

High-bandgap silicon-carbon ultrathin films for semitransparent PV devices

Rita Masagué Comellas and Isabel Teixidó Moreno

The objective of the project is to optimize ultrathin films of a-SiC_x:H for their application in transparent solar cells. It focuses on investigating the correlation between carbon content and bandgap in a-SiC_x:H films. The analysis involved studying the optical properties and composition of various samples. The films were prepared using the PECVD technique, and their reflectance and transmittance were measured using a double-beam spectrophotometer. To ensure greater precision, absorbance was also measured using the PDS technique. Additionally, the actual concentration of each sample was determined using XPS measurements.

Key words: a-Si:H, bandgap, absorbance, photo generation

I. INTRODUCTION

Conventional photovoltaic (PV) technologies face limitations due to their surface dependence, requiring critical raw materials and in some cases the use of toxic precursors. These constraints hinder their use on diverse surfaces, such as building facades, where aesthetic and other considerations are taken into account. To overcome these obstacles, alternative concepts like transparent photovoltaics (TPV) have emerged. TPV selectively absorb UV and/or IR light while minimizing or completely avoiding the absorption of visible light. This makes TPV devices essentially transparent to the human eye while harvesting wavelengths out of the visible light spectrum, thus expanding the deployment of PV technologies while increasing the proportion of clean energy in the overall energy mix [1]. The UPC research group MNT-Solar is involved in a project for PV integration into ceramics. This project, named FOTO-CER, aims to obtain transparent photovoltaic finishes for obtaining safe, efficient and clean energy through the envelope of buildings while maintaining the aesthetic of the material. FOTO-CER is a public-private collaborative project granted under the call MISIONES [2].

The proposed TPV device is a solar cell composed of ultrathin films. The structure, starting from the bottom, is a glass substrate, followed by fluorine-tin-oxide (FTO), zinc oxide (ZnO), hydrogenated amorphous silicon carbide (a-SiC_x:H), vanadium oxide (V₂O₅), and a layer of aluminum-doped zinc oxide (AZO). FTO and AZO are Transparent Conductive Oxides (TCOs) that serve as electrodes in the solar cell. FTO, known for its higher conductivity compared to AZO, enables efficient electron transport. On the other hand, ZnO acts as an electron-selective contact, promoting the extraction of electrons at the cathode. The a-SiC_x:H film works as the absorber layer and V₂O₅ functions as a hole-selective contact, allowing for effective collection of holes in the anode.

Our work is focused on optimizing the a-SiC_x:H film by increasing the carbon content, which we expect to result in higher bandgap. So one would also expect the

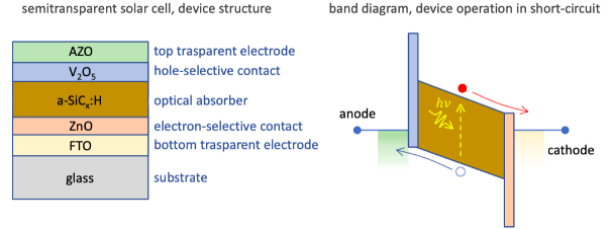


FIG. 1. Schematic of the device structure for the semitransparent solar cells that are the final objective of this work (left). Operation of the solar cell in short-circuit conditions (right).

samples with more carbon to be more transparent, as there is a trade-off between photocarrier generation and transparency.

II. EXPERIMENTAL

In order to study the properties of a-SiC_x:H films, two sets of samples were made. The first set consisted of (relatively) thick films ($\sim 0.4 \mu\text{m}$), and the second set was of ultrathin films (the kind that would be used in solar cells). For each set we took different concentrations of carbon, so that we could study the effect that it had on the material.

The a-SiC_x:H samples were made using the Plasma Enhanced Chemical Vapor Deposition (PECVD) technique. This technique consists of the deposition of thin films onto a substrate by introducing a precursor gas into a vacuum chamber that is subjected to a plasma discharge. The plasma activates the precursor gas, causing it to decompose and form a thin film on the substrate surface. PECVD is usually used in the manufacturing of electronic devices and integrated circuits for depositing materials such as amorphous silicon, among others. This technique has advantages such as low deposition temperatures ($200 \text{ }^\circ\text{C} < T < 400 \text{ }^\circ\text{C}$) and high deposition rate. However, the deposition rate varies depending on the Si/C phase ratio, meaning that the thickness of the samples were different (for the same deposition time). Our depositions were done under

a pressure of 0.5 mbar, at a temperature of 400 °C and with a power of 6W.

