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Study of He-induced nano-cavities as sinks of oxygen for forming silicon-on-insulator

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In the present work, a Cz–Silicon wafer is implanted with helium ions to produce a buried porous layer, and then thermally annealed in a dry oxygen atmosphere to make oxygen transport into the cavities. The formation of the buried oxide layer in the case of internal oxidation (ITOX) of the buried porous layer of cavities in the silicon sample is studied by positron beam annihilation (PBA). The cavities are formed by 15 keV He implantation at a fluence of 2×10^{16} cm^{-2} and followed by thermal annealing at 673 K for 30 min in vacuum. The internal oxidation is carried out at temperatures ranging from 1073 to 1473 K for 2 h in a dry oxygen atmosphere. The layered structures evolved in the silicon are detected by using the PBA and the thicknesses of their layers and nature are also investigated. It is found that rather high temperatures must be chosen to establish a sufficient flux of oxygen into the cavity layer. On the other hand high temperatures lead to coarsening the cavities and removing the cavity layer finally.

Keywords: positron annihilation, nanocavity, oxygen diffusion, silicon dioxide
PACC: 6180J, 7870B, 6170A

1. Introduction

Positron annihilation spectroscopy (PAS) performed with a slow positron beam is a powerful technique for probing open volume defects in solid.[1] The PAS is also used to study extensively the formation, evolution and electronic structure of defects in elemental and compound semiconductors.[2,3] In particular, in the Doppler broadening experiments with positron beams, the one-dimensional momentum distribution of the positron electron annihilating pairs is measured by using the PAS. The narrowing of the momentum distribution is an indication of positron trapping in vacancies and vacancies cluster defects.

The low-cost and high-quality thin layers of single crystal silicon-on-insulator (SOI) are available and have been used to fabricate semiconductor devices that are characterized mainly by increasing hard radiation, improving device performances while reducing latch-up and parasitic capacitance.[4,5] Recently, low dose separation by implanted oxygen (SIMOX) technology has developed rapidly to improve the quality of the SIMOX wafers and to reduce the production costs.[6] The process is carried out in two steps: firstly a high-equality planar buried oxide (BOX) is obtained by implanting silicon at a much low dose of 4×10^{17} cm^{-2} and thermally annealing at 1573 K. It is almost one-fifth of high-dose SIMOX;[7] Secondly, the BOX is further grown through the ITOX.[8] It is known that BOX thickness increases due to the oxygen diffusion into the wafer in an Ar/O_2 atmosphere, through a surface silicon-oxide layer and a superficial silicon layer.[9] There is an alternative economical way to employ a buried cavity layer as the nucleation site for BOX. The growth of cavities and their thermal evolution when He ions are implanted into Si have been investigated.[10,11] So in this paper, we concentrate on the nanocavity that is formed by using the 15 keV He implantation at a fluence of 2×10^{16} cm^{-2} and subsequently the pre-thermal annealing to 673 K in vacuum, then thermal annealing at varying temperature in a dry oxygen atmosphere which facilitates the nucleation and growth of SiO_2 precipitates. The buried oxide layer is studied by using the PAS.

2. Experimental procedure

The starting material in our study was 4-in n-type (100)-oriented, Czochralski-grown silicon (Cz–

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Si) wafer (P-doped, 0.6–0.79 Ωcm). The sample was implanted with 15 keV He ions at a fluence of $2 \times 10^{16}\,\mathrm{cm}^{-2}$ and room temperature. The sample was cut into $10 \times 10\,\mathrm{mm}^2$ and annealed at 673 K for 30 min, which led to a band of cavities at a depth of 80–250 nm.[12] Internal oxidation of the pre-annealed samples was performed in a quartz tube within a tubular furnace under an oxygen gas flow at temperatures varying from 1073 to 1473 K for 2 h.

