On the determination of the interface density of states in a-Si:H/a-$Si_{1-x}C_x$:H multilayers

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This paper deals with the determination of the interface density of states in amorphous silicon-based multilayers. Photothermal deflection spectroscopy is used to characterize two series of a-Si:H/a-$Si_{1-x}C_x$:H multilayers, and a new approach in the treatment of experimental dada is used in order to obtain accurate results. From this approach, an upper limit of 10^{10} cm^{-2} is determined for the interface density of states.

1. INTRODUCTION

One of the most interesting aspects of amorphous semiconductor multilayers is their application in studying the interfaces between different a-Si:H based alloys, because of the great number of interfaces that a multilayer structure can contain. There are several magnitudes, such as the additional hydrogen content at interfaces [1,2] or the density of states (DOS) per interface [3-7] that can be estimated from measurements of series of multilayers with different geometries and number of interfaces.

In particular, the DOS per interface is a valuable parameter used to define the optoelectronical quality of interfaces. One of the most suitable techniques for the measurement of DOS is photothermal deflection spectroscopy (PDS). However, the use of PDS to determine the DOS per interface requires accurate determination of the surface DOS (i.e. the DOS at air/multilayer and multilayer/substrate interfaces) and the strong assumption of a constant surface DOS in spite of the geometry of the multilayer [4]. Other complications can arise from the more defective material in the multilayer (usually the alloy), whose contribution to the measured total DOS can obscure the smaller contribution from the DOS at interfaces.

In this paper, the DOS at a-Si:H/a-$Si_{1-x}C_x$:H interfaces is estimated from the characterization by PDS of two series of multilayers with variable mean composition. A novel approach is used to determine the DOS per interface and thus avoid the obscuring effects of the surface DOS and the silicon-carbon alloy DOS. This treatment gives an upper limit of 10^{10} cm^{-2} to interface DOS, which demonstrates the high quality of these interfaces.

2. EXPERIMENTAL

Two series of a-Si:H/a-$Si_{1-x}C_x$:H multilayers with variable mean composition were studied. One presented a constant a-$Si_{1-x}C_x$:H layer thickness of 37 Å and a variable a-Si:H layer thickness (between 7 and 147 Å). The other presented a constant a-Si:H layer thickness of 55 Å and a variable a-$Si_{1-x}C_x$:H layer thickness (between 9 and 205 Å). The number of elementary pairs of layers was varied in order to obtain approximately the same total thickness ($\approx$ 0.5 μm) in all the multilayers. The carbon content of alloy layers was 0.36 as determined from XPS measurements.

The samples used in this study were deposited by RF glow discharge in a reactor described elsewhere [8]. The most significant feature of this reactor is an automated substrate holder which permits removal of the substrates from plasma influence during the gas-exchange process. This feature was also used to obtain up to four samples of homogeneous material with different thicknesses but prepared under identical conditions in order to determine the surface DOS of both materials.

The DOS was obtained from the excess absorption in the low absorption zone from photothermal deflection spectroscopy (PDS) measurements. The absorption spectra were obtained from the PDS signal as described elsewhere [9]. The DOS was calculated by integrating the spectra between 0.95 and 1.50 eV and the constant used in the calculation was 7.9×10^{15} cm^{-2} eV^{-1}.

3. RESULTS AND DISCUSSION

Before analyzing the measurements of multilayers, several homogeneous samples of each material with thicknesses ranging from 0.5 to 2.5 μm were measured. From these measurements the bulk and surface DOS were accurately obtained. The a-Si:H layers used in the multilayers presented a bulk DOS of 1.2×10^{16} cm^{-3} and a surface density of 8.5×10^{11} cm^{-2}. These values were respectively 8.5×10^{16} cm^{-3} and 2.7×10^{12} cm^{-2} for the a-$Si_{1-x}C_x$:H layers. The surface DOS was associated with the states in the air/layer and layer/substrate interfaces.

