EVIDENCE OF DEFECT MIGRATION AND CLUSTERING IN MeV HEAVY ION DAMAGED SILICON

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ABSTRACT

We have studied electrically active defects created by MeV heavy ion implantation in n-silicon. The buried damaged layer, created by implanting Ar^+ ions of energy 1.45 MeV and doses in the range 10^{13}-10^{14} cm^{-2} at room temperature, is embedded within the depletion layer of a Schottky diode. The defects are characterized using capacitance-voltage (C-V), current-voltage (I-V) and deep level transient spectroscopy (DLTS). Large concentration of electrically active defects are found to occur in a region several microns beyond the ion range or the damage profile predicted by Monte Carlo simulations. The dominance of a single trap in the damaged region is established from hysteresis effect in C-V, space charge limited conduction in forward I-V characteristics and DLTS results. With annealing in the temperature range of 400-600C, the observed changes in defect charge profile indicate that the effective electrical interface moves progressively towards the surface. C-V characteristics have been simulated using model charge profiles which suggest presence of a compensated region and a sharp negatively charged defect profile at a distance much larger than that expected from ion range. Our results constitute experimental evidence of migration and clustering of interstitial related defects, even at room temperature in case of high dose irradiation.

INTRODUCTION

Ion implantation is one of the most important processing tools in silicon integrated circuit (IC) technology. Recently, implantation at MeV energies has emerged as a preferential tool for precise positioning of dopants, control of lifetime, production of amorphous layers, improved well structures and isolation structures through buried layers [1,2]. It is known that for applications involving high dose implants, defects produced in as-implanted layers control subsequent evolution of defects and extent of relaxation of the disordered layer [3]. Hence a knowledge of physics of defect process in the buried layer has become a significant concern. Though a variety of structural tools have been used to study such layers [4], electrical characterization has often been limited to conductivity measurements [5] except for very few recent studies using deep level transient spectroscopy (DLTS) [6]. This is mainly due to lack of convenient test device structure, and limitations in use of conventional electrical characterization techniques to study these layers.

In this article, we report the study of defects in deep buried, damaged layers produced by MeV heavy ion implantation in n-Si. We show that a dominant electrically active defect occurs in large cncentrations at distances much beyond the ion range, and argue that their origin lies in formation of clusters of migrating interstitials .

EXPERIMENTAL

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

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with 1.45 MeV Ar^+ ions (having an approximate mean range of 1.23 μm as calculated from TRIM [7]) using a 2 MeV Van de Graaff accelerator. Ion doses of 5 x 10^{13} cm^{-2} and 1 x 10^{14} 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 10^9 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 70° 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.

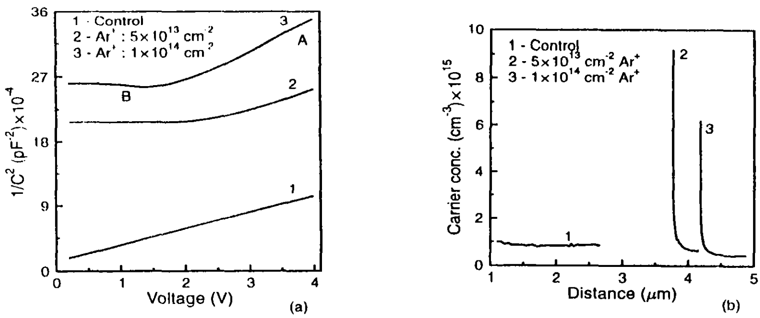


Fig.1(a) Typical C-V characteristics at 300K for n-Si Schottky diode before and after iradiation with various doses of Ar^+ ions.(b)Apparent carrier concentration profile obtained of curves of (a)

