Influence of Pre-Existing Structures and Ion-Implantation Conditions on the Formation of Amorphous Silicon

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Introduction

Stable defects are introduced into Si by nuclear collisions in ion beam processing. These defects are known to be pernicious to semiconductor devices and so have become a major issue as the integrated circuit industry moves towards smaller device dimensions and lower thermal budgets. It is essential then to understand the influence that ion implantation has on the structure of the target material in order to minimize defects in the active device region and to further understand their role in materials.

Previous studies have shown that the implant temperature and the ion fluence has a strong effect over the type and amount of irradiation induced disorder.[1] Therefore, these parameters will be varied over a wide range in order to better understand this influence. Also, we can study the role of defects in a controlled environment via the use of structural relaxation which has in part been attributed to the annihilation of non-equilibrium defects.[2] Structural relaxation has the effect of decreasing the strain energy and is related to the topology of the material which can be described by the RMS bond angle deviation. This can be measured directly by Raman spectroscopy.[3]

The conditions under which the Si substrates were prepared involved varying the substrate temperature during implantation and the self-ion-implantation dosages at a fixed energy. The implants were performed into both crystalline silicon (c-Si) and relaxed amorphous silicon (a-Si). The structure of the silicon was then characterized by its vibrational properties as measured by the Raman spectrometer. Rutherford Backscattering Spectrometry and Channeling (RBS-C) was also used to determine the density and layer thickness of the samples giving us further information about its amorphous state.

In surveying a range of ion induced effects we are also investigating the influence that pre-existing nanocavity structures have on the formation of a-Si. In particular, Raman Spectroscopy will be used to characterize the formation of amorphous material around the cavities at different ion doses. Nanocavities are used for the gettering of transition metal impurities and defects and are found to collapse upon irradiation due to plastic flow in a-Si.[4] Again, RBS-C will be employed to record the effect of ion implantation.

The following paper will only present our results on ion-implantation into relaxed a-Si and c-Si at an implant temperature of 77K.

Experiment

In this study Cz Si(100) p-type wafers of a resistivity ranging between 1 − 10Ωcm were used. A thick amorphous layer was prepared by ion implantation of $^{28}\text{Si}^+$ ions at energies of 0.5, 1.0 and 2.0 MeV using a 1.7 MeV NEC ion implanter. During these implants the substrates were affixed to a stage held at 77K with silver dag to ensure good thermal contact. The samples were then annealed for 45 minutes at a temperature of 500°C in vacuum. This had the effect of relaxing the amorphous layer. A region
Figure 1: a) The Stokes Raman Spectra for relaxed a-Si (top) and c-Si (bottom). b) The Stokes Raman spectra for relaxed a-Si (bottom), implanted relaxed a-Si (100keV $^{28}$Si$^+$ ions to a fluence of $1 \times 10^{17}$ at 77K), and the same implant into c-Si (top). Indicated are the peak position and peak half width.

which overlapped both relaxed a-Si and c-Si was then irradiated with 100keV $^{28}$Si$^+$ ions to fluences ranging from $1 \times 10^{13}$ to $1 \times 10^{17}$cm$^{-2}$ while the substrates were held at temperatures of 77K, 293K, or 373K. Raman spectra were then taken using the University of Melbourne Dispersive Raman Microprobe at integration times of 1000s. The 514.5nm line of a continuous wave Ar$^+$ ion laser was used to irradiate the sample in a backscattering geometry. The Raman laser had a spot size of $1\mu m \times 1\mu m$ with a power of 0.6mW at the sample surface to avoid heating effects. The scattered light was spectrally resolved onto a CCD camera where the gratings were arranged in a double subtractive mode.

Results and Discussion

Raman Spectroscopy is quite sensitive to transformations from the crystalline to amorphous phase. This point is illustrated in Figure 1(a) which shows typical spectra for relaxed a-Si and c-Si. The c-Si Raman spectrum is determined by wavevector selection rules. A strong single one-phonon band at 520.2cm$^{-1}$ dominates the underlying second-order Raman characteristics. The intensity of this peak is polarization dependent and is attributed to the creation of the triply degenerate long wavelength optical phonons. On irradiation the intensity of this line will decrease as more light will be scattered from a disordered material. It’s general shape will also become skewed and shift towards lower wavenumbers with the build up of damage and the ultimate breakdown of selection rules. These effects will be studied more closely in the nanocavity Raman spectra with the use of the Phonon Confinement Model.[5]

The a-Si spectrum reflects the full vibrational Density-of-States (DOS). It consists
Figure 2: a) Half width of the TO Raman peak as a function of dose for both relaxed a-Si and c-Si (open circles) irradiated at a temperature of 77K. b) Position of the TO Raman peak as a function of dose. Indicated are typical values of Relaxed a-Si.

of a transverse optical (TO) phonon peak at $\sim 470 \text{cm}^{-1}$ whose existence requires tetrahedral symmetry to be present in the amorphous structure. Features on the lower wavenumber shoulder of the TO peak are attributed to longitudinal optical (LO) and longitudinal acoustic (LA) phonon bands.

The evolution of the TO peak was followed as the ion dose was increased. In particular, its peak position shift and half width. The half width to the high wavenumber side of the peak was measured (as indicated in Figure 1b) to avoid the LO and LA like features. It can be seen that once the relaxed a-Si is irradiated to high doses its Raman spectra becomes identical to that of its as-implanted counterpart.

The range of 100keV Si ions in Si is 1500Å with the peak in $(\frac{dE}{dx})_{\text{nuclear}}$ occurring at a depth of $\sim 1000\text{Å}$ as calculated by SRIM. These depths are within the expected probe depth ($\sim 1600\text{Å}$) of the Ar laser in a-Si. For implantation into relaxed a-Si, the 100keV ions cause de-relaxation of the continuous random network (CRN) structure. This leads to increased bond-angle distortion and defect incorporation and results in the observed shift in the TO position and width, as shown in figure 2. For implantation into c-Si the 100keV ions initially generate isolated zones of a-Si which coalesce into a continuous amorphous layer with increasing dose. Amorphous layers produced at elevated implantation temperatures where dynamic annealing may play a vital role are yet to be analyzed.

The trends observed here are qualitatively similar to those observed by Roorda et al.[7] for 5.5MeV implantation into relaxed a-Si where the ion range is far beyond the probe depth of the laser. As expected, in the case of our 100keV implants, the relatively small depth range of the ions causes the range at which the TO position exhibits the
most dramatic shift to occur at lower doses than that observed by Roorda. We are currently examining our data in more detail to see if the differences between data sets can be related to the expected changes in the a-Si network. We expect that the trends observed in samples implanted at room temperature and above will provide a better picture of what is happening in the material.

Conclusion
This study investigated the influence of ion implantation conditions on the structure of a-Si. It was found that keV implants display qualitatively similar behaviour to the MeV implants produced by Roorda et al. as seen by Raman analysis. Using this tool we will be able to characterize the effect of ion induced damage at a range of ion doses and temperatures where dynamical annealing may play a vital role in determining the resultant structure.

Samples produced with different ion doses and at different ion implantation temperatures are yet to be analyzed. Subsequent RBS-C spectra will be obtained in order to determine the density and layer thickness of the samples to correlate this with the Raman spectra. Thus, the effect of ion implantation temperature and dose on the resultant amorphous structure will be determined as well as a comparison between keV and MeV implants.

Using the same analytical tools as above the collapse of nanocavities is yet to be examined.

REFERENCES