CHARGE REDISTRIBUTION AND DEFECT RELAXATION IN HEAVILY DAMAGED SILICON STUDIED USING TIME ANALYZED TRANSIENT SPECTROSCOPY

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ABSTRACT

We have carried out electrical characterization of defects in heavily damaged silicon, where damage is created by MeV heavy ions at doses near but below amorphization threshold. Trapping kinetics over several orders of magnitude in time have been monitored using isothermal spectroscopy called Time Analyzed Transient Spectroscopy (TATS). Two distinct effects regarding the nature of changes in density of states in the gap have been demonstrated. Firstly, we show that charge redistribution among multiple traps occur such that only the occupancy of the deeper states increase at the cost of shallower ones for long time filling. Secondly, a novel defect relaxation mechanism is observed for samples with relatively lower damage. A trap is seen to exhibit progressive deepening in energy with increase in filling time, finally stabilizing for large filling times. From the athermal nature of associated TATS peaks, it is argued that the relaxation involves large entropic contribution to free energy. The necessity of using a time domain relaxation spectroscopy such as TATS in the study of different mechanisms of relaxation is demonstrated.

INTRODUCTION

In regions of implant induced damage in silicon, it is of both technological and fundamental significance to determine i) the density of states (DOS) in the gap, and ii) nature of relaxation of defects in presence of disorder [1,2]. However, limitations of popular defect characterization methods such as DLTS have restricted the domain of studies to cases of low damage. We have used time analyzed transient spectroscopy (TATS) [3], an isothermal spectroscopic technique, to study DOS and nature of relaxation of defects in heavily damaged buried layers created using MeV heavy ions.

Damage is created in n-silicon using heavy ion beams of Ar⁺ (1.45 MeV, dose 10¹³-10¹⁴ cm⁻²) and Au⁺ (4.6 MeV, dose 5x10⁹ cm⁻²) at room temperature, and Schottky barrier devices are made for capacitance based transient studies. The doses are high enough to create heavy damage without amorphization. Constant-capacitance voltage transients are analyzed using TATS to monitor trapping kinetics of defects.

Trapping kinetic studies, using variable filling pulsewidth technique over five orders of magnitude in time at low temperatures, show that evolution of occupancies of multiple traps are coupled. The coupling is shown to be due to charge redistribution from shallower to deeper states mediated via conduction band. In addition, we describe results indicating occurrence of a novel hierarchical defect relaxation mechanism.

DESIGN AND PRINCIPLE OF EXPERIMENTS

Phosphorus doped epitaxial silicon wafers of resistivity 2-5 Ω-cm on n⁺ substrates were used for the present study. These wafers were irradiated from front side at room temperature with 1.45 MeV Ar⁺ ions (having an approximate mean range of 1.23 μm) using a 2 MeV Van de Graaff accelerator. Ion doses of 5 x 10¹³ cm⁻² and 1 x 10¹⁴ cm⁻², which are just below amorphization threshold, were used to create damage. Few wafers were
irradiated with 4.5 MeV Au⁺ ions at a dose of 5 x 10⁹ cm⁻² for comparison with Ar⁺ ion case. Schottky diodes were formed with evaporated gold dots on irradiated wafers. The diodes receiving only the heat treatment of 700°C for 30 minutes for curing epoxy contacts will be referred to as as-implanted samples. Some mounted devices were oven annealed at a relatively low temperature of 160°C for 30 minutes. Capacitance measurements were carried out using Boonton capacitance meter (Model 72B) operated at 1 MHz. The transient data were analyzed using conventional DLTS to estimate trap activation energy and capture cross-section.

We have recently shown inter-relationship [3] between various DLTS family of spectroscopies wherein spectroscopy is viewed in terms of differential operators. For example, we have shown that the differential operator corresponding to \( \frac{\partial}{\partial \ln(t)} \) i.e. differentiation of the transient with respect to \( \ln(t) \) gives rise to DLTS in the temperature domain (with \( 1/T \) as the spectroscopic axis). The difference operator corresponding to this would give rise to a DLTS-like operation in the \( \ln(t) \) domain and is known as Time Analyzed Transient Spectroscopy (TATS), where the first order spectrum is given by

\[
S(t) = C(t, T) - C(t + \gamma, T) \quad (1)
\]

where \( C(t, T) \) represents the isothermal transient at temperature \( T \) and \( \gamma \) is an experimentally chosen constant defining the width of the moving rate window. For exponential transient of time constant \( \tau \), \( S(t) \) has a maximum when plotted against \( \ln(t) \) and it occurs at a time \( t_m \) given by the relation,

\[
\tau = \left[ \frac{\gamma}{\ln(1 + \gamma)} \right] t_m \quad (2)
\]

