Nondestructive Characterization of Semiconductor Multilayers

Christopher Pickering

This article reviews the use of spectroscopic ellipsometry (SE) for determining layer thicknesses, compositions, and surface and interface roughness of complex multilayer structures. An indirect technique, SE relies on an accurate database of dielectric functions and cross-correlation with destructive techniques. Examples shown here use recent data on strained and relaxed \( \text{Si}_{1-x} \text{Ge}_x \), strained and relaxed \( \text{In}_{x} \text{Ga}_{1-x} \text{As} \), and unstrained \( \text{In}_{1-x} \text{Al}_{x} \text{As} \), obtained from single epilayers, to analyze SE data from both lattice-matched and pseudomorphic multilayer structures. The SE method has great potential for in-line and in-situ use, leading ultimately to real-time process control.

INTRODUCTION

Advanced semiconductor materials and complex multilayer structures are under study for improved device performance and incorporation of novel optoelectronic functions into microelectronic systems. For ultimate performance, precise control is required of layer parameters such as thickness, composition, interface sharpness, etc. These are conventionally assessed by destructive, time-consuming methods on selected monitor wafers. Research is now under attention since they are noninvasive, and can be used in any way to develop rapid, nondestructive techniques that can be used in-line to characterize each wafer after each process or control it in real time.

Optical techniques are receiving much attention since they are noninvasive, nondestructive, and can be used in any transparent ambient. Ellipsometry has the advantage of high sensitivity due to the measurement of the phase of the reflected light and, since it is inherently a double-beam technique, it is relatively unaffected by instrumental drift due to source fluctuations, etc. Because the penetration depth of the optical probe is a strong function of the wavelength, spectroscopic ellipsometry (SE) can provide information on thicknesses of several layers in multilayer structures, as well as compositions and strain through measurement of critical point transition energies, and surface or interface roughness. This review will introduce the theoretical basis and experimental technique and indicate how the parameters of interest are extracted by modeling the experimental data. Since SE is indirect, it relies on an accurate database of reference dielectric functions and cross-correlation with destructive techniques, such as cross-sectional transmission electron microscopy (XTEM), Rutherford backscattering (RBS), and x-ray diffraction (XRD), to validate the information obtained, particularly for new materials. Examples of this approach will be given for III-V and Si-based alloy multilayer systems. The use of SE for in-situ monitoring and control will also be discussed.

THEORETICAL BACKGROUND

Figure 1 shows a linearly polarized light beam incident at a surface at an oblique angle of incidence, \( \phi \). In general, the reflected light has phase changes that are different for electric field components polarized parallel (p) and perpendicular (s) to the plane of incidence, resulting in elliptically polarized light. Ellipsometry measures this state of polarization, and theoretical modeling is then used to determine dielectric functions and thicknesses of the reflecting structure. Further modeling of the dielectric function data gives information on compositions, strain, etc.

Ellipsometry measures the complex reflectance ratio, written as

\[
\rho = \frac{r_p}{r_s} = \tan \psi \exp(i\Delta)
\]

where \( \psi \) and \( \Delta \) are the amplitude ratio and phase difference, respectively, of the p and s components and are the ellipsometric parameters (often given as \( \tan \psi, \cos \Delta \)) measured as described in the next section. The reflectance coefficients are directly related to the optical constants of the surface by assuming the ambient is air \( (n_{\text{air}} = 1) \),

\[
\begin{align*}
\hat{r}_p &= \frac{n \cos \phi_s - \cos \phi}{n \cos \phi_s + \cos \phi} \\
\hat{r}_s &= \frac{\cos \phi_s - n \cos \phi}{\cos \phi_s + n \cos \phi}
\end{align*}
\]

where \( n = n + i k \) is the complex refractive index. The angle of refraction may be obtained using Snell’s Law,

\[
sin \phi_i = n_{\text{air}} \sin \phi_t
\]

Thus, if the sample is an ideal bulk, the real and imaginary parts of the complex refractive index or the dielectric function, \( \varepsilon = \varepsilon_1 + i \varepsilon_2 \), may be calculated from the measured \( \Delta \) and \( \psi \) values and a knowledge of the incidence angle, using

\[
\hat{\varepsilon} = \hat{n}^2 = \sin^2 \phi \left\{ 1 + \tan^2 \phi \left[ (1 - p)/(1 + p) \right] \right\}
\]

\( \hat{n} \) and \( \hat{\varepsilon} \) are simply related by

\[
\varepsilon_1 = n^2 - k^2 \quad \text{and} \quad \varepsilon_2 = 2nk
\]

