Rapid photoreflectance spectroscopy for strained silicon metrology

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We present an improved photoreflectance (PR) spectroscopy technique upon the prior art in providing a rapid acquisition method of the PR spectrum in a simultaneous and multiplexed manner. Rapid PR (RPR) application is the on-line monitoring of strained silicon. Shrinkage in the silicon bandgap is measured and converted to strain, using theoretical models. Experimental RPR results are in good correlation with Raman spectroscopy. © *2008 American Institute of Physics.*
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I. INTRODUCTION

Strained silicon (sSi) refers to silicon in which strain is engineered locally in a device structure or globally across a wafer by a local or global stress to accelerate electrons, which allows manufacture of faster devices.[1] Faster sSi transistors due to increased electron mobility and velocity have already been proven.[2] As a result, the technology of strain engineering is being widely used to speed carrier mobility in transistor channels in order to increase the drive currents.

Globally sSi on a wafer comprises a very thin layer of single-crystal silicon strained by pseudomorphic growth up to a critical thickness on a relaxed Si_xGe_{1-x} stressing layer of wider lattice constant dependent on the Ge mole fraction x. In all global sSi technologies with one exception, the strain in the silicon is described as biaxial, the result of two effects, namely, the expansion of the silicon lattice due to the wider lattice constant of the relaxed $Si_{1-x}Ge_x$ layer, which is tensile stressing it, and the contraction of the silicon lattice in the vertical direction because of its behavior as a near-perfect Poisson solid. These two strain effects, hydrostatic tension, and uniaxial compression, will be presently shown to be mirrored by two competing effects in the electronic band structure in the vicinity of the E_1 critical point of silicon, whose combined effect is measurable by photoreflectance[3] (PR) spectroscopy.

More recently, it has been demonstrated[4] that such a sSi layer can be transferred onto an SiO_2 buried oxide layer, using the SmartCut™ process technology of SOITEC, while retaining the strain to form a strained silicon-on-insulator (SSOI) wafer.

X-ray diffractometry (XRD) (Ref. 5) and Raman spectroscopy (RS) (Ref. 6) have been used for strain measurement in silicon. The former suffers from excessive measurement time, and the latter from resolution issues. PR spectroscopy[7] provides a useful alternative to XRD and RS to meet the requirements of substrate and device manufacturers for a nondestructive in-line strain metrology tool. In this letter, we report for the first time the application of a new method of PR, called rapid PR (RPR), on the measurement of strain in sSi with a high degree of accuracy in a sufficiently short time for application as an on-line production quality assurance tool.

PR is an optical modulation spectroscopy technique in which the reflectance of a material such as a semiconductor is altered significantly by means of the periodic photoinjection of charge carriers. The perturbation is optically applied by means of a modulated light beam, the so-called pump beam.

II. EXPERIMENTAL RESULTS AND MODELS

PR spectroscopy $(\Delta R/R)$ requires the simultaneous detection of a small modulated reflectance (ΔR) signal and a large time-invariant reflectance signal R. Even at parts of the spectrum where it is significant, ΔR is relatively small compared to the unmodulated reflectance (R), of the order of several to hundreds parts per million. Various sources of optical and electrical noises will be present and these dominate the ΔR signal. However, the ΔR signal is always present at the known modulation frequency and so methods of frequency-discriminating signal recovery are typically employed to detect a signal at this known frequency. Therefore, phase sensitive lock-in amplification was required for the measurement of the ΔR signal in PR spectroscopy and the measurement was to be made at different times for each wavelength, so that the $\Delta R/R$ spectrum was therefore generally recorded in a serial spectral mode. This limited the practical speed of the PR measurement and precluded its widespread industrial application in high-speed production line inspection of semiconductor wafers.

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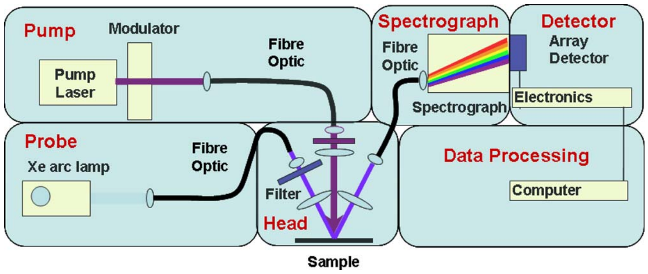

FIG. 1. (Color online) RPR setup showing the signal acquisition of all wavelengths in parallel.