Doppler broadening positron annihilation spectrum as a function of incident energy E of positron was measured by using a high-purity Ge (HPGe) detector at room temperature under a vacuum of about 10^{-5} Pa at the Key Laboratory of Nuclear Analysis Techniques, Institute of High Energy Physics, Chinese Academy of Sciences. The PBA results were described in terms of two parameters (S and W). The S-parameter gives the fraction of annihilations with low-momentum (mostly valance) electrons and provides the information on the value of open volume. The W-parameter is a measure of the fraction of annihilations with the high-momentum core electrons, and it is sensitive to the chemical composition of the atoms around the annihilation site.[13] The S-parameter was calculated as the ratio of the counts in the central area of the peak ($|E\gamma\text{-}511| \leq 0.44$ keV) to the total area of the peak ($|E\gamma\text{-}511| \leq 3.45$ keV).The experimental data were analysed with the aid of the program VEPFIT[14] that contains an algorithm simulating positron implantation, diffusion, trapping, and annihilation. The layered structures, which correspond to positrons annihilated in the surface, in the damaged layer produced by the He-ion implantation, and in the bulk undamaged layer beyond the range of He-ion distributions were measured. Hence the S-parameter corresponding to a given positron energy E can be expressed as a linear combination of three terms.[15]

$$S(E) = S_\mathrm{s} f_\mathrm{s}(E) + S_\mathrm{b} f_\mathrm{b}(E) + S_\mathrm{d} f_\mathrm{d}(E), \qquad (1)$$

where $f_\mathrm{s}(E), f_\mathrm{b}(E)$ and $f_\mathrm{d}(E)$ are the positron annihilation probabilities in the surface, in the bulk, and in the defects, respectively. $S_\mathrm{s}, S_\mathrm{b}, S_\mathrm{d}$, are the characteristic values of S for positrons annihilating in the surface, in the bulk, and in a defect.

The mean incident depth of positron is assumed to follow a power law $x = AE^n\rho$, where x is in nm, E is the incident energy of positron in keV, and ρ is the density of material in $\mathrm{g/cm}^3$ (which is $2.33\,\mathrm{g/cm}^3$ for Cz–Si material). The constant A was found empirically to be $3.5\,\mu\mathrm{g/cm}^2$ and $n = 1.7$.[16]

3. Results and discussion

The concentration profiles of implanted atoms in the Cz–Si host matrix are obtained by using the Monte Carlo simulation code, TRIM program.[12] From Fig.1 one can see that the peak positions of the distribution profile for vacancies and helium in the Cz–Si sample implanted with 15 keV He ions are located at about 150 and 230 nm, respectively.

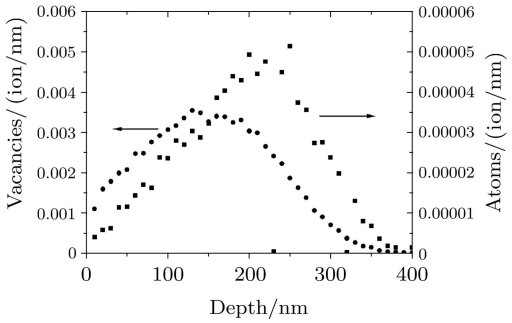


Fig.1. Monte Carlo simulation results of the depth distribution of He and vacancies in Cz–Si implanted with 15 keV He ions.

The S-parameter that is related to annihilation with valence electrons shows the highest values of its sensitivity for vacancies and cavities. Shown in Fig.2(a) are the analyses of incident energy of positron for the oxidation of the samples containing a buried cavity layer at several temperatures. The curves of S-parameter versus incident energy of positron are shown for a pristine sample and the samples oxidized at temperatures ranging from 1073 to 1473 K. In the pristine sample, a gradual increase of S from low values of S to bulk values is found. The low value of S-parameter is due to the oxidation of the sample surface.[17] The changes result from the creation of cavities which are induced by implantation with He ions after annealing.[18] It is shown that the sample contains a buried cavity layer after thermal annealing at 1073 K in a dry oxygen atmosphere. There is a nearly straight line of S-parameter at the incident energies of positron ranging from 3 to 6 keV, which is the profile of the vacancies as calculated by TRIM (see Fig.1). But the value of S-parameter at 3 keV is larger than those in a range of 3.5 to 5 keV. It is different from that for the sample with a buried cavity layer.[19] The value of S is normalized to the Si bulk value S_b, i.e. $S_\mathrm{n} = S/S_\mathrm{b}$. The values of normalized S as a function of incident energy E of positron are shown in Fig.2(b). The maximum value of S decreases abruptly in the case of thermal annealing at

