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ELLIPSOMETRIC STUDY OF Si_{1-x} Ge_x ALLOY

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ABSTRACT

A report on ellipsometric studies of $Si_{0.5}$ $Ge_{0.5}$ and $Si_{0.7}$ $Ge_{0.3}$ thin films is described. The samples were earlier prepared from SiGe disks of 3" diameter using RF magnetron sputtering and the films were deposited onto glass substrates at room temperature. Some of the optical properties were investigated using an ellipsometer. In this method, we investigate the changes in refractive indices, *n* and extinction coefficients, *k* with film thickness as well as the relevant dielectric constant, ε. The results showed that, at a wavelength of 632.80 nm, *n* was found to increase with an increase of the germanium contents.

INTRODUCTION

Recently, the properties of alloys of silicon and germanium have become the subject of a great deal of interest [1]. Electronic devices incorporating strained epitaxial films of that material can be much faster than devices that exclusively use silicon [2]. The film can be grown by molecular beam epitaxy (MBE) or by ultrahigh vacuum chemical vapor deposition (UHVCVD). Since the 1960's, several studies of the optical parameters of SiGe alloys have been performed [3]. Using SE (spectroscopic ellipsometry), Humlicek *et al.* [3] have produced a series of pseudodielectric ($\varepsilon=\varepsilon_1 + \varepsilon_2$) functions for a number of bulk $Si_{1-x}Ge_x$ alloys with composition x = 0.22, 0.39, 0.51, 0.64, 0.75, 0.83, and 0.91, and determined the critical point energies by fitting the numerically differentiated dielectric functions.

The purpose of this paper is therefore to present an ellipsometric studies of SiGe film on glass substrates. Ellipsometer (DRE EL X-02C) was used to measure ψ and Δ at a wavelength 632.8 nm and a nominal incident angle of 70^o. An ellipsometric measurement yields ψ and Δ, which are the intensity ratio and the phase difference between the *p* and *s* directions (parallel and perpendicular to the plane of incidence, respectively) when quasi-monochromatic light reflects at a surface [4]. The refractive index of the glass substrate is known (1.5116-0.0000*i*) [5]. The unknowns are the real and imaginary part of the refractive index and film thickness.

EXPERIMENTAL METHOD

Thin films of $Si_{1-x}Ge_x$ alloys of different compositions x were prepared from SiGe disks of 3" diameter using a sputtering unit (NEVA) in Ar atmosphere. Before admitting Ar into the sputtering chamber, it was pumped to a pressure of 10^{-5} Torr using an oil diffusion pump. The argon pressure was maintained at 7.5×10^{-3} Torr. Sodium glass was used as substrates. They were chemically cleaned and, after mounting in the sputtering chamber, they further cleaned by plasmaglo for 10 min before deposition. A

99.999 % purity targets of $Si_{0.5}\,Ge_{0.5}$ and $Si_{0.7}\,Ge_{0.3}$ were used. The films were annealed for 1 hour at 500 °C in argon environment at atmospheric pressure. The composition was determined on selected samples by Energy Dispersive X-ray Fluorescence Spectrometry (EDXRF) and X-Ray diffraction, to provide a correlation to ellipsometry measurements.

Ellipsometer was operated under oblique incidence in reflection configuration (sometimes in *T* configuration). It always needs very smooth films and substrates of homogeneous thickness and composition. In some cases, a small roughness will not disturb the measurement and could be taken into account in the calculation. The complex effective dielectric function ε of the composite films can be calculated by solving the implicit system of the two Fresnel formulae describing *R* and *T* as functions of complex index, *n,* thickness *d*, and wavelength λ:

$$R = f\,(n, k, d, \lambda), \quad T = g\,(n, k, d, \lambda)$$

or similarly with Δ and for ψ ellipsometric measurements [6].

