Brewster angle spectroscopy: A new method for characterization of defect levels in semiconductors

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A new optical method which allows the identification of electronic defects in semiconductors is presented. Deep level characterization is done by detecting changes of the Brewster angle induced by optically excited transitions involving defects. An empirical model is developed which correlates the minima of the derivative of the Brewster angle as a function of photon energy with the energetic locations of defects in the semiconductor gap. Contactless room-temperature measurements on n-GaAs (100) and p-InP (111) clearly reveal defects with high accuracy, including the well known EL2 and EL12 centers in GaAs. The applicability of the method for semiconductor device technology processes is discussed.

The analysis of electronic defects is of crucial importance for semiconductor materials development. The need for deep level characterization in electronic devices and their components has led to the establishment of a series of detection methods. Among those, techniques such as deep level transient spectroscopy (DLTS),14 photocapacitance spectroscopy (PCS),5-7 electroreflectance (ER)5,8 and photoluminescence (PL)5,10 require either sample contacting or cooling. Other methods, for instance, electron spin resonance (ESR),11-13 photoreflectance,14 photothermal deflection spectroscopy15 and standard reflectivity measurements are limited in sensitivity and/or applicability.

The technique presented here is based on the optical properties of semiconductors below the band-gap energy. If, in a first approximation, the semiconductor is viewed as a dielectric in this energy range, the reflectivity for light polarized parallel to the plane of incidence should vanish. The presence of an absorbing defect can be mathematically modeled as a harmonic oscillator, influencing the reflectivity $R_p$ and the Brewster angle $\phi_B$. The calculation performed below shows that for a given oscillator strength, the changes in $\phi_B$ are larger than in $R_p$. Therefore, a measurement of $\phi_B$ versus photon energy is characterized by a higher sensitivity.

The influence of an absorbing center on $R_p$ and $\phi_B$ can be calculated assuming Lorentz oscillatory behavior.16,17 For the complex dielectric constant

$$\tilde{\varepsilon} = \varepsilon_1 - i\varepsilon_2 = \varepsilon_{\infty} + \sum_{j} \frac{s_j}{\omega_j^2 - \omega^2 + i\omega \Gamma_j}$$  \hspace{1cm} (1)

where $\omega_j$: frequencies of the absorbing centers; $\Gamma_j$: damping; $s_j$: oscillator strength; the Brewster angle can be determined analytically and is described by the function $\phi_B = \arcsin \left( \frac{1}{\sqrt{\varepsilon_1}} \right)$ which will be given in the appendix. For comparison of the change in $\phi_B$ and the change in $R_p$ we also give the analytical relationship of $R_p = R_p(\varepsilon_{\infty}, \omega_B, \omega)$ in the Appendix.

Figure 1 shows data obtained by incorporation of a simulated defect in a semiconductor band tail region. The data were calculated using several Lorentz oscillators at $E_g = 1.56$ eV (band gap) and above to simulate typical semiconductor behavior such as for GaAs. A small oscillator (defect center) with an oscillator strength $s = 5 \times 10^{-5}$ and a damping of $\Gamma = 50$ meV at 0.75 eV.
The defect contribution is assumed to be almost undetectable in the ε2 spectrum [Fig. 1(a)]. The calculation shows that the minimum of $d\phi_E/dE$ reveals the energetic position of the defect level at 0.75 eV. For higher detection sensitivity, we suggest to use the second derivative $d^2\phi_E/dE^2$, where the inflection point identifies the defect level position $E_D$. [Figs. 1(e) and 1(f)]. The spectral changes in $R_p$ also displayed in Fig. 1(c) are seen to be smaller than those in $\phi_E$ [Fig. 1(d)].

The experimental arrangement is schematically shown in Fig. 2. As a light source a tungsten iodine lamp with a Kratos monochromator was used. The light beam is split into a reference and a signal channel, detected at $D_1$ and $D_2$, respectively. The signal beam is polarized parallel to the plane of incidence, using a Glan–Thompson polarizer $P$. The polarized light is focused onto the sample held at an angle $\phi$ close to the Brewster angle $\phi_B$. The reflected intensity is detected by a cooled Si-(0.4–1 μm) or Ge detector (0.8–1.7 μm). For analysis of the reflected intensity and the Brewster angle position, the signal at $D_2$ was measured as a function of the angle $\phi$. The minimum was determined by a least squares fit and the according reflectivity $R_p$ was determined by comparison with the signal at detector $D_1$. Standard lock-in technique was used for data analysis. The accuracy of the method depends critically on the angular resolution of the goniometer table on which the sample is mounted. The mechanical specification yields a resolution better than $2 \times 10^{-3}$ deg. The step motor limitation results in a resolution of $4 \times 10^{-3}$ deg. To determine the first and second derivative of the measured Brewster angle spectra a specific algorithm based on a compensation parabola method (quadratic least square fit) was used.18

In Fig. 3, data recorded on n-GaAs (100) are displayed. For comparison the spectral dependence of $\phi_E$ itself is also shown in the figure. The inflection point of the second derivative of the Brewster angle with respect to the photon energy locates the energetic position of a series of levels, among them defects at the energetic position of the well known EL1,19 and EL2 centers.20 Additional levels determined by photocapacitance measurements6 are also reproduced with high accuracy.

Figure 4 gives an analogous dataset for InP(111). Here, too, the inflection point of $d^2\phi_E/dE^2$ determines $E_D$ with high accuracy as evidenced by comparison with literature data.21 It should be noted that two conditions have to be fulfilled simultaneously for unambiguous identification of $E_D$: inflection of $d^2\phi_E/dE^2$ and a minimum in $d\phi_E/dE$. The Brewster angle spectroscopy (BAS) allows the identification of deep levels in the semiconductors and insulators at room temperature. The method is particularly suited in areas where bulk semiconductors have to be analyzed as, for instance, materials preparation for photovoltaics and photoelectrochemistry. The limitations of the method with respect to number and/or concentration of absorbing centers cannot be estimated at present but it
appears that the sensitivity is among the highest compared to other deep level detection experiments. For development of semiconductor materials for photosensitive devices such as solar cells and detectors, BAS provides a powerful tool in the materials optimization process.

Appendix: The analytical expression for the Brewster angle in the case of a complex dielectric function is derived from the third order equation

\[ y^3 + \left( \frac{|\varepsilon|^4 - 3|\varepsilon|^2}{2|\varepsilon|^2 + 2\varepsilon_1} \right) y^2 - \left( \frac{|\varepsilon|^4}{|\varepsilon|^2 + \varepsilon_1} \right) y + a = 0 \]

with \( y = \sin^2 \phi_B \) and \( \alpha = \frac{|\varepsilon|^4}{2|\varepsilon|^2 + 2\varepsilon_1} \). The solution is straightforward and will be given elsewhere. The corresponding equation for the reflectivity, \( R_p \), is developed from the Fresnel equations:

\[ R_p = \frac{\mu + |\varepsilon|^2 \cos^2 \phi - \cos \phi (\mu + \sin^2 \phi) \sqrt{2(\mu + \kappa)}}{\mu + |\varepsilon|^2 \cos^2 \phi + \cos \phi (\mu + \sin^2 \phi) \sqrt{2(\mu + \kappa)}} \]

\[ \mu^2 = |\varepsilon|^2 - 2\varepsilon_1 \sin^2 \phi + \sin^4 \phi \text{ and } \kappa = \varepsilon_1 - \sin^2 \phi. \]

\( \phi \) denotes the angle of incidence.