Reliability in Modeling of Spectroscopic Ellipsometry

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(Received September 19, 2000; accepted October 10, 2000)

Spectroscopic ellipsometry (SE) [1, 2] is a powerful non-destructive technique to determine the structure of silicon-based materials such as amorphous silicon (a-Si) and hydrogenated amorphous silicon (a-Si:H). In analyzing the SE spectra, the Bruggeman effective medium approximation (EMA) [3, 4] is usually used to model a thin film as a mixture of amorphous silicon and voids. In these models, however, precise knowledge of the dielectric functions of the various components is required in order to obtain reliable estimation of the structural parameters. This requirement is particular critical to the amorphous component because the structure of amorphous silicon is known to depend considerably on the preparation procedures [5]. So far, the dielectric functions used for modeling a-Si$_{1-x}$ :H$_x$ have been based on certain dielectric functions without consideration of the preparation method. It may not be clear, particularly for thin films of amorphous silicon prepared by novel method, whether it is relaxed or unrelaxed dielectric functions which are appropriate for the modeling. In the present work the scope of the problem is assessed by constructing dielectric functions for relaxed and unrelaxed a-Si$_{1-x}$ :H$_x$ thin films using measured a-Si dielectric functions, and fitting, respectively, using simulated dielectric functions for bulk unrelaxed and relaxed a-Si$_{1-x}$ :H$_x$ on the surface roughness and void concentration parameters.

The tetrahedron model [3, 4] is applied to construct the complex dielectric functions for relaxed ($\varepsilon = \varepsilon_{1r} + i\varepsilon_{2r}$) and unrelaxed ($\varepsilon = \varepsilon_{1ur} + i\varepsilon_{2ur}$) a-Si$_{1-x}$ :H$_x$, by using the dielectric functions for relaxed and unrelaxed a-Si [5], respectively. For details we refer to the work of Mui and Smith [3], [4]. The complex dielectric functions constructed for relaxed and unrelaxed a-Si$_{1-x}$ :H$_x$ components with various hydrogen concentrations are shown in Fig. 1. It is seen that the relaxed and unrelaxed spectra exhibit different peak position and amplitude. Moreover, as the hydrogen content increases, the complex dielectric functions shift to higher photon energy with lower peak values.

The complex dielectric functions for the relaxed (unrelaxed) a-Si$_{1-x}$ :H$_x$ film are constructed using a three-layer structure: the first layer is a surface roughness layer, modeled using the EMA, consisting of 50% voids, 50% layer 2. Layer 2 is modeled using the EMA, consisting of a mixture of relaxed (unrelaxed) a-Si$_{1-x}$ :H$_x$ and voids. The substrate is smooth silicon dioxide (SiO$_2$). Fractional void concentrations in layer 2 are varied from 0.01 to 0.26 in the simulations. The thickness of layer 1 is set to be 0.001 $\mu$m, while the film thickness (layer 2) is fixed at 1 $\mu$m. The incidence angle is set to be 75$^\circ$. The constructed complex dielectric functions for relaxed a-Si$_{1-x}$ :H$_x$ films are then fitted using unrelaxed a-Si :H spectra, applying a nonlinear regression based on the Levenberg-Marquardt method [6], and vice-versa. In order to avoid interference caused by the interface, the fits are done above 1.75 eV. We denote the void concentration and the thickness of the surface roughness by $C_{\text{void}}$ and $T_R$ respectively. The fitting error of the void concentration and the thickness of the surface roughness are denoted by $\Delta C_{\text{void}}$ and $\Delta T_R$, respectively, i.e.

$$C_{\text{void}} = |C_{\text{void}}^{\text{constructed}} - C_{\text{void}}^{\text{fit}}|,$$

similarly for $\Delta T_R$.

In order to reveal the quality of the modeling, we define

$$\theta = \frac{\Delta C_{\text{void}}}{C_{\text{void}}} + \frac{\Delta T_R}{T_R},$$

as a measure for the reliability of the modeling. The fits are done for the case (1) that $T_R$ is fixed and only $C_{\text{void}}$ is a fitting parameter (the contribution to $\theta$ consists only of the error in $C_{\text{void}}$), and (2) for the case that both $C_{\text{void}}$ and $T_R$ are fitting parameters. The indicator $\theta$ for the first case, obtained from the best fit is shown in Fig. 2a. It is seen that, at low void concentration, the values of $\theta$ obtained by the modeling based on the use of relaxed spectra are reduced by approximately a factor of two in comparison to those ($\theta_{\text{un}}$) by using unrelaxed spectra. However, all curves are found to converge at high void concentration. It can be concluded that at low void concentration,
a modeling using relaxed spectra, in general, reduces the mis-estimation of the void concentration. However, for structure with high void concentration, modeling using either relaxed or unrelaxed spectra will introduce roughly the same error.

The indicator $q$ for the case of fitting with $C_{\text{void}}$ and $T_R$ is shown in Fig. 2b. It can be seen that, by allowing $T_R$ to be a fitting parameter, $q_r$ reduces by a factor of two in comparison to those in Fig. 2a. It is seen that, at $C_{\text{void}} < 0.06$, $q_r$ are smaller than $q_{ur}$, however, at $C_{\text{void}} > 0.06$, $q_r$ turns out to be larger than $q_{ur}$. These results indicate that the mis-estimation of the structural parameters introduced by the modeling can be minimized by choosing particular dielectric functions for a specified range of void concentration. If the a-Si$_{1-x}$:H$_x$ samples contain a low void fraction, spectra of relaxed a-Si$_{1-x}$:H$_x$ should be used, while in the case of high void concentration, unrelaxed is better. The presence of hydrogen in the structure barely changes the fitting results.

In summary, we investigate the mis-estimation of the structural parameters of a-Si$_{1-x}$:H$_x$ thin films in the fitting of spectroscopic ellipsometry. The results indicate that using of unsuitable dielectric functions in determining the structure of an a-Si$_{1-x}$:H$_x$ thin film of unknown compositions will lead to errors. For most of device-quality a-Si$_{1-x}$:H$_x$ films which contain a low void fraction, fitting by use of relaxed spectra will, in general, result in a more reliable determination of the structure than using unrelaxed spectra.

References