RESULTS AND DISCUSSION

Figure 1(a) shows a typical $1/C^2$ vs. V plot at room temperature for unimplanted and Ar^+ ion implanted samples with two different doses. As expected for unimplanted samples, the curve is linear in the measured voltage range indicating uniformity of shallow dopant concentration. However, for implanted sample a linear region (A) occurs at high voltage and a nonlinear or flatter region (B) occurs at lower voltages . The nature of the curves are qualitatively similar for both samples irradiated with low dose (5 x 10^{13} cm^{-2}) and high dose (1 x 10^{14} cm^{-2}) of Ar^+ ions. As depletion width (W) is proportional to 1/C, a larger W for implanted sample compared to unimplanted sample. Moreover, for high dose implanted sample zero bias depletion width is larger compared to low dose case. Fig.1b. shows the *apparent* carrier concentration as a function of width of the depletion region deduced from standard analysis of slopes of the curves in Fig.1a. The sharp rise in concentration profile is due to presence of a flat region in C-V. This feature is an artefact due to large trap density in a region of depeletion layer. TRIM simulatons predict the range of the ion to be 1.23μm with no significant damage beyond 1.5μm. Note that the edge of the depelion layer is at distnaces much larger from the surface than predicted by TRIM simulations. This was found to be a characteristic feature of highly damaged samples using heavy ions.

The fact that the unusual features in C-V are indeed controlled by trap dominated regions within the depeltion layer become clear from Fig.2(a). which shows hysteresis behaviour of C-V depending on both direction and rate of voltage sweep. The C-V characteristic is identical for

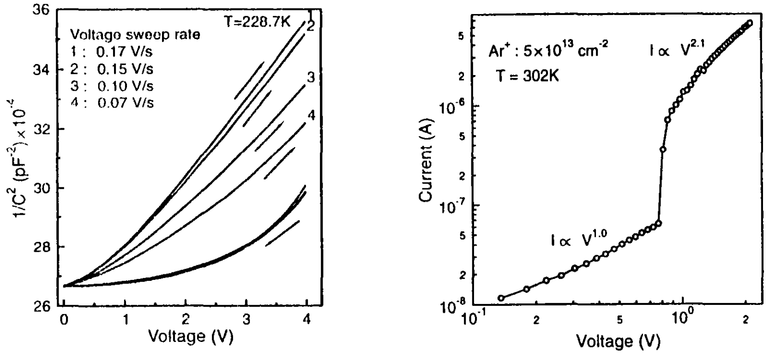
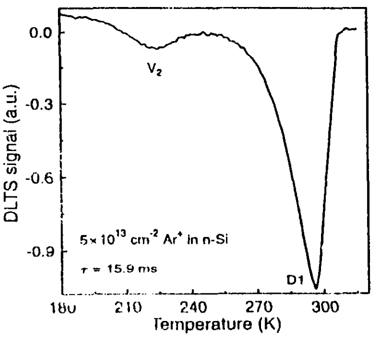


Fig.2. **(a)** C-V characteristics with decreasing and increasing bias showing hysteriesis effect in Au^+ implanted n-Si. Arrows indicate the direction of voltage seeep and different set of curves were obtained for different degrees of for bias injection. **(b)** Forward I-V characteristics of irradiated sample showing ohmic and space charge limited current regions.

different sweep rates when the voltage is decreased owing to fast capture process at the traps, while it is different on increasing the voltage since it is now controlled by rate of emission of the trapped charge. Indeed the hysteresis behaviour is observed for voltage sweep rates comparable to or faster than the trap emission rate at that temperature. It is confirmed from transient measurements that the trap time constant at the measured temperature is comparable to the voltage sweep duration. Note that the depletion width is larger when the reverse bias is increased after allowing capture during C-V measurements indicating that the dominant centres capture majority electrons and hence act as the dominant deep acceptors in the damaged layer.

