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Spectroscopic Ellipsometry

An Ellipsometric Study of the Optical Constants of C60 & C70 Thin Films

Application Note

Material Science SE35

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Abstract

Spectroscopic ellipsometry (SE) is used to determine the optical constants of C60 and C70 thin films over the range 0.6-6.5eV (i.e. 190-2100nm). The information provided by the optical constants allows for a better understanding of the electronic structure of these materials.

Introduction

Since their discovery in 1985, fullerenes, such as C60 and C70, have attracted attention in material science, electronics, and nanotechnology. A fullerene is any molecule composed of carbon in the form of a hollow sphere, an ellipsoid, a tube or other various shapes. Spherical fullerenes are also called buckyballs, and they resemble the balls used in football. Cylindrical fullerenes are called carbon nanotubes, or buckytubes. Moreover, there are different fullerene derivatives which are created in order to enhance the perfomance and the efficiency of the devices in which they are used. The most common fullerene derivatives is $PC_{60}BM$, which is used in organic solar cells.

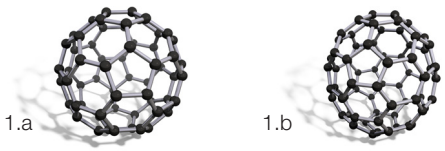


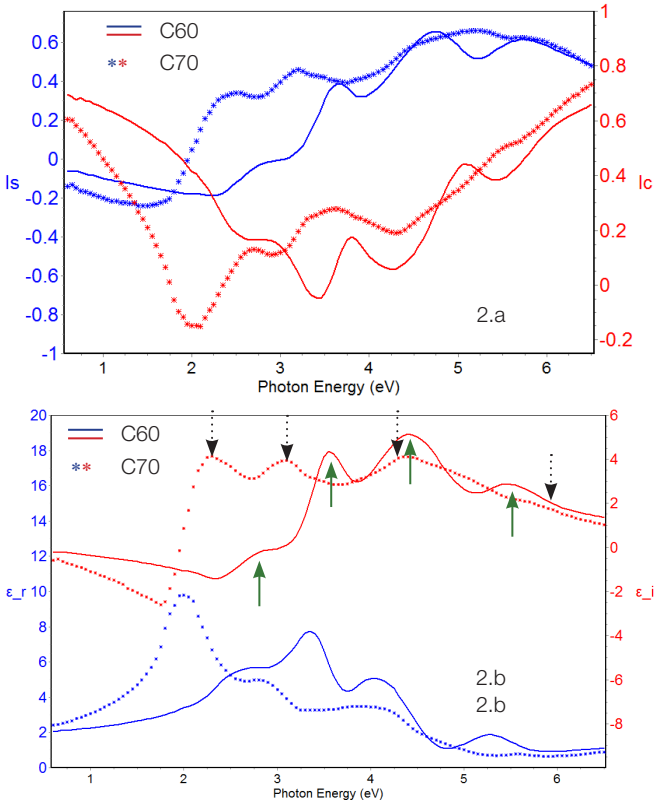
Figure 1: C60 (a) and C70 (b) fullerenes

Experiment

Two samples of thin layers of C60 and C70 fullerenes, coated on a glass substrate, have been measured using the HORIBA Scientific UVISEL 2, a Phase Modulated Spectrosopic Ellipsometer, at an angle of incidence of 70° over a spectral range of 0.6 – 6.5eV (i.e. 190 nm to 2100 nm). From these ellipsometric measurements and through modeling using the HORIBA Scientific DeltaPsi2 software, the thickness and most importantly, the optical constants of these layers were determined.
These samples were measured directly, without any special sample preparation, and the backside reflections due to the glass substrate were collected and taken into account in the model.

Before discussing the modeling aspects, one can learn valuable information from looking at the raw ellipsometric measurements, (Is, Ic) (also related to (Ψ,Δ)) shown in figure2.

This data represents a fingerprint of the sample, describing its electronic structure, including information about microstructure, density, absorption peaks and thickness. From these ellipsometric spectra we can transform (Is,Ic) (or (Ψ,Δ)) by direct inversion to the pseudo dielectric function <ε>, which is shown in figure 3. For an ideal bulk sample, <ε> corresponds to the real dielectric function, ε of the material. For other, non-ideal samples, the pseudo dielectric function can be used to extract information regarding the interference oscillations and the contrast in index of refraction. In the example shown here, the pseudo dielectric function enables one to locate the energies of the absorption peaks, which will used in the dispersion function for modeling.