The results corresponding to the DOS measured in our multilayers are shown in Figure 1. These results are plotted as a function of the varying thickness. An increase in DOS when the a-$Si_{1-x}C_x$:H layer thickness increases (and consequently when the number of interfaces decreases) is observed (samples represented by circles). In the other series, the DOS decreases when the a-Si:H layer thickness increases (and consequently the number of interfaces decreases).

The different behaviour in the two series when the number of interfaces is varied highlights the main role of the total a-$Si_{1-x}C_x$:H thickness in determining the measured DOS.

Several contributions to DOS are expected in multilayer structures. Two of them are the bulk DOS of the materials used (N_s^{Si} and N_s^{SiC}), another is the surface DOS corresponding to the air/multilayer and multilayer/substrate interfaces (N_{surf}), and, finally, the contribution of the interfaces between elementary layers (N_i):

$$N_s d = N_s^{Si} d_{Si} n + N_s^{SiC} d_{SiC} n + N_i (2n-1) + N_{surf}$$

where d is the total thickness of the multilayer, n is the number of bilayers, and d_{Si} and d_{SiC} are the thicknesses of elementary layers.

The weight of each contribution has to be considered to obtain an estimation of the interface DOS. In our case, from the usual values reported for the interface DOS in a-Si:H/a-$Si_{1-x}C_x$:H multilayers (3-5×10^{10} cm^{-2}) [3-6], we can expect that the increase in the total DOS due to the interface states will be much lower than the weight of the bulk a-$Si_{1-x}C_x$:H DOS or the surface DOS. In addition, some authors have suggested that the multilayer structure could affect the surface roughness with respect to homogeneous layers [10], so the assumption of the same value for this surface DOS as in homogeneous layers should be relaxed.

To avoid these problems, our treatment of the experimental results assumes that a) the volume DOS in the a-Si:H layers in a multilayer structure did not change with respect to homogeneous layers, and b) any value for the interface DOS in a reasonable range (between 5×10^{8} and 10^{11} cm^{-2}) is possible. From the assumption of these two values, we have fitted the dependence observed for each series with two parameters: the a-$Si_{1-x}C_x$:H bulk DOS and the surface DOS. The goodness of the fit is evaluated by means of an error function calculated as the average deviation of the measured DOS from the DOS obtained from the optimal parameters of the fit. This fit was performed to different values of the interface DOS in the above mentioned range, and gave a continuous dependence for the best fit values of the parameters (N_s^{SiC} and N_i) and the error function.

The results from this treatment applied to the series with constant a-$Si_{1-x}C_x$:H layer thickness and constant a-Si:H layer thickness are respectively shown in Figures 2 and 3.

In both cases, the error function increases suddenly when the interface DOS is assumed to be more than approximately 2×10^{10} cm^{-2}. This value is an upper limit to the interface DOS in our case, but also the reasonability of the fitting parameters and the consistency between the results of the two series have to be analyzed. For example, it does not seem very likely that the best-fitting values of the volume a-$Si_{1-x}C_x$:H DOS in Figure 2 could be lower than the volume DOS assumed for the a-Si:H layers. Moreover, the surface DOS and the volume a-$Si_{1-x}C_x$:H DOS are expected to be very similar in both series, and not much different from the values estimated from homogeneous layers.

In Figures 2 and 3, the curves corresponding to the volume a-$Si_{1-x}C_x$:H DOS intersect at a value of 8.8×10^{16} cm^{-3}, which corresponds to an interface DOS of 2.2×10^{9} cm^{-2}, and the surface DOS curves intersect at a value of 1.4×10^{12} cm^{-2}, which corresponds to an interface DOS of 5.7×10^{9} cm^{-2}. The values for the interface DOS are very close, and the values of the volume a-$Si_{1-x}C_x$:H DOS and the surface DOS are consistent with those measured from homogeneous layers, which indicates the correctness of this method. The interface DOS values are below 10^{10} cm^{-2}, one of the lowest values reported, which demonstrates the high quality of these interfaces.