Further evidence of trap controlled nature of the depletion layer comes from forward I-V characteristic curve as shown in Fig.2(b) which displays a near ideal case of crossover from ohmic conduction to square law space charge limited conduction regime at the voltage corresponding to trap filled limit (V_{TFL}). The nearly vertical rise in current accompanying the trap filling is an indicator that the associated defect is a discrete level [10]. In this case, it must be due to the dominant defect which controls hysteresis in C-V and is also observed in large concentration in DLTS spectra as shown later. These results also show that the sample structure under study is akin to a *p-i-n* diode where *p* is replaced by a metal and *i* region is nearly intrinsic due to presence of traps in the damaged region.

A typical DLTS spectrum for a sample irradiated with MeV Ar^+ ions is shown in Fig.3(a). For the chosen rate window two majority carrier related peaks labeled V_2 and D1 are observed in the temperature range 90K-310K, irrespective of ion species and dose. In some of them a weak signal corresponding to A center (oxygen-vacancy pair) [8] is also detected. Note that the doses used are considerably high so as to produce large concentration of defects. The peak labeled V_2 is a well known peak due to divacancy center $V_2\{-/0\}$ observed in all ion irradiation processes in n-Si [8]. The peak labeled *D1* is a newly observed feature [9] and it is the most dominant among all other peaks shown in these samples. The defect responsible for peak D1 occurs consistently in large concentration in all our samples.



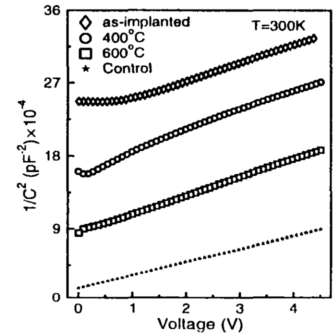


Fig.3. (a) A typical DLTS plot of Ar^+ irradiated sample showing divacancy V_2 and midgap acceptor D1. **(b)** Comparison of C-V characteristics at 300K of unimplanted, as-implanted and n-Si . The implantation dose was $5x10^{13}$ ions $/cm^{-2}$.

This defect has not been observed so far mostly because, to our knowledge, no other DLTS study uses unannealed samples with as high doses as in our case. An unusual feature in the DLTS lineshape of D1 is the distorted peak shown in Fig.3(a). Though exact estimation of trap parameter using time constants obtained from DLTS peaks may not be possible due to possible nonexponentiality in transient, ignoring effects of nonexponentiality on time constant evaluation, DLTS analysis shows that it is a midgap level with capture cross-section typical of a neutral trapping center. However, a more accurate analysis shows that trap energy varies in the range of E_c -0.49 eV to E_c -0.52 eV depending on the sample condition i.e. degree of disorder and low temperature relaxation [9]. For both annealed and lower dose implanted samples, the energy is deeper indicating that the defect is in more relaxed configuration. The degree of filling seem to increase for the relaxed material showing larger peak height in DLTS. This dependence of trap energy on process parameters is a strong indicator that the corresponding defect is a large complex or clusters. The dependence on process parameters is also clearly observed in C-V characteristics of samples undergoing progressive annealing. Such a comparison is shown if Fig.3(b). Note that unusually large zero bias depletion widths (and hence the location of the traps controlling C-V) progressively recover towards control sample on annealing. Further the temperature range of annealing (400°C-600°C)itself suggests that dominant defects controlling electrical behavior are point defects, since extended defects begin annealing out only temperatures above 1000°C. Hence the clusters formed in this damage regime seem to behave as point defects prior to their evolution to fully fledged extended defects such as dislocation loops.

In order to explain experimental features in C-V curves, we have used model charge profiles on the basis that dominant midgap acceptor D1 would cross the Fermi level within the depletion layer. These simulations, the details of which would be published elsewhere, show that the irradiation damage produce two regions :(i) a compensated region with most dopants being deactivated, and (ii) a sharp negatively charged (*occupied*) defects in large concentration close to the depletion edge. The resulting energy band diagram and C-V curve, obtained from solving Poisson's equation, are shown in Fig.4. Note that the flatness in $1/C^2$ vs. V in simulated curves correspond to the Fermi level meeting large concentration of acceptors within the depletion layer. This enables voltage changes during C-V to be accommodated by suitable occupancy changes in the narrow region of E_T-E_F crossing. Hence our simulation points to the fact that there exist an effective electrical interface between trap dominated and nearly defect free region within the depletion layer. The peak labeled D1 is a newly observed feature and it is the most dominant among all other peaks observed in these samples. Recall that the depletion edge is at a distance much larger than the expected range of ions.