Figures 2: (a) shows the raw ellipsometric data for C60 and C70 and (b) shows the pseudo dielectric function for C60 and C70.

Figure 2b above shows the first absorption peak, in ε_i, for C70 at a lower energy than for C60. For C70, the absorption peaks are centered around ~2.3eV , ~3.1eV, ~4.4eV and ~5.5eV, whereas for C60, the absorption peaks are centered around ~2.9eV, ~3.55eV, ~4.4eV and ~5.45eV (the absorption peaks are shown in figure 2b, with black arrows representing the absorption peaks for C70 and green arrows representing the absorption peaks for C60).

From these observations, the complex refractive index (n, k) of C60 & C70 thin films have been determined using a summation of several Tauc Lorentz oscillators [1].

The model used for these two samples consisted of four layers : ambient / C60 or C70/Glass/ void . This model structure takes into account the backside reflection from the glass substrate.

The fit results for C60 and C70 are displayed in figures 3 & 4. The thickness of the films was found to be 35.1 nm for C60 and 57.1nm for C70.

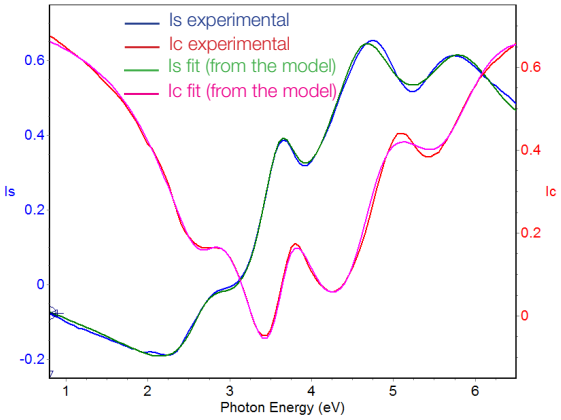


Figure 3: Fit results – C60/glass with experimental (Is,Ic) data in red and blue and fitted (Is,Ic) generated by the model in green and pink

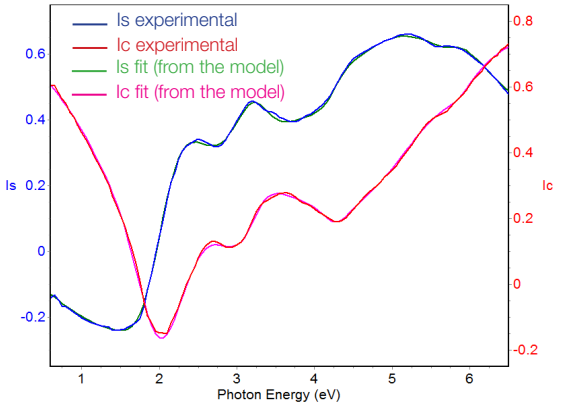


Figure 4: Fit results – C70/glass with experimental (Is,Ic) data in red and blue and fitted (Is,Ic) generated by the model in green and pink

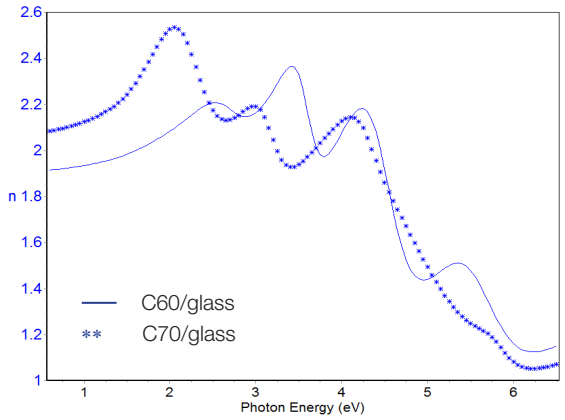


Figure 5a: n=f(E) for C60 and C70 thin film

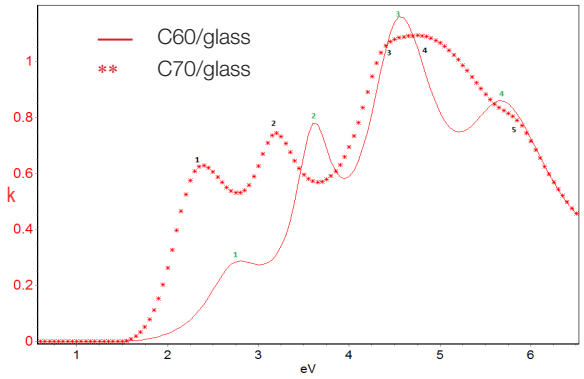


Figure 5b: k=f(E) for C60 and C70 thin film

Absorption peaks	Energy (eV)	
	C60	C70
TL 1	2.692	2.217
TL 2	3.569	3.144
TL 3	4.460	4.295
TL 4	5.601	4.692
TL 5		5.816
Thickness (nm)	35.1	57.1