Therefore, the thicker films were not only done so that we could more easily and accurately measure the properties of the material, but were also crucial so that we could calculate the deposition time for the ultrathin films. We took four samples for each type of layer with different SiH₄/CH₄ gas phase ratio (given in standard cubic centimeters): for sample 1 is 36/12, for sample 2 is 32/16, for sample 3 is 28/20 and for sample 4 is 20/28.

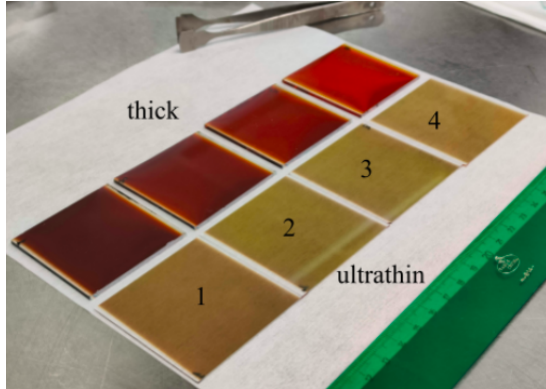


FIG. 2. Ultrathin and thick films made with the PECVD technique.

At first, a profilometer was used to measure the height of the thick layers by using a shadow caused by a small piece of silica. However, the results were very noisy so they were dismissed and we turned into using interference fringes to calculate the thickness. The deposition rate for each gas phase ratio was measured on the thick samples using the transmittance spectrum and interference fringes (also used to calculate the thickness and refractive indexes). With this information, the corresponding deposition time for the ultrathin samples was calculated after we fixed the deposition time for the first sample (at 4 minutes).

In order to measure the transmittance and reflectance of the ultrathin films, a double beam spectrophotometer was used (an equipment from a UB research group that kindly agreed to collaborate with us). The working principle of this instrument is that one of the beams passes through the sample and the other one passes through the reference. To eliminate systemic errors, the first measure is done without an actual sample present. The measurement instrument employs an ideal diffuser as a reference, which is an integrating sphere, while a barium oxide, a highly reflective and white material, serves as the reflector reference.

The absorbance of the thick films has been also measured by Photothermal Deflection Spectrometry (PDS) [3]. This technique is capable of directly measuring the

optical absorbance of the films with an extraordinary sensibility. The working principle is that non-radiative recombination heats the medium close to the sample, which induces a change of its refractive index. This causes the deflection of a laser probe beam parallel and very close to the film surface. And with the resulting angle difference one is able to calculate the absorbance.

Finally, a X-ray Photoelectron Spectroscopy (XPS) was done to measure the real concentrations of our samples. XPS consists of bombarding a sample with X-ray photons causing the emission of electrons from the outermost atomic layers, which are then collected and their kinetic energies are measured. XPS can determine the binding energies of the electrons and identify the elements present in the sample by analyzing the measured kinetic energy. So, XPS is a powerful technique to know the composition of a material's surface. However, the data could not be analyzed in time for this report. The work is in progress and we intend to present the main conclusions in the presentation.

III. RESULTS AND DISCUSSION

The results are summed up in table I. Nonetheless, the explanation behind each calculation is explained over the following paragraphs.

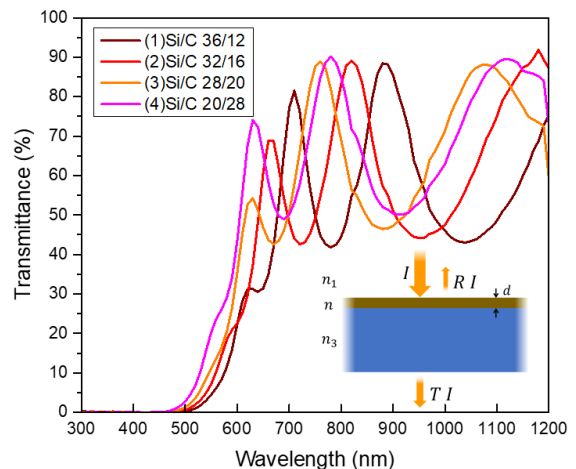


FIG. 3. Transmittance spectra of thick a-SiC_x:H films studied in this work.