1073 K; the value of S-parameter is about 0.8% larger than that of S_b. In the sample containing a buried cavity layer after annealing at 1273 and 1473 K, the main peaks of S-parameter occur at 1.7 and 2.7 keV, respectively. The value of S in the buried cavity layer is lower than that of S_b. It indicates that vacancy-type defects disappear in the proximity of the surface which acts as a sink for oxygen to form a buried oxide. The shift of main peak of S-parameter is mainly due to the agglomeration of smaller cavities and vacancies present from the surface of the sample down to the cavity layer. On annealing at 1273 K or 1473 K, the change in value of S-parameter is different from that in the case of annealing at 1073 K, which indicates that the cavities have been modified because they have been reduced in size and changed by decoration with oxygen. Since voids and cavities in silicon can be an efficient getter centre for oxygen and metals,[20,21] when the samples containing a buried cavity layer are annealed at a high temperature in a dry oxygen atmosphere, the oxygen will be dissolved and diffuse into the stable buried layer to be trapped, thereby forming multivacancy-multioxygen (V_xO_y) complexes and oxide. The growth rate of the internal oxide is limited by the diffusion of oxygen from the Si/SiO_2 interface. The flux of oxygen diffusing to the cavity layer may be described simply as

$$J_O = D_O C_O N_{si}/L_{cav} \tag{2}$$

where D_O is the diffusivity of oxygen in Si, C_O is the equilibrium oxygen concentration at the Si/SiO_2 interface, N_{SI} the atom density of Si, L_{cav} the distance between the interface and the cavity layer. According to Ref.[22], the value of D_O varies from 0.9×10^{-10} to $3 \times 10^{-8}\,cm^2/s$ when the annealing temperature changes from 1073 to 1473 K. N_{si} is $2.33\,g/cm^3$, and L_{cav} is about 100 nm. It is known that V_xO_y complex can migrate at temperatures above 1073 K.[23] It leads to the formation of oxygen clusters and oxygen precipitates (SiO_x, $x < 2$), resulting in a large decrease in the value of S parameter. Above 1273 K, the SiO_x dissociates through the reaction $SiO_x \rightarrow Si + SiO_2$.[24] Therefore the excess Si interstitials are formed at the buried oxide layer where extended defects are produced, which leads to a shift of the main peak of S parameter at 2.7 keV when the sample is thermally annealed at 1473 K.

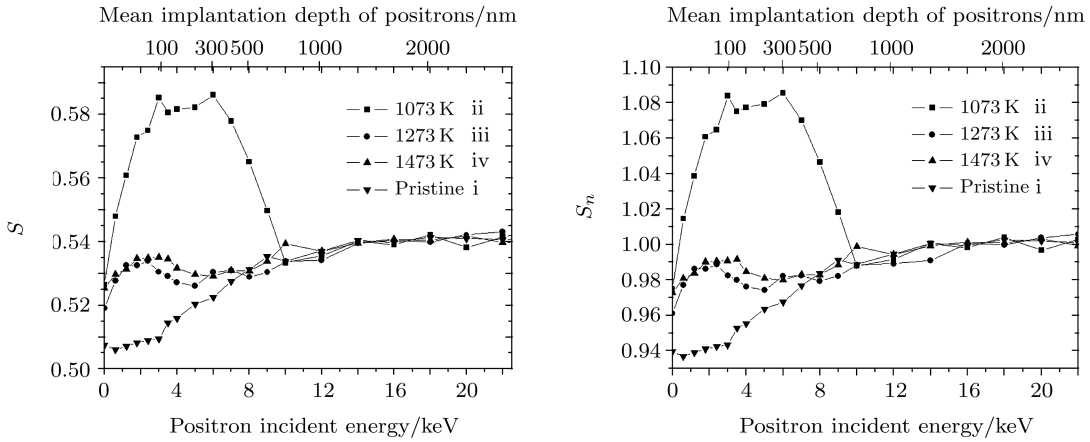


Fig.2. Curves for S and normalized S parameters, separately, vs. incident energy of positron for Si/SiO_2 structures fabricated by dry oxidation, where panel (a) shows the value of S-parameter as a function of the incident energy of positron (bottom axis) and the mean implantation depth of positron (top axis), panel(b) describes the S_n parameter vs. incident energy E of positron (bottom axis) and the mean implantation depth of positron (top axis). Data in the insets correspond to the following cases: pristine (i), after implantation of $2 \times 10^{16}\,cm^{-2}$ 20 keV helium and pre-annealing at 673 K in vacuum, then additional annealing, separately, at 1073(ii), 1273 (iii) and 1473 K(iv) in a dry O_2 atmosphere.