The ellipsometer used in these experiments is an automated rotating compensator ellipsometer in the polarizer-sample-compensator-analyzer (PSCA) configuration. A He-Ne laser (632.8 nm) was used as a light source, and a photomultiplier tube as a detector. The ellipsometry was done using an incidence angle of 70 °C. Calculated (Δ, ψ) trajectories were fitted into ellipsometry measurements to estimate the refractive index. The refractive index of the glass substrate was taken to be 1.5116-0.0000*i*. The submonolayer Ellipsometer EL X-02C is an optical instrument, which can measure the change of polarization of laser light after reflection at a surface with highest precision and accuracy. By use of a new measurement algorithm the instrument is especially useful for the measurement of submonolayers. This ellipsometer uses the Minsearch Algorithm which is based on a very fast error corrected stepper motor with 360 000 steps/rotation. The absolute precision of the stepper motor is 0.002° (this is about 100 times better precision than the precision of an uncorrected stepper motor). The maximum speed is 720 000 steps/s.

Ellipsometry measures the change in the polarization state of a linear polarized incident light beam upon reflection from the sample surface. The experimentally measured parameters are tan ψ and cos Δ, defined by [4];

$$\tan\psi = |\rho|; \Delta = \arg\rho; \rho = \frac{R_p}{R_s}$$

where R_p and R_s are the sample's complex reflection coefficients for parallel and perpendicular (to the plane of incidence) polarized light. Tan ψ and cos Δ are measurements of amplitude ratio and phase differences respectively, between the p and s components of polarized light reflected from the surfaces.

The dielectric function ε, the refraction index (n) and the absorption coefficient (k) can be directly obtained from the measurements of ρ with the following relations [4];

$$\varepsilon = \left[1 + \left(\frac{1-\rho}{1+\rho}\right)^2 .\tan^2\Phi\right].\sin^2\Phi$$

$$\varepsilon = \varepsilon_1 + i\varepsilon_2\,;\ \varepsilon_1 = n^2 - k^2\,;\ \varepsilon_2 = 2nk.$$

where ε_1 and ε_2 are the real and imaginary parts [4].

The principle of Minsearch-Ellipsometry is shown in Fig. 1. A nearly linear polarized laser beam passes polarizing components, hits the sample, passes the polarizing prism that is mounted on the hollow shaft of a stepper motor and hits the detector. The sample substrate and the thin layer on the sample influence the state of polarization of the

reflected beam. Fig. 2 shows the state of polarization of an elliptical polarized light wave.
:race of the field strength vector shows
:s *Ellipticity* ε and *Orientation* θ.

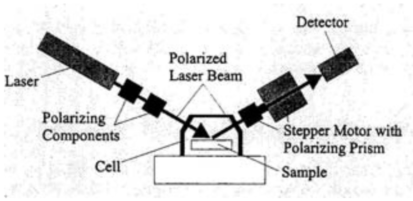

Fig.1: Principle of Minsearch-Ellipsometer

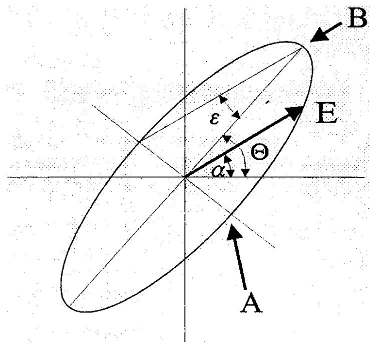

Fig.2: Elliptical polarization of a light wave

RESULTS AND DISCUSSIONS

The most common optical functions include, for any photon energy ħω or wavelength λ, the complex dielectric function $\varepsilon = \varepsilon_1 + \varepsilon_2$ and the complex refractive index $N = n+ik = \sqrt{\varepsilon}$. The dielectric function links the macroscopic electric displacement D and field E via D = εE = E + 4πP, where P is the induced dipole-moment density. Since the polarization (measured by P) due to different physical mechanisms is approximately additive, ε is the appropriate function to deal with an additional polarisability superposed on the intrinsic background (such as plasma of free carriers in doped materials or impurities). The complex refractive index is useful to describe the wave propagation, including the reflections at interfaces of layered structures. The intensity of a wave traversing a distance d in a homogenous medium of extinction coefficient k is attenuated by the factor exp (-K*d*), where K = $4\pi k/\lambda$ is the absorption coefficient. Thus, 1/K is a convenient measure of the penetration depth [7].