Figure 3 shows the transmittance spectra of the series of thick films deposited on glass varying the Si/C gas phase ratio. The interference fringes of each spectra can be used to calculate the thickness and refractive index of each layer. A detailed description of this procedure, applied to similar films deposited on transparent glass substrates, has been reported in the literature [3].

First, the refractive index (n) of the film can be calcu-

lated as:

$$N = \frac{n_1^2 + n_3^2}{2} + 2n_1n_3 \frac{T_M - T_m}{T_M T_m}, \quad n = \sqrt{N + \sqrt{N^2 - n_1^2 n_3^2}} \quad (1)$$

Where n_1 and n_3 are the refractive indexes of air and glass, and T_M and T_m are the maximum and minimum transmittance values at a given wavelength (one of these values needs to be estimated).

Furthermore, the interference order of the peaks l can be fitted allowing a highly precise calculation of the thickness of each layer (Figure 4):

$$\frac{l}{2} = 2d \frac{n}{\lambda} - m_0 \quad (2)$$

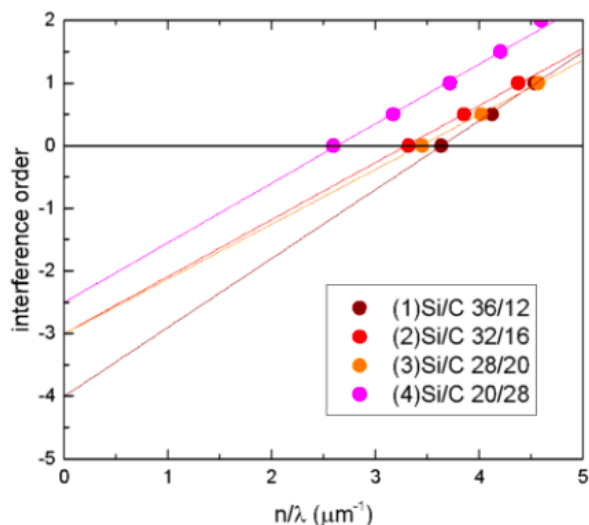


FIG. 4. Linear fit from the analysis of interference fringes to calculate the film thickness.

Finally, the strong attenuation of transmittance spectra at short wavelengths is related to band-to-band optical absorption. This region can be used to calculate the absorption coefficient, which can be fitted in Figure 5 by the Tauc's law [4]:

$$\sqrt{h\nu\alpha} = B(h\nu - E_g) \quad (3)$$

As it was expected, the bandgap energy increases as we add more carbon to the films. The results from the analysis of transmittance spectra are summarized in Table I.

The absorbance of the series of thick films has been also measured by Photothermal Deflection Spectrometry (PDS) [5]. The corresponding spectra are shown in Figure 6, which confirm the increase of the bandgap as more carbon is incorporated into the films.

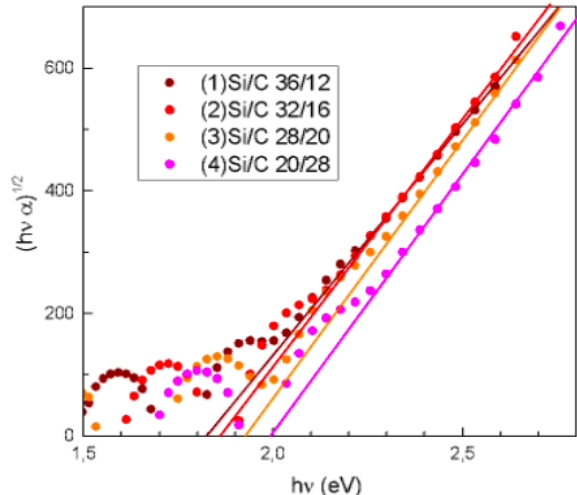


FIG. 5. Tauc's law applied to the series of thick samples varying the Si/C ratio.