Unfortunately, real materials are not ideal and there is usually at least an overlayer present consisting of a native oxide or roughness. In this situation, the determined \( \hat{\varepsilon} \) is the pseudo-dielectric function, written \( \langle \varepsilon \rangle = \varepsilon_{\text{eff}} + i \varepsilon_p \), which is a mathematical representation of a uniform material with the same optical properties as the composite.
The situation is more complex. A physically rough interface, where there is no atomic intermixing, can be represented by the Bruggeman effective medium approximation (EMA). In this case, the effective $\varepsilon$ is obtained from

$$f\left(\frac{\varepsilon - \varepsilon_m}{\varepsilon_0 + 2\varepsilon_m} + \frac{\varepsilon - \varepsilon_0}{\varepsilon_0 + 2\varepsilon_0} + \ldots = 0 \right) \quad (8)$$

where $f_1$, $f_2$, etc., are volume fractions of constituent phases, $a$, $b$, etc., with $f_a + f_b + \ldots = 1$. The EMA also may be used to model a rough surface as a mixture of the bulk material with voids. If the mixing is on an atomic scale, however, as in a true alloy, the EMA cannot be used. This is because alloying produces a change in the band structure and shifts in the energy gaps, or critical point (CP) transition energies. This is illustrated in Figure 2, which shows reference spectra for strained Si$_x$Ge$_{1-x}$ obtained by SE. The peaks in the spectra are due to strong absorption occurring at $E_1$, $E_1 + \Delta_1$ ($E_1^\text{Si}$) transitions near 3.25 eV and $E_2$, transitions at 4.25 eV. The $E_1$, $E_1 + \Delta_1$ peaks move monotonically to lower energy with increasing $x$. A physical mixture of Si and Ge using the EMA would produce $\varepsilon$ spectra with two $E_1$ peaks at the energies characteristic of the constituents. To represent an alloy, an interpolation procedure is used based on polynomials for the variation of each CP as a function of composition. Reference spectra at discrete compositions are required, and then $\varepsilon$ spectra for arbitrary compositions can be obtained by averaging the two spectra closest in composition, above and below $x$. A nonlinear shift of their energy scales brings each CP into coincidence with the database, the composition of a layer may be obtained as an additional fitting parameter. The CP peaks strongly depend on crystallinity, doping, and temperature. The sharp peaks indicate crystallinity, and very high doping, $\sim 10^{12}$ cm$^{-3}$, also causes broadening.

Spectroscopic ellipsometry owes its ability to measure buried interfaces to the variation in penetration depth with wavelength, as shown in Figure 3 for crystalline Si(c-Si). The minimum penetration depth in the ultraviolet near the $E_1$ and $E_2$ CPs is $\sim 100$ Å since the absorption coefficient ($\alpha = 4\pi k/\lambda$) is $\sim 10^4$ cm$^{-1}$. This is typical for direct transitions away from the Brillouin zone center, which occurs at similar energies for III-V compounds. At energies below $E_1$, the penetration depth increases rapidly to several µm in c-Si and to $\sim 1$ µm at $E_0$, the fundamental energy gap at $\Gamma$, which occurs at $\sim 1.45$ eV in GaAs, for instance. The absorption coefficient is $\sim 10^4$ cm$^{-1}$ for $E_0$ and it can be observed weakly. In c-Si the fundamental gap is indirect with $\alpha \sim 10^4$ cm$^{-1}$, which is too weak to be observed. Thus, a useful approach to data analysis is to fit short-wavelength data with a model incorporating the surface layer with an oxide or roughness overlayer, then to extend the fit for longer wavelengths to incorporate buried layers. The simplest model should be used with abrupt interfaces. The quality of the fit will then indicate if interface layers are required. One must investigate by simulations the sensitivity of the spectra to the parameters to avoid correlations that can occur in over-complex models.

**EXPERIMENTAL TECHNIQUE**

Commercially available automatic wavelength-scanning SE instruments use a rotating prism (polarizer or analyzer) or a photoacoustic modulator (phase-modulation ellipsometry) to modulate the intensity of the reflected beam. A typical arrangement based on a rotating polarizer is shown in Figure 4. The angle of incidence can be varied over the angle range 45–80°, but 75°, close to the pseudo–Brewster angle, usually gives highest sensitivity. The source is a broad-band xenon lamp. A 3 mm diameter beam with $<0.5$ mrad divergence is produced by a system of mirrors and passes through a quartz Rochon polarizer. The reflected beam passes through a Glan–Taylor calcite analyzer and is focused onto the entrance to an optical fiber connected to a 0.75 m prism/grating monochromator with typical resolution $0.5$ Å at $\lambda = 300$ nm. The detector is a photon-counting multi-alkali photomultiplier operating over the range 240–930 nm. A linearly polarized beam is produced by the polarizer, which after reflection is generally elliptically polarized. The intensity after the fixed analyzer produced by the polarizer rotating at 40 Hz is a sine wave given by

$$I(t) = I_0 \left(1 + \frac{\alpha}{2} \cos 2\pi t + \beta \sin 2\pi t\right) \quad (9)$$