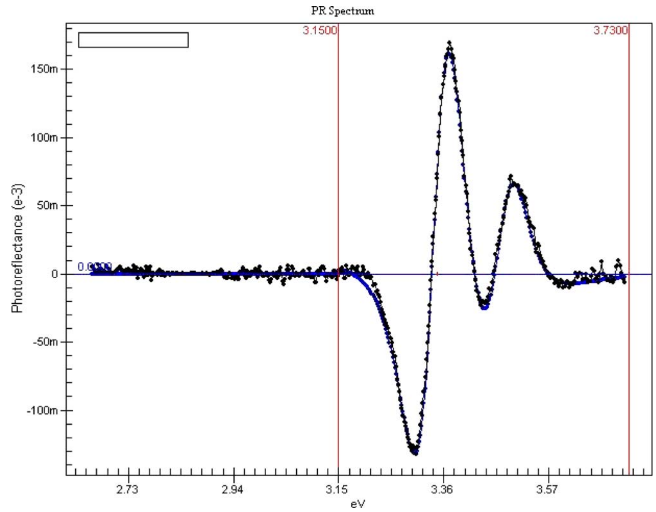

FIG. 2. (Color online) A typical RPR spectrum on 200 Å SSOI wafer. The blue line corresponds to the theoretical fit [Eq. (1)]. The goodness of fit is $R^2=0.995$. The acquisition time of the entire 512 pixels over the 2.7 to 3.6 eV is 10 s.

In this paper we present a RPR technique where the measurement time is 100 to 500 times faster than that of the conventional serial PR method. We overcame a major difficulty in the PR spectrum acquisition, namely, the slowness of the measurement. The main application of such development is the in-line measurement of strain in sSi wafers including SSOI and silicon-germanium on insulator. We measure the direct bandgap energy of the sSi layer and convert its value to strain using a theoretical model. Our results are also correlated with RS results.

Figure 1 describes the experimental setup of the RPR spectrometer. A probe light source generates an incident probe beam and directs it through optical components onto a sample. The modulated reflected probe beam is filtered down to the bandpass region of the spectrum in the region of the E_1 transition of silicon at approximately 3.4 eV, routed to the sample as a blue-UV beam through optical components including fiber optics and, after reflection from the sample, is dispersed into its constituent wavelengths by a spectrograph. The dispersed wavelengths are detected by an array of probe beam detector pixels, each detector pixel detects light from a narrow range of the constituent wavelengths of the probe beam such that the entire array of detector detects light over a broader wavelength range of the probe beam. The light signal can be measured simultaneously by multiplexing the readout using a sufficiently fast electronics system to read the signal from each detector at a sampling rate sufficiently fast to provide multiple samples of the modulated reflectance during a single modulation cycle.

The pump beam is modulated by a mechanical chopper. The electronics system is capable of reading the modulated reflectance ΔR signal as well as the unmodulated reflectance R signal from each pixel of the detector array in sufficiently rapid succession such that multiple measurements of the ΔR signal can be made within a single period of the modulation cycle. In this way, the system allows the simultaneous measurement of the PR signal at all wavelengths in parallel by means of multiplexing the readout. The acquisition time for the entire spectrum is approximately 1.03 ms; this acquisition is averaged at a few thousand times in order to improve the signal to noise ratio, depending on the measured structures.

Figure 2 shows a typical RPR spectrum recorded on a typical nominal 200 Å top (strained) silicon layer thickness SSOI wafer[7] acquired during 10 s. The spectrum is measured over the spectral range of the Si direct bandgap energy which is 2.8 to 3.7 eV and is fitted to a summation of two low field PR line shapes, each modeled using the approximation due to Aspnes known as the "third derivative functional form",[8] in which the critical point dimensionality is 2-d, and index parameter $m=3$:

$$\frac{\Delta R}{R}_{\mathrm{PR}}(E) = \mathrm{Re}[Ae^{i\theta}(E - E_g + i\Gamma)^{-3}]. \quad (1)$$

This is an appropriate model given the negligible electro-optic effect and absence of the Franz–Keldysh oscillations in the silicon PR spectra. In Eq. (1), A is an amplitude factor, θ is a line shape phase factor, E_g is the bandgap energy, and Γ is the broadening energy parameter. The fitted parameters results are summarized in Table I. The two transitions measured by fitting the RPR spectrum correspond to the light hole (LH) and heavy hole (HH) direct bandgaps. According to the theory,[9] the hydrostatic tensile strain shifts the interband transition (L band) energy, and the compressive uniaxial strain along the normal to the wafer lifts the degeneracy of the valence band, leading to split LH and HH bands, and a splitting of the transition occurs.

The behavior of the energy shift of the E_1 and associated transitions under hydrostatic strain and the splitting in the

TABLE I. Fitting parameter results of Eq. (1).