The peak value of the TATS signal is a measure of the strength of the exponential. One of the principal advantages of time domain spectroscopy such as TATS is that the lineshape of a peak is independent of the trap parameters or the range of time and temperature. This is in contrast to DLTS or any other temperature scanning spectroscopy. For better resolution of multiple emission time constants, TATS can be performed using a higher order spectroscopies. The electrical transient studies reported here are carried out in a typical system, described elsewhere in more detailed, includes a fast Boonton capacitance meter (72B) and digitizer (Keithley 194). The system is automated and is capable of acquiring 20,000 sampling points for transients over four orders of magnitude in time typically from millisecond to hours. All spectroscopic operations as described above are implemented using software after complete acquisition of the transients.

Experimentally our motive behind the measurements that we describe in this paper was to monitor relative trap occupancies of multiple trap with different filling time duration, in order to investigate the nature of coupling between the trap levels observed in this irradiated Si. In conventional cases where more than one deep level is present in the material under study, the occupancies of the deep levels (i.e. as monitored by the magnitude of the TATS peak) increase monotonically with filling time and saturates for large filling times indicating its concentration. The sample is taken to zero-bias for a predetermined certain duration ranging from 100 µs to few seconds, and the resulting transient is monitored. One set of measurements constitute use of many different filling times at a fixed temperature.

**TRAPPING KINETICS AT LOW TEMPERATURES: CHARGE REDISTRIBUTION**

Figure 1 shows first order TATS spectra for a typical irradiated sample in which the faster peak corresponds to divacancy \( V_2 \), and the slower the peak P2 is a midgap acceptor trap D1 recently observed [4] in high dose irradiated silicon. The peak corresponding to divacancy is
composed of two different peaks P1 and P2. Often in literature [5] it has been associated with two different defects. Our higher order TATS analysis also confirms this conclusion. To quantitatively evaluate occupancy changes of all the three peaks P1A, P1B and P2, we use first order TATS spectra for filling times varying over five orders in magnitude. The successive frames in Fig. 1 correspond to such spectra for progressively increasing filling times. Note that peak D1 initially increases primarily at the expense of peak P1A and then saturates. The relative concentration of the constituents have been evaluated by fitting contributions from three different defects. The emission time constants are experimentally determined and only the relative concentrations are treated as free parameters. The relative occupancies obtained from the analysis has been plotted as a function of logarithm of filling time in Fig. 2 for two different doses. The occupancies of peak P1A initially increase going through a maximum, significantly enough, at filling times approximately equal to its emission time constant. The increase of peak D1 occurs when P1A starts decreasing. Peak P1B also goes through a maximum and its contribution is small to the growth of peak D1. These broad features are common to both the samples irradiated to different doses.

In the present case, the key observation is that the shallower states lose charges to the deeper ones, and that too for filling times larger than their characteristic emission time. Also note that only the height of the peaks change and not their time constants. These observations are sufficient to pin down the mechanism to redistribution of charges through multiple trapping. For filling times $t_f$ shorter than time constant of emission $\tau_e$ of a particular level, the occupancy increases in proportion to the product of its capture constant and number density of empty states. For $t_f > \tau_e$, emitted electrons from a shallow trap is recaptured by deeper states with increase in filling time. Similar charge redistribution has been earlier invoked for multiple traps associated with DX centers [6,7] and amorphous silicon [8]. In all these cases the necessary condition for observation of the mechanism of charge redistribution.

![Fig. 1. First order TATS spectra at 217.6K for different filling times ($t_f$) showing progressive changes in occupancy for high dose $1 \times 10^{14}$ cm$^{-2}$ implanted sample. Peak P1 is fitted (dotted line) to two different centers P1A and P1B, and peak P2 corresponding to defect D1 is fitted to a Gaussian (FWHM 25 meV) broadened peak with separate dotted line in frame e.](image-url)
Fig.2. Occupancy of individual peaks as a function of filling time for samples with doses (a) $5 \times 10^{13}$ cm$^{-2}$ and, (b) $1 \times 10^{14}$ cm$^{-2}$ of Ar' ion. Arrows indicate measured emission time constants for the corresponding peak.

