Optical effects of doped top layers in silicon-on-insulator structures formed by ion implantation

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Arsenic ions were implanted into silicon-on-insulator (SOI) structures at an incident energy of 100 keV to a dose of 2×10^{15} cm⁻². Conductive top layers were formed in the SOI structures after annealing at 1200 °C for 20 s. Infrared reflection spectra in the wave number range of 1500–5000 cm⁻¹ were measured and interference fringes, related to free-carrier plasma effects, were observed. By detailed theoretical analysis and computer simulation of infrared reflection spectra, the carrier concentration, the carrier mobility, and the carrier activation efficiency were obtained. The physical interpretation of the results and a critical discussion of the sensitivity of the data, fitted to variation in the parameters, are given.

1. Introduction

The synthesis of silicon-on-insulator (SOI) structures by ion implantation for very large-scale integrated (VLSI) circuits has received considerable attention in recent years [1]. The technique of ion implantation is currently being developed to form SOI structures with a high quality, single-crystal silicon layer on an insulating layer. Until now the properties of SOI structures formed by nitrogen or oxygen implantation into silicon were mainly determined by transmission electron microscopy (TEM), secondary ion mass spectroscopy (SIMS) and Rutherford backscattering spectroscopy (RBS). There are no reports of optical characterization of the doped top silicon layer.

In the present work, optical properties of the doped top silicon layer have been investigated. Infrared (IR) reflection interference measurements were employed to determine the free-carrier plasma effects. By detailed theoretical analysis and computer simulation of the IR reflection interference spectra, the carrier concentration and mobility of the doped top layer have been obtained. Physical interpretation of the results and a critical discussion of the sensitivity of data fitted to variation in the parameters, are also given.

2. Experimental procedure

Device grade $\langle 100 \rangle$ -oriented high-resistivity singlecrystal silicon wafers were implanted with O⁺ ions at an incident energy of 170 keV to a dose of 1.8×10^{18} cm⁻². During implantation, the wafer was maintained at 500–550 °C. After implantation, thermal annealing at 1300 °C for 5 h was used to allow for solid-phase epitaxial regrowth of the top silicon layer and for the formation of the continuous buried oxide layer. Arsenic ions at an incident energy of 100 keV to a dose of 2×10^{15} cm⁻² were implanted into the top silicon layer. After implantation, rapid thermal annealing (RTA) at 1200 °C for 20 s was used in order to allow for the formation of the conductive top layers. Resistivity was measured by using an ASR-100C/2 spreading resistance probing (SRP) system. IR reflection interference measurements were made at room temperature by means of a Perkin-Elmer 983 double-beam spectrometer for the frequency range $1500-5000 \text{ cm}^{-1}$. The quoted accuracy of the Perkin-Elmer is +1% in absolute reflection. The reflection was measured with the beam at near normal incidence to the implanted surface. Multiple reflections between the front and rear surfaces was eliminated by the coarse back surface. To obtain the absolute reflection, R, from the sample, the energy reflected from the sample was compared with that reflected from a high-quality front surface of an aluminium mirror.

3. Results and discussion

Before presenting the experimental and theoretical results, it will be useful to discuss some features of the model which have been developed to analyse the reflection interference spectra. After RTA processes, the implanted arsenic ions become electrically active as donors and there will be a distribution of free carriers within the implanted region. Free-carrier plasma effects will cause interference effects in the IR reflection spectra. If n_i and k_i are the refractive index and extinction coefficient of the implanted region, the optical constants n_i and k_i at lower frequency are dominated by the free-carrier plasma [2]. Therefore, calculation of the optical constants n_i and k_i must include the dispersion effects produced by a free-carrier plasma: n_i



Figure 1 (a) The Infrared reflection spectrum of the sample implanted with 100 keV arsenic ions to a dose of 2×10^{15} cm⁻² and annealed at 1050 °C for (\bigcirc) 20 s and (\longrightarrow) the best-fitting curve. (b) The calculated carrier concentration profile.

