Estimation of the dielectric properties of low-k materials using optical spectroscopy

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The dielectric function spectra of low dielectric constant (low-k) materials have been determined using spectroscopic ellipsometry, near-normal incidence spectroscopic reflectometry, and Fourier transform infrared transmission spectrometry over a wide spectral range from 0.03 to 5.4 eV (230 nm to 40.5 μm wavelength region). The electronic and ionic contributions to the overall static dielectric constant were determined for representative materials used in the semiconductor industry for interlayer dielectrics: (1) FLARE—organic spin-on polymer, (2) HOSP—spin-on hybrid organic-siloxane polymer from the Honeywell Electronic Materials Company, and (3) SiLK—organic dielectric resin from the Dow Chemical Company. The main contributions to the static dielectric constant of the low-k materials studied were found to be the electronic and ionic absorptions. © 2001 American Institute of Physics.
SiLK I—organic dielectric resin from the Dow Chemical Company. SiLK is an aromatic hydrocarbon polymer with a dielectric constant of 2.65. The low-\(k\) layers were prepared on single-crystal silicon wafers using the standard spin coating procedure. Other details have been reported in Refs. 11 and 12.

Spectroscopic ellipsometry, near-normal incidence spectroscopic reflectometry, and infrared transmission spectrometry were combined to determine the optical functions of the low-\(k\) materials over a wide spectral range 0.03–5.4 eV covering the ultraviolet, visible, near- and midinfrared regions. A computer controlled four-zone null ellipsometer was employed in the spectral region from 1.5 to 5.4 eV (230–840 nm wavelength region). The ellipsometric measurements were completed with near-normal incidence reflectometry in the spectral range from 0.5 to 6.5 eV (190 nm to 2.5 \(\mu\)m wavelength region) obtained using a double beam spectrometer (Shimadzu, UV-3100 PC). The simultaneous fit of ellipsometric and reflectivity data decrease the correlation between a layer thickness and parameters describing optical functions.11,14,15 The measured normal incidence transmission spectra were obtained using a Fourier-transform infrared spectrometer in the spectral region from 0.03 to 0.52 eV (247–4194 cm\(^{-1}\) wave number region).

In this study, we used a relative transmittance.12 The optical functions of the single-crystal Si substrate were taken from Ref. 16. The measured data were fitted to the model dielectric function

\[
\varepsilon(E) = \varepsilon_{1\times} + \frac{A E_1^2}{E_1^2 - E^2} + \sum_n \frac{A_n E_{0n}^2}{E_{0n}^2 - E^2 + i \Gamma_n E_{0n}},
\]

where the first term \(\varepsilon_{1\times}\) and the second Sellmeier term describe the dispersion in the visible and near-infrared regions. \(A\) and \(E_1\) denote the amplitude and the energy of the absorption peak outside the measured range. The sum of damped harmonic oscillators corresponds to the infrared absorption structure. For example, the \(n\)th absorption peak is described using amplitude \(A_n\), the Lorenz resonant frequency \(E_{0n}\), and the width \(\Gamma_n\).
and the broadening parameter $\Gamma_n$. The model dielectric function (2) exactly fulfills the Kramers–Kronig dispersion relations and gives the simple static limit:

$$\varepsilon(E \to 0) = \varepsilon_1 + A + \sum_n A_n.$$  \hfill (3)

We stress the main advantages of our spectroscopic data processing: (i) Dielectric function dispersion in the visible and near-infrared regions was parameterized using the Sellmeier term. Consequently, the electronic contribution to the static dielectric constant is equal to $\varepsilon_1 + A - 1$. An estimation of the electronic contribution as the square of the refractive index measured at a fixed wavelength in the visible range would be only rough approximation. (ii) The dielectric function in the infrared region was parameterized using the sum of damped harmonic oscillators [Eq. (2)], because the transmission is influenced by both the real $\varepsilon_1$ and imaginary $\varepsilon_2$ parts of the complex dielectric function. (iii) The measured infrared transmittance data were fitted to a model including incoherent reflections in the thick silicon substrate. (iv) The thicknesses of low-$k$ layers, used for infrared transmission data fits, were precisely obtained from a simultaneous fit of the ellipsometric and reflectivity data.

Figures 1, 2, and 3 show the dielectric function spectra obtained for FLARE, HOSP, and SiLK low-$k$ materials, respectively. The parameters obtained are listed in Tables I, II, and III including the layer thickness $t$ and the parameters from Eq. (2). According to Eq. (3), the static dielectric constant and its electronic and ionic contributions were estimated and summarized in Table IV for the low-$k$ materials studied. Figure 4 shows a comparison between the dielectric constants obtained using Eq. (3) and the values given by the manufacturers. The static dielectric constants obtained from the spectroscopic data for FLARE (2.78), HOSP (2.57), and SiLK (2.66) correspond very well to the values given by the manufacturers.

![Contributions to the dielectric constant](image)

**TABLE IV.** Electronic and ionic contributions to the static dielectric constants of the low-$k$ materials studied are shown. Values in brackets represent the contributions related to the value given by low-$k$ material manufacturers.

<table>
<thead>
<tr>
<th>Low-k material</th>
<th>$\varepsilon_1 + A - 1$</th>
<th>$\sum A_n$</th>
<th>Total dielectric constant</th>
</tr>
</thead>
<tbody>
<tr>
<td>FLARE (2.8)</td>
<td>1.70 (60.7%)</td>
<td>0.08 (2.9%)</td>
<td>2.78 (99.3%)</td>
</tr>
<tr>
<td>HOSP (2.5)</td>
<td>0.86 (34.4%)</td>
<td>0.71 (28.4%)</td>
<td>2.57 (102.8%)</td>
</tr>
<tr>
<td>SiLK (2.65)</td>
<td>1.63 (61.5%)</td>
<td>0.03 (1.2%)</td>
<td>2.66 (100.4%)</td>
</tr>
</tbody>
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**References:**