The W-parameter has been shown to be extremely sensitive to the annihilation with oxygen core electrons. Plotted in Fig.3 are the curves for W-parameter versus the mean implantation depth of positrons (top axis) for the samples after oxidation at the temperatures varying from 1073 to 1473 K. It can be seen that the sample containing a buried cavity layer has a low value of W-parameter after thermal annealing at 1073 K. It indicates that no buried oxide has been formed. However, on thermal annealing at

1273 or 1473 K, the value of W-parameter increases abruptly in the defect layer, and it is close to the value at the surface corresponding to the top oxide, indicating the formation of the buried oxide when the sample is thermally annealed at 1273 or 1473 K. The W value and oxide layer both increase with annealing temperature.

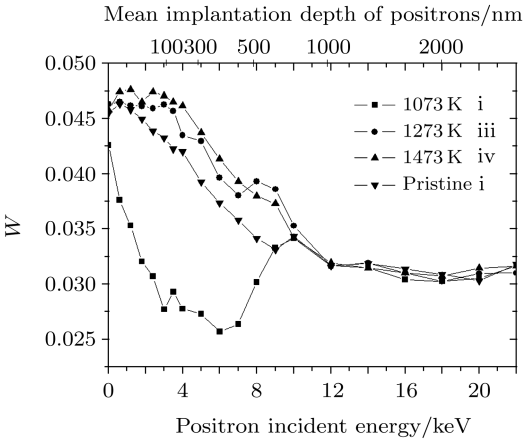


Fig.3. Curves for W-parameter as a function of incident energy of positron (bottom axis) and mean implantation depth of positron (top axis), separately. Data in the inset correspond to the following cases: pristine (i), after implantation of $2 \times 10^{16}\,\mathrm{cm}^{-2}$ 20 keV helium and pre-annealing at 673 K in vacuum, then additional annealing, separately, at 1073 (ii), 1273 (iii) and at 1473 K (iv) in a dry O_2 atmosphere.

Shown in Fig.4 is an S–W map, where all the characteristic values are obtained during oxidation of the samples for the cavity layer. The characteristic values of the cavity layer change gradually from cavities to coordinates, clearly deviating from those for silicon and lying at a point between SiO_2 and Si after 1273 K oxidation. However, the further increase of temperature to 1473 K leads the value of S to increase, which indicates that the internal oxidations of the cavities are not stable at this temperature.[25]

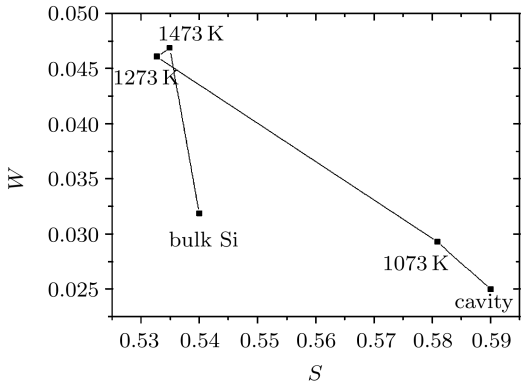


Fig.4. The S–W map, where the characteristic values are obtained during the oxidation of silicon with a buried layer at the indicated oxidation temperatures.

4. Conclusions

A novel technique for producing a high-quality and low-cost silicon-on-insulator has been described. With this method, a buried cavity layer in silicon is formed first by using the implantation with helium ions, and then by transporting the oxygen into the cavity to produce a buried oxide layer. The oxidation of silicon with a buried cavity layer is monitored by PAS. The 15 keV helium ions are implanted into the silicon and, subsequently, the implanted silicon is thermally annealed at 673 K for 30 min, thereby leaving a buried cavity layer at about 80–250 nm from the surface. The chosen conditions, i.e. temperature and dry oxygen, are sufficient to grow a complete buried oxide layer by means of internal oxidation, especially the oxidation that takes place at 1273 K. At 1473 K, the internal oxidations of cavities are unstable.

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