and $k_{\rm I}$ are functions of carrier concentration profile $N_{\rm c}(x)$, damping constant $\gamma(x)$ and frequency, ω . As a result of the SODDIS (simulation of dopants diffussion in SIMOX) calculation, the implanted ion distributions are uniform after annealing at 1200 °C for 20 s [3]. The optical constant $n_{\rm I}$ and $k_{\rm I}$ of the top layer can be calculated based on the carrier concentration, $N_{\rm c}$. The complex dielectric function, $\varepsilon_{\rm I}$, for the *i*th layer can be written

$$\varepsilon_{I} = \varepsilon'_{I} + i\varepsilon''_{I} = (n_{I} - ik_{I})^{2}$$
$$= \varepsilon_{IO} - \varepsilon_{IO}\omega_{PI}^{2}/(\omega^{2} - i\gamma_{I}\omega)$$
(1)

where $\varepsilon_{IO} = n_0^2$ is the dielectric constant for $\omega \gg \omega_{pI}$. The second term is the dielectric response for free carriers where γ_I is the damping constant; γ_I was taken as [4]

$$\gamma_{\rm I} = N_{\rm CI} e^2 / (m_{\rm e}^* \sigma_{\rm I} F_{\gamma}) = N_{\rm C} \rho_{\rm I} e^2 / (m_{\rm e}^* F_{\gamma})$$
 (2)

where σ_1 and ρ_I are experimental values of the conductivity and resistivity of the top layer; F_{γ} is a fitting parameter and was determined in the fitting process; m_e^* is the conductivity effective mass of free carriers in silicon; and ω_{ot} is the plasma frequency of the top layer

$$\omega_{\rm pI}^2 = N_{\rm c} e^2 / (\varepsilon_{\rm IO} \varepsilon_{\rm O} m_{\rm e}^*) \tag{3}$$

Factoring Equation 1 for ε_1 into its real and imaginary parts gives

$$\varepsilon'_{\rm I} = n_{\rm I}^2 - k_{\rm I}^2 = \varepsilon_{\rm IO} [1 - \omega_{\rm pI}^2 / (\omega^2 + \gamma_{\rm I}^2)]$$
 (4)

$$\varepsilon_{\rm I}^{\prime\prime} = 2n_{\rm I}k_{\rm I} = \varepsilon_{\rm IO}\gamma_{\rm I}\omega_{\rm pI}^2/[\omega(\omega^2 + \gamma_{\rm I}^2)] \qquad (5)$$

Solving Equations 4 and 5 for the refractive index, $n_{\rm I}$, and extinction coefficients, $k_{\rm I}$, gives

$$n_{\rm I} = [\epsilon_{\rm I}'/2 + (\epsilon_{\rm I}'^2 + \epsilon_{\rm I}''^2)^{1/2}]^{1/2}$$
(6)

$$k_{\rm I} = \left[-\epsilon_{\rm I}'/2 + (\epsilon_{\rm I}'^2 + \epsilon_{\rm I}''^2)^{1/2} \right]^{1/2} \tag{7}$$

TABLE I Parameter values for best fit curves of Fig. 1

$N_{\rm co}({\rm cm}^{-3})$	<i>n</i> ₀	D _I (µm)	n _B	D _B (µm)
5.8×10^{19}	3.59	0.22	1.69	0.39

The frequency-dependent refractive index of the substrate, n_s , is given by [5]

$$n_{\rm S} = [4.1476 + 5.8876 \times 10^9 / (27973^2 - L^2)]^{1/2}$$
(8)

where L is the wave number. The extinction coefficients are zero for the wave number range $1500-5000 \text{ cm}^{-1}$. A computer code was established to calculate the interference at normal incidence in reflection R from a multilayer thin-film model described above [6]. The code computes R for an arbitrary number of layers having indices of refraction n, extinction coefficient k, and layer thickness D. The doped top silicon layer of SOI structures was taken as one uniform layer of index $n_{\rm I}$, extinction coefficient $k_{\rm I}$, and thickness $D_{\rm I}$. The buried layer was taken as one uniform silicon oxide layer of index $n_{\rm B}$ and thickness $D_{\rm B}$. Because the back surfaces of the SOI samples were coarse lapped, the substrate was taken to be an infintely thick layer of index $n_{\rm S}$.

The experimental reflection spectrum was fitted by using the computer code which adjusted the values of parameters of the multilayer thin-film model to minimize the reduced chi-square, χ^2

$$\chi^2 = \sum_{i=1}^{N} (R_{i, \text{measured}} - R_{i, \text{calculated}})^2 / (N - N_p)$$
 (9)

where N is the number of data points of the experimental reflection spectrum and N_p is the number of parameters of the model described above. In fitting of the data, it was found that the values of the parameters of the model such as the carrier concentration of the



top silicon layer, $N_{\rm C}$, the refractive index of silicon of the top layer, n_0 , the refractive index of the buried silicon oxide layer, $n_{\rm B}$, and the thickness of the buried layer, $D_{\rm B}$, were well defined while maintaining a good fit to the data.

