detection limit at 400 °C. At temperatures around ∼300 °C, several new levels form but they exhibit rather low concentrations and anneal out at ∼400 °C.

Minority carrier transient spectroscopy (MCTS) was also carried out to monitor the lower part of the bandgap. A dominant level was observed at E_v +0.35 eV and associated with the C_iO_i pair [11]. However, the MCTS results did not reveal any correlation between the strength of this level (or any other level in the lower part of the bandgap) with the annealing of V_2 and VO.

Prominent features of the annealing curves in Fig. 2 are the influence by ion mass on the decrease of the V_2(−/0) peak and the increase of the V_2(=/−) and VO peaks in the temperature range of 150–250 °C. As described previously, several models have been proposed to explain the effect of ion mass on the generation and annealing of the V_2 and VO centers. Firstly, assuming that several overlapping levels contribute to the V_2(−/0) signal (model (ii)), the annealing data can be interpreted as a dissociation of the additional centers, $V_n \rightarrow nV$, resulting in an increase of the VO, V_2(=/−) and V_2(−/0) signals. Secondly, in the strain model (model (i)), where crystal strain prevents motional averaging of V_2 promoting the V_2(−/0) state over V_2(=/−), the reduction of the V_2(−/0) signal in the temperature range of 150–250 °C can be due to migration of V_2. This may lead to formation of other defects, such as larger vacancy clusters ($nV_2 \rightarrow V_{2n}$). However, Fig. 2(a)–(d) do not show a corresponding rise in any other defect level and thus, the vacancy clusters must either be electrically inactive or having levels not detectable by DLTS. Further, the annealing is also expected to decrease the crystal strain, resulting in an increased amplitude of the V_2(=/−) peak. Thirdly, in the local compensation model (model (iii)), the annealing data can be interpreted in a similar way as for the strain model, where agglomeration of V_2 centers into larger defect clusters occur, resulting in a reduction of the local carrier compensation and a corresponding increase in the population of the V_2(=/−) and VO states. In addition, it has been shown in Ref. [8] that the DLTS amplitude of the V_2(−/0) level is artificially enhanced in compensated samples and this effect is expected to decrease with annealing.

In this context, it can be noted that according to the value for the diffusion constant of V_2 given by Mikelsen et al. [12], annealing for