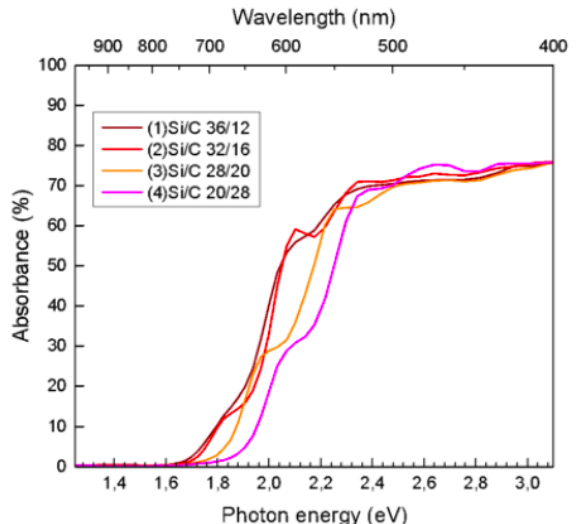


FIG. 6. Absorbance spectra of the series of thick films measured by the PDS technique.

Figure 7 shows the transmittance and reflectance spectra for the series of thin a-SiC_x:H films. In this series the deposition time has been adjusted to obtain a thickness of about 30 nm in all cases. This is the thickness used for absorbing layers implemented in devices, as the one depicted in Figure 1. The inset shows the absorbance of these films that can be calculated as:

$$A = 100\% - R - T \quad (4)$$

Compared to the irradiance spectra of one-sun [6] (inset), these curves indicate that the semitransparent solar cells basically make use of the blue-ultraviolet region of the spectrum.

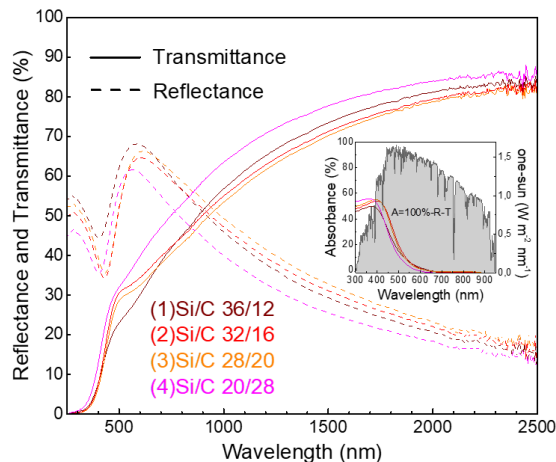


FIG. 7. Optical characterization for the series of thin a-SiC_x:H films. The inset compares the absorbance of these layers to the reference irradiance of the sun.

TABLE I. Series of thick a-SiC_x:H films prepared in this work including results from optical characterization.

SiH ₄ /CH ₄ Gas Flow (sccm)	Refractive Index n	Thickness d (μm)	Deposition Rate r_d ($\text{\AA}/\text{s}$)	Bandgap E_g (eV)
36/12	3.2	0.55	2.3	1.82
32/16	3.1	0.45	1.9	1.86
28/20	3.0	0.44	1.8	1.92
20/28	2.9	0.47	1.9	2.00

As shown in Table I, the refractive indexes decrease

with the increase of carbon concentration. However, the bandgap increases, as we expected. The properties in terms of transparency are visible in figure 2, where clearness increases with carbon concentration. Though the difference from one sample to the next one can be rather subtle, the tendency is clear.

IV. CONCLUSIONS

The bandgap energy increases with the concentration of carbon as does the transmittance and, thus, the transparency. The results yielded from this research, led the UPC group to use ultrathin silicon-carbon films with a higher carbon content for their current solar cell device than they did initially (the current proportions are 20/28 sccm in SiH₄/CH₄ gasflow). It is clear that this is an interesting research line that could lead to tangible improvements in our society and should be further explored.

V. FINAL NOTE

The opportunity to take part in this project has been very gratifying. Not only we had the chance to work in an actual lab and take part in an experiment, but we also explored an interesting topic hand in hand with amazing researchers.

We must thank the UPC research team Cristobal Voz, Eloi Ros, Pablo Ortega and Quim Puigdollers for guiding us through this project and being always of great help. And also thanks to the UB team, with JM Asensi, for letting us use their equipment and collaborating with us.

VI. REFERENCES

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