Modelling of the Optical Spectra of CVD-deposited Silicon Films For Solar Cell Applications

E. Malainho, M. I. Vasilevskiy, J. P. Alpuim, S.A. Filonovich
Centre of Physics, University of Minho, 4710 - 057 Braga, Portugal
id1960@alunos.uminho.pt

In contrast with crystalline solids, the quasimomentum conservation is relaxed for amorphous semiconductors, leading to a substantial difference in their optical properties. The Tauc model [1] was developed for the description of the optical properties of such systems, based on the following assumptions: (i) parabolic shape of the density of states (DOS) in the valence and conduction bands, (ii) relaxation of the *k* selection rule for optical transitions, and (iii) the energy-independent transition matrix element. This model enables one to estimate the optical band gap (E_g) of amorphous materials using the so called Tauc plot, $(\alpha E)^{1/2}$ versus E (α is the absorption coefficient and E the photon energy).

However, despite the Tauc model's simplicity, for materials presenting oscillatory transmittance spectra, the linear fit to the spectral region above the gap is not obvious, bringing a significant uncertainty into the evaluation of E_g. Silicon films with sub-500 nm thickness, deposited on glass substrates for solar cells applications using Chemical Vapour Deposition (CVD), are within such group. Taking this fact into account, the present work has been developed with the scope of modelling the samples' transmittance spectra and the evaluation of E_g of the hydrogenated amorphous silicon (a-Si:H).

First, we introduced some modifications in the traditional Tauc model by taking into account the absorption tail below the gap, produced by the fluctuations of the band edges. We used the approach [2] usually taken for heavily doped crystalline semiconductors with direct band gap, although the energy scale of the tail cannot be obtained theoretically and has to be considered as a fitting parameter in our case. By constructing the imaginary part of the dielectric function ($\hat{\varepsilon}$) of the amorphous silicon from the tail-added joint DOS, the real part of $\hat{\varepsilon}$ was obtained using the Kramers-Krönig relation. Given this, the optical transmittance and reflectance spectra were calculated using the standard approach for multilayer structures taking into account all the multiple reflections at the interfaces.

We have achieved a good agreement between the theoretical and the experimental transmittance spectra. This has enabled us to determine self-consistently the band gap values for a-Si:H films grown in different conditions. The results show that E_g is influenced by the percentage of hydrogen added during the film deposition, since E_g increases with the hydrogen concentration.

References:

[1] Morigaki, K., Physics of Amorphous Semiconductors, Imperial College Press and World Scientific Publishing, (1999).
[2] Shklovskii, B. I., Efros, A. L., Electronic Properties of Doped Semiconductors, Springer, (1984).