Table 1: Absorption peak energies and thickness for C60 and C70 thin films studied here

The determination of the optical band gap for C60 and C70 was obtained by a Tauc plot calculation, which is included in the DeltaPsi2 software, according to the following equation:

$(\alpha h\nu)^n = A(h\nu - Eg)$

where A is a constant, $h\nu$ is photon energy, Eg is the allowed energy gap, and n = ½ for an allowed direct transition.

The optical band gap of C60 was calculated and found to be 2.41eV, and the optical band gap for C70 was found to be 2.01 eV.

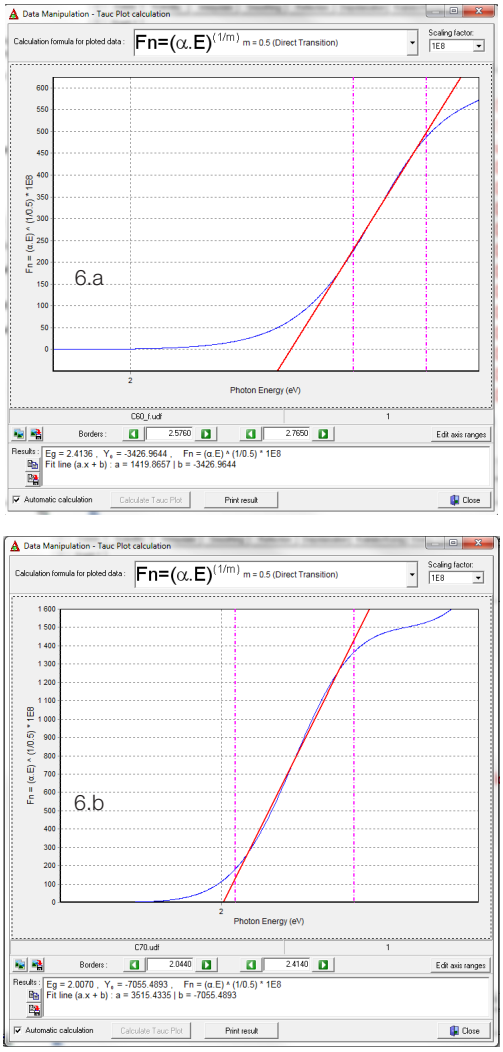


Figure 6: Optical band gap determination from Tauc plot calculation for C60 (a) and C70 (b)

Conclusion

This study has shown the ability to determine optical constants of C60 and C70 thin films over a range of 0.6-6.5 eV, by using spectroscopic ellipsometry. Once the raw ellipsometric data, Is and Ic, are collected, a simple inversion of the data to determine the pseudo dielectric function leads to valuable information to aid in building a suitable model for analysis of the ellipsometric data. In this case, the pseudo dielectric function provided starting energy values for the absorption peaks seen in both C60 and C70 thin films, and this allowed for the use of a dispersion consisting of a summation of Tauc-Lorentz oscillators. Also, ellipsometry analysis allowed for the determination of thickness of the C60 and C70 thin films, as well as a band gap value for each. Moreover, as the HORIBA Scientific UVISEL 2 phase modulated spectroscopic ellipsometer has no moving parts during acquisition, the collection of backside reflections due to the glass substrate has been included and taken into account in the model using a special feature of the HORIBA Scientific DeltaPsi2 software.

References

[1] G.E.Jellison, F.A.Modine, Phys.Rev., 69(3), 371-374(1966).
[2] J.Tauc, Menth A 1972 Non Cryst. Solids 569 8
* (Is,Ic) observables linked to (Ψ,Δ) with the following formula:

$$Is = \sin 2\Psi.\sin\Delta \quad \& \quad Ic = \sin 2\Psi.\cos\Delta$$

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