This fact means that a slight variation in the surface DOS due to changes in the surface roughness or in the technological process (for example, the manipulation of the substrates during the cleaning process or the temperature of the reactor when the samples are removed) could obscure the interface DOS.

This means that accurate measurement of the interface DOS is very difficult, and that only an upper limit to this can be obtained.

The lower weight of the interface DOS with respect to the volume DOS in a-$Si_{1-x}C_x$:H layers is consistent with the behaviour of the photoconductivity observed in these samples, which suggests that recombination takes place mainly in the alloy layers [11].

4. CONCLUSIONS

The DOS of two series of a-Si:H/a-$Si_{1-x}C_x$:H multilayers was measured by PDS. A treatment of the results, which did not assume pre-determined values for the volume DOS in alloy layers or for the surface DOS, gave an upper limit to the interface DOS of 10^{10} cm^{-2}. This value is very low, and implies an important difficulty in accurate determination, and a very low weight of this contribution compared with others such as the surface DOS or the volume DOS in defective a-$Si_{1-x}C_x$:H layers.

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REFERENCES

1. R. Schwarz, T. Fischer, P. Hanesch, T. Muschik, J. Kolodzey, H. Cerva, H.L. Meyerheim and B.M.U. Scherzer, Appl. Surf. Sci., 50 (1991) 456.
2. W.A. Lanford and B. Abeles, Nucl. Instr. and Meth. B, 15 (1986) 390.
3. A. Asano, T.Ichimura, M. Oshawa, H. Sakai and Y. Uchida, J. Non-Cryst. Solids, 97&98 (1987) 971.
4. A. Asano, T. Ichimura, Y. Uchida and H. Sakai, J. Appl. Phys., 63 (1988) 2346.
5. P. Fiorini, M. De Seta and F. Evangelisti, J. Non-Cryst. Solids, 114 (1989) 732.
6. N. Bernhard, M. Kirsch, R. Eigenschenk, M. Bollu, C. Wetzel, F. Müller and R. Schwarz, Mat. Res. Soc. Symp. Proc., 192 (1990) 237.
7. S. Wang and R. Cheng, J. Non-Cryst. Solids, 114 (1989) 702.
8. J. Bertomeu, J.M. Asensi, J. Puigdollers, J. Andreu and J.L. Morenza, Vacuum, 44 (1993) 129.
9. N.M. Amer and W.B. Jackson, in: Semiconductors and Semimetals, Vol. 21. Hydrogenated Amorphous Silicon, part B, Ed. J.I. Pankove (Academic Press, New York, 1984) p. 83.
10. H. Itoh, S. Matsubara, S. Muramatsu, N. Nakamura, T. Shimada and T. Shimotsu, Jpn. J. Appl. Phys., 27 (1988) L24.
11. J. Bertomeu, J. Puigdollers, J.M. Asensi, J.C. Delgado and J. Andreu, Mat. Res. Soc. Symp. Proc., 297 (1993) in press.

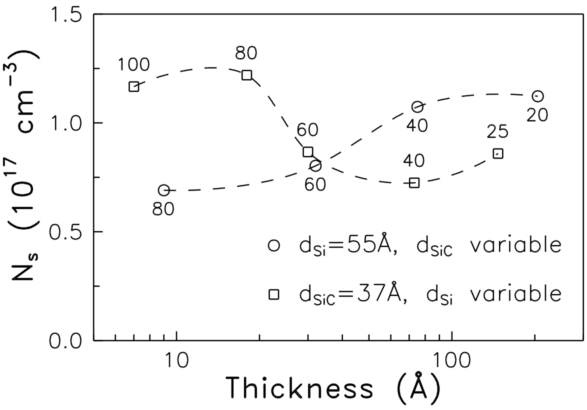

Figure 1. Measured density of states for the two series of multilayers as a function of the varying thickness. The labels indicate the number of elementary pairs of layers.