Fig. 1a shows the IR reflection spectrum for the SOI sample implanted with 100 keV As ions to a dose of 2×10^{15} cm⁻² and annealed at 1200 °C for 20 s. The full curve in Fig. 1a shows the results of fitting



Figure 2 (a) The calculated IR reflection spectra for deviation of the parameters away from the best-fitting parameters of the sample of Fig. 1. Variation of concentration with depth is shown in the inset, in (a): $N_{\rm eo}$: (----) 5.8×10^{19} cm⁻³, (---) 7×10^{19} cm⁻³, (---) 3×10^{19} cm⁻³. Variation of the refractive index with depth is shown in the insets in (b-e).

the reflection spectrum using the theoretical model. The non-linear least-square adjusted curve is in good agreement with the reflection spectrum. Also shown is the distribution of free carrier as the fitting function in Fig. 1b. Parameter values for the best fit curve in the figure are listed in Table I. The mobility for the top layer can be calculated by the usual expression $\mu_{\rm I} = e/(m_e^* \gamma_{\rm I})$; the computed mobility is 110 cm² V⁻¹ s⁻¹.

Variations in IR reflection spectra caused by deviation in $N_{\rm C}$, $D_{\rm I}$, $n_{\rm O}$, $D_{\rm B}$ and $n_{\rm B}$ away from the bestfitting parameters in Table I are now discussed. Fig. 2 shows the computer-generated IR reflection spectra for various $N_{\rm c}$, $D_{\rm I}$, $n_{\rm O}$, $D_{\rm B}$ and $n_{\rm B}$. It shows that the IR reflection spectrum is sensitive to the parameters of the theoretical model mentioned above. This is of great importance, in that it provides an estimate of the sensitivity of this method to the carrier concentration of the top silicon layer and parameters of SOI structures.



Figure 3 The calculated IR reflection spectra for various N_c : (----) 10^{20} cm⁻³, (---) 10^{19} cm⁻³, (---) 10^{18} cm⁻³, (---) 10^{17} cm⁻³ (---) 10^{16} cm⁻³.



Figure 4 (\triangle) The infrared reflection spectrum of the SOI sample and (—) the besting fitting curve. The variation of the refractive index with depth is shown in the inset.

TABLE II Parameter values for best fit curves of Fig. 4

$N_{\rm co}({\rm cm}^{-3})$	n ₀	$D_{\rm I}(\mu{\rm m})$	n _B	$D_{\rm B}(\mu{\rm m})$
< 1 × 10 ¹⁷	3.54	0.22	1.69	0.39

The electrical activity, η , of the implanted arsenic can be obtained from the ratio of the integral of the best-fit carrier profile to the implanted dose, ϕ

$$\eta = N_c D_I / \phi \qquad (10)$$

This gives values of 64% for an implant dose of 2×10^{15} cm⁻². Fig. 3 shows computer-generated IR refelction spectra for $N_c = 1 \times 10^{20}$, 1×10^{19} , 1×10^{18} , 1×10^{17} and 1×10^{16} cm⁻³. It shows that when $N_{\rm c} < 1 \times 10^{17} \, {\rm cm}^{-3}$, the IR reflection spectrum is insensitive to free-carrier plasma effects. Fig. 4 shows the IR reflection spectrum of the SOI sample. The full curve in Fig. 4 shows the results of fitting the reflection spectrum using the theoretical model. Also shown is the refractive index profile of the SOI samples as the fitting function. Parameter values for the best-fit curve in the figure are listed in Table II. It should be noted that the refractive index of silicon of the top layer of the SOI sample implanted with arsenic ions is larger than that of the SOI sample. Therefore, there is a defective top silicon layer after arsenic ion implantation and the RTA process [3].

4. Conclusion

Optical properties of the doped top layers of SOI structures have been studied. IR reflection spectra in the wave number range $1500-5000 \text{ cm}^{-1}$ were measured and interference fringes related to free-carrier plasma effects were observed. By detailed theoretical analysis and computer simulation of the IR reflection interference spectra with the model described in the text, the carrier concentration and mobility of the top layer were obtained. The calculated results show that the IR reflection spectra are very sensitive to the parameters of the model given in the text. Our investigation indicates that IR reflection interference spectra fitted with a suitable model are very useful and that is an effective method for analysis of the doped top silicon layer of SOI structures.

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