EVIDENCE OF NOVEL DEFECT RELAXATION: TRAPPING KINETICS IN RELAXED MATERIAL

During the course of filling time experiments, a novel phenomena was consistently observed in samples with either low dose implantation or those partially relaxed after annealing. It was most strikingly observed in (i) low dose Au' ($5 \times 10^{13}$ cm$^{-2}$) implanted n-Si and (ii) Ar' implanted samples in which partial relaxation was induced by annealing at 400°C for 30 minutes. The presence of a damaged region with comparatively lesser degree of disorder is common to these set of samples.

Figure 3(a) shows CC-TATS spectra at room temperature for a series of filling times $t_f$ varying from 20 ms to 1 minute. The well formed peak shown in the figure is due to a new distinct peak whose time constant is strongly dependent on the filling time, becoming slower for longer duration of filling pulses. Note that the time constant of emission changes 4-5 orders of magnitude as does the filling time. Also note that the height of the new peak is approximately similar for all different filling times showing that the corresponding defect is located in the same region and has nearly the same degree of occupancy irrespective of duration of pulse. These observations are indicative of occurrence of hierarchical relaxation through continuous metastable states, stabilizing in a state with the longest time constant. In any case, these results imply that the emission time constant is dependent on resident time of electron in the defect site. This dependence on history is a signature of a non-Markovian process possessing a memory of the duration the electron spends at the occupied defect [9].

Another intriguing feature of this phenomena is that the time constant is nearly temperature independent for any particular filling time, $t_f$. This is illustrated in Fig 3(b) where TATS spectra for a filling time of 1s are shown for different temperatures varying over 30K. The time constant of major peak on the left of the figure does indeed change as would be expected of a normal thermally activated process. However, the peaks that evolves with $t_f$ does not show shift in time constant with temperature. This shows that the process associated with the relaxation is nearly athermal. From the athermal nature, we conclude that the part of the free energy changing with defect relaxation can be considered to be proportional to temperature $T$. In Fig 4, we show dependence of $\tau$ on $t_f$ indicating a power law dependence. The effective energy associated with
the relaxation can be written as $U_{\text{eff}} \sim k_B T \ln[(1+t_f/t_{\text{eff}})^\alpha]$, where it is characterized by an effective time constant of relaxation $t_{\text{eff}}$ and exponent $\alpha$.

Fig. 3 (a) Filling time dependence of the major peak for $\text{Ar}^+$ irradiated 400°C annealed n-Si at $T=274.1K$. (b) CC-TATS spectra for different filling time $t_f$ at a fixed temperature showing evolution of a new peak whose time constant increases with increasing filling times.

The nature of this energy term also suggests that it can be viewed as an entropic term contribution to the measured enthalpy [10]. Physically it would mean that traps undergoing relaxation during electron occupation have a distinct entropy, most probably owing to changes in degeneracy factor.

Though the mechanism which drives this novel relaxation is not clear, a plausible physical scenario as visualized by Cohen and coworkers [9] can be described. With capture of a carrier a positive polarization cloud in the vicinity of the defect deepens the potential well and emission is monitored from this deepened state in absence of capture. During the capture pulse, successive emission and capture events can drive the defect to relax continuously to more stable states if the polarization cloud is unable to follow this process rapidly. In other words a relaxation process much slower than emission or capture processes would have the memory of net duration of occupation.

Fig. 4. Power law dependence of $\tau$ and $t_f$ for spectra shown in Fig. 3(a). Solid line refers to a best fit to relation $U_{\text{eff}} \sim k_B T \ln[(1+t_f/t_{\text{eff}})^\alpha]$.
CONCLUSIONS

Two distinct trap related phenomena in ion damaged silicon have been demonstrated. The phenomenon of charge redistribution among multiple traps have been shown to occur through trapping kinetics studies over 5-6 orders of magnitude in time. At relatively higher temperature, for partially relaxed samples, a novel defect relaxation process is observed where defect energy progressively deepens with trap filling time and this process is nearly athermal. It is important to reiterate here that isothermal spectroscopy such as CC-TATS is absolutely essential in study of phenomena such as described in this chapter. In a temperature scanning spectroscopy, such as DLTS, sensitivity to filling time and its temperature dependence on one hand, and possible occurrence of athermal process on the other can completely distort manifestation of such phenomena beyond recognition.

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REFERENCES