Hence it is abundantly clear that the trap D1, being present in large concentration in high dose implanted samples, is responsible for the unusual features in C-V. Its origin possibly involves higher order complexes of intrinsic defects. Recently, it has been shown from molecular dynamic simulations and high resolution electron microscopy observations that accumulation of di-interstitial pairs occur in heavy ion implanted layers leading to homogeneous amorphization beyond a threshold dose [4]. Further Privitera *et al.* [11] have recently demonstrated long range room temperature migration of Si self-interstitials. More recently, atomistic calculations and experimental studies on point defect evolution strongly suggest formation of interstitial type defect clusters in high dose implanted Si [12].

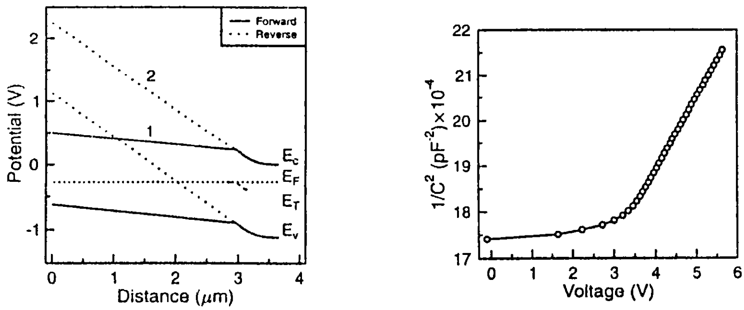


Fig.4. Typical calculated (a) energy band diagram and (b) corresponding simulated C-V characteristics for a Schottky diode with one midgap acceptor trap level at energy E_T.

Since we have observed the major defect (D1) to be lying much beyond the TRIM predicted profile, there is a strong indication of possible involvement of migrating interstitials forming clusters. It is highly likely that the migrating interstitials become immobile on forming clusters and therefore produce a sharp edge in the trap profile which occurs close to the edge of the depletion layer. The sensitivity of enrage level of D1 to processing conditions such as dose, annealing etc. [9] also suggest that D1 level is due to clusters formed during large injection of interstitials. Furhter, the depletion width is observed to shrink towards surface on annealing the samples in the temperature range of 400-600C indicating recovery of clusters of different sizes as annealing temperature is increased. The size of the clusters seem to depend on the distance form the damaged region (corresponding to the range of the implanted ions).

More vigorous correlated studies are required to establish size and distribution of clusters involved. Specifically, as has been pointed out by Benton et al [6], it is perplexing to note that the electrical defect spectra is nearly always dominated by a single point defect-like D1 though one expects large variation in cluster sizes. It appears to us that variation in cluster size is mainly spatial being dependent on migration from the point where interstitials are injected. Since electrical studies are mainly from a narrow region of E_T-E_F crossing (which acts as an effective electrical interface), these methods only sample clusters of specific size in a particular experiment. The detection of standard divacancy centers at such large distances also raises the question whether cluster formation process itself involves maintaining certain saturation level of divacancy in the region.

CONCLUSION

We have studied high dose MeV Ar^+ ions implanted n-Si using electrical characterization methods. On the basis of unusual and interesting features such as hysteresis in C-V characteristics, trap filled limit space charge conduction and large peak height in DLTS signal we argue that a high concentration of trap is located in regions deeper than the region directly modified by implantation. This major defect is a midgap acceptor level and its origin lies in formation of clusters from interstitials migrating away from the region of heavy damage.

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