A_{LH} (a.u.)	θ_{LH} (rd)	E_{LH} (eV)	Γ_{LH} (meV)	A_{HH} (a.u.)	θ_{HH} (rd)	E_{HH} (eV)	Γ_{HH} (meV)
0.126	3.5	3.346	84	0.054	3.6	3.476	86

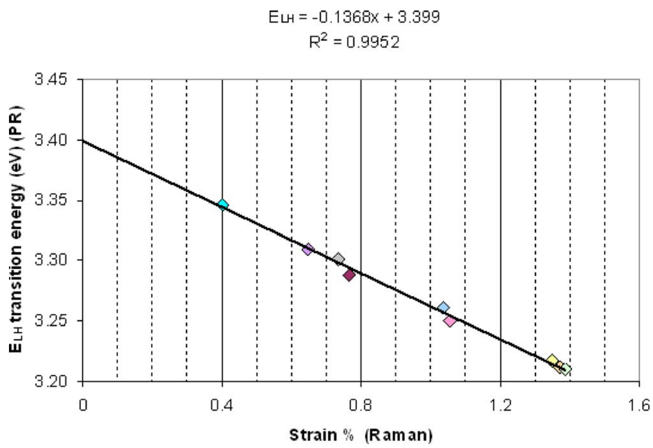

FIG. 3. (Color online) LH direct energy gap measured by RPR as a function of strain measured by RS.

energy shift due to the uniaxial strain contribution have been described[10] by a relationship based on extensive analysis of the electroreflectance response of silicon under uniaxial stress.

$$\Delta E = \sqrt{1/3}D_1^1(\varepsilon_\perp + 2\varepsilon_\parallel) \pm \sqrt{2/3}D_3^3(\varepsilon_\perp - \varepsilon_\parallel), \tag{2}$$

where $\pm$ sign is applied as + to obtain the shift in the HH and LH branches, $\varepsilon_\perp$ is strain along [001] direction (perpendicular to growth), and $\varepsilon_\parallel$ in-plane strain. Also D_1^1 is the hydrostatic deformation potential, measured by Kondo and Moritani[10] as −9.8 eV, and D_3^3 is the intraband strain deformation parameter along [001], having a value of 4.7 eV. The relationship may therefore be rewritten as

$$\Delta E = -5.658(\varepsilon_\perp + 2\varepsilon_\parallel) \pm 3.837(\varepsilon_\perp - \varepsilon_\parallel). \tag{3}$$

The (001) strain tensor elements take the form[8]

$$\varepsilon_{xx} = \varepsilon_{yy} = \varepsilon_\parallel = \frac{a_0(\mathrm{Si}_{1-x}\mathrm{Ge}_x) - a_0(\mathrm{Si})}{a_0(\mathrm{Si})}, \tag{4}$$

$$\varepsilon_{zz} = \varepsilon_\perp = -2\frac{C_{12}}{C_{11}}\varepsilon_\parallel, \tag{5}$$

$$\varepsilon_{xy} = \varepsilon_{xz} = \varepsilon_{yz} = 0, \tag{6}$$

where x is the germanium concentration, C_{11} and C_{12} are the elastic constants, and the Bir–Pikus Hamiltonian for a G_1 type band has the form[11]

$$a_0(\mathrm{Si}_{1-x}\mathrm{Ge}_x) = a_0(\mathrm{Si}) + 0.200\,326x(1-x) + [a_0(\mathrm{Ge}) - a_0(\mathrm{Si})]x^2. \tag{7}$$

Therefore the lower energy branch of the split transition shifts according to

$$\Delta E = E_{\mathrm{LH}} - 3.4 = -0.1375\varepsilon_\parallel(\mathrm{eV}), \tag{8}$$

where $\varepsilon_\parallel$ is expressed in percentage strain (dimensionless). As a result, the strain value is calculated using the bandgap shift of the E_{LH} transition compared to the unstrained silicon direct bandgap (3.4 eV), in that particular case we found 0.395%. It is conventional to quote the tensile strain in the plane of the wafer.

Note that in order to check the consistency of our strain measurements, the RPR results were compared to RS. A series of sSi wafers with different thicknesses and growth conditions were measured by RS and RPR. Figure 3 shows the LH bandgap energy measured by RPR as a function of the strain value measured by RS. The actual calibration against the range of RS values gives a calibration result of 3.399 and −0.1368 eV as unstrained silicon bandgap and conversion factor, respectively. These values are well within the range permitted by the experimental error in the determination of the deformation potentials.

III. CONCLUSION

In conclusion, we have demonstrated the capability of the PR technique to measure the tensile in-plane strain in biaxially strained SSOI wafers. A decrease in the acquisition time by a factor of 100 to 500 was achieved making this a nondestructive technique suitable for in-line sSi metrology. A decrease and split (E_{LH} and E_{HH}) in the silicon bandgap are observed upon tensile strain. Based on theoretical models, the *e*-LH transition (E_{LH}) value is converted to biaxial tensile strain, which is in good agreement with RS results.

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