Δ and ψ values of each SiGe-layer were obtained for two different stoichiometries. Figure 3(a) and (b) shows an example of the Δ-ψ plot simulation diagram of such a layer system for $Si_{0.7}Ge_{0.3}$ and $Si_{0.5}Ge_{0.5}$ respectively. The color of the simulation curve will change for every 10 nanometer. Experimental results of Δ and ψ for sample $Si_{0.7}Ge_{0.3}$ are shown in Fig. 3(a); the results for $Si_{0.5}Ge_{0.5}$ are very similar. The points denote the measurement data, the full curve represents a simulation based on a single-layer model. By analyzing a number of Δ-ψ curves corresponding to the films of different germanium content, the complex refractive index of the material as a function of wavelength can be obtained. No error analysis can be made with this diagram since Δ and ψ describe the sample behavior and not the measurement system. The errors of the different ellipsometer types can be directly analyzed from a corresponding $\Theta = f(\varepsilon)$ diagram.

For calculation, the substrate index is taken as $\acute{N}$ = 1.5116-0.0000*i*. The obtained values of the complex dielectric function $\varepsilon_1 + \varepsilon_2$, and complex refractive index n + *i*k are listed in Table 1. The fourth and fifth columns show the measured ellipsometric data Delta (Δ) and Psi (Ψ) whereas the 9th column displays the layer thickness, *d* in nanometer.

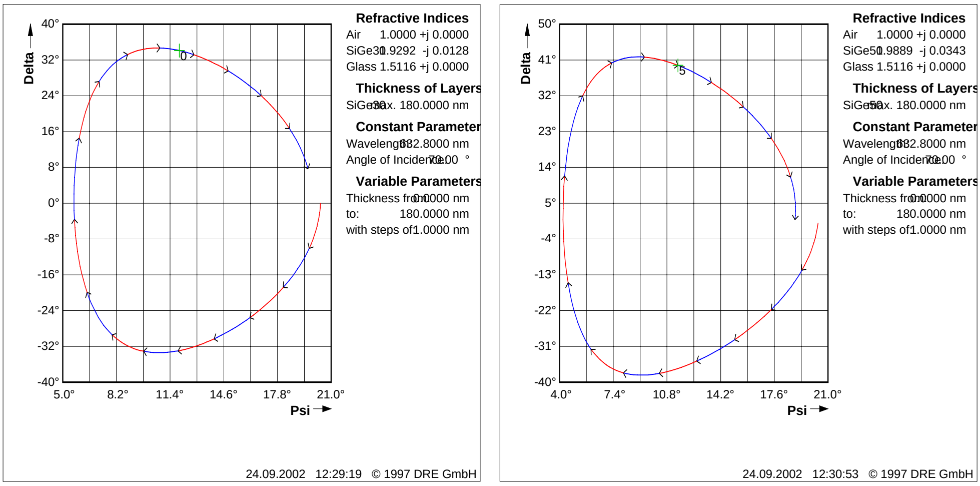

Figure 3: (a) Si0.7Ge0.3 and (b) $Si_{0.5}Ge_{0.5}$ on glass - Simulation of layer thickness dependent of Δ and ψ. The color of the simulation curve changes for every 10 nm.

Column 5 in Table 1 shows the differences of refractive index, *n* at 1.96 eV of SiGe films on glass substrate as a function of germanium content. It is clear from column 5 that the real <n> part of complex refractive index increases as a function of germanium content, *x*. Here, the real part of refractive index for $Si_{0.7}Ge_{0.3}$ and $Si_{0.5}Ge_{0.5}$ layer system was obtained in the range of (1.9154-1.9292) and (1.9714-1.9889) respectively. Results from XRD suggest that the increases in the values of the reflection may due to the SiGe layer that was not completely changed to alloys, as seen in very weak peaks. From the XRD spectrum (to be published), the result shows that amorphous film is formed when deposition temperature is low (<500 ºC), however polycrystalline film could be obtained when heat-treatment is applied (500 ºC).

From column 7, we observe that ε_1 increases with the Ge content. The value of ε_1 and ε_2 for SiGe thin films obtained in the present experiment show that real part of dielectric function, ε_1 is in the range of 3.668757 to 3.721649 for $Si_{0.7}Ge_{0.3}$ and 3.886417-3.954547 for $Si_{0.5}Ge_{0.5}$. The dependence of the estimated refractive index and dielectric constants of $Si_{1-x}Ge_x$ on the Ge fraction is compared with previous work on bulk, primarily polycrystalline $Si_{1-x}Ge_x$ [7]. The XRD results suggest the inconsistent values compare to previous research. The lower values observed occasionally on $Si_{1-x}Ge_x$ alloys are likely to be due to the scattering of the probing beam on inhomogeneties of the composition (and, consequently, refractive index), which directs the part of transmitted light to pass the detector.

Column 9 shows the average thickness of both samples with different Ge content. It can be seen that the average thickness of $Si_{0.5}Ge_{0.5}$ was 131.6498 nm while average thickness for $Si_{0.7}Ge_{0.3}$ was found to be 138.04824 nm. The results shows that the effects of SiGe alloys are highly influenced by the growth temperature that can be controlled by preparation condition and post annealing, and also composition and thickness of the films.

There are currently two available databases for $Si_{1-x}Ge_x$ in the literature [3,7]. J. Humlicek *et al.* [3] have published the results of measurements of bulk $Si_{1-x}Ge_x$ grown by the Czochralski method (heated 1500 °C) and also of thick films grown by liquid-phase epitaxy. The ellipsometric technique has been used to measure the $Si_{1-x}Ge_x$ alloys throughout the whole composition range [3]. However, there is a variation between a sample grown on a silicon substrate and another sample of similar composition grown on a glass substrate. Therefore, in our analyses, Ref. [3] spectra taken from bulk sample will be used in which the author claimed that the optical properties of strained SiGe alloys on Si are quite different from those of the unstrained alloys while for bulk sample measurement. The real refractive index of relaxed $Si_{1-x}Ge_x$ as a function of x can be measured by;

$n = 3.42 + 0.37x + 0.22x^2$ and

$k = 0.094 + 0.033x + 0.089x^2$.

As compared to present experiments, the results show that the surface film of SiGe is of lower refractive index than the bulk and thus, it is noted that the points lie off the theoretical curve. Further improvements may be realized through variations in composition ($0<x<1$) using Si substrate and growth temperatures up to 550 °C.

Table 1 : List of measurement data

No	Information	Δ/°	Ψ/°	*n*	*k*	ε_1	ε_2	Thickness/ nm
1	$Si_{0.7}Ge_{0.3}$	34.108	11.9492	1.9292	0.0128	3.721649	0.049388	136.2517
2		33.9612	11.9515	1.9161	0.0062	3.671401	0.02376	138.3796
3		34.0000	11.9539	1.9170	0.0078	3.674828	0.029905	138.5695
4		34.0835	11.9486	1.9154	0.0000	3.668757	0.00000	138.8421
5		33.9625	11.9521	1.9201	0.0033	3.686773	0.012673	138.1983
6	$Si_{0.5}Ge_{0.5}$	39.6544	11.498	1.9889	0.0343	3.954547	0.136439	129.9701
7		39.6578	11.4982	1.9735	0.0085	3.89463	0.03355	131.6980
8		39.6612	11.5013	1.9732	0.0075	3.893462	0.029598	132.0364
9		39.6567	11.4957	1.9714	0.0007	3.886417	0.00276	131.7907
10		39.6493	11.5000	1.9744	0.0111	3.898132	0.043832	131.3297

CONCLUSION

To conclude, the complex refractive index at the wavelength 623.8 nm (1.96 eV; red line of He-Ne laser) of SiGe films on glass substrates has been determined as a function of Ge fractions of x using submonolayers ellipsometry. We find the real part of the refractive index to change with increasing germanium content. It is to be emphasized that the accuracy of the measurement is specific to a sample. It may be seen from the theoretical curves that this depends very much on the optical thickness of the surface film and the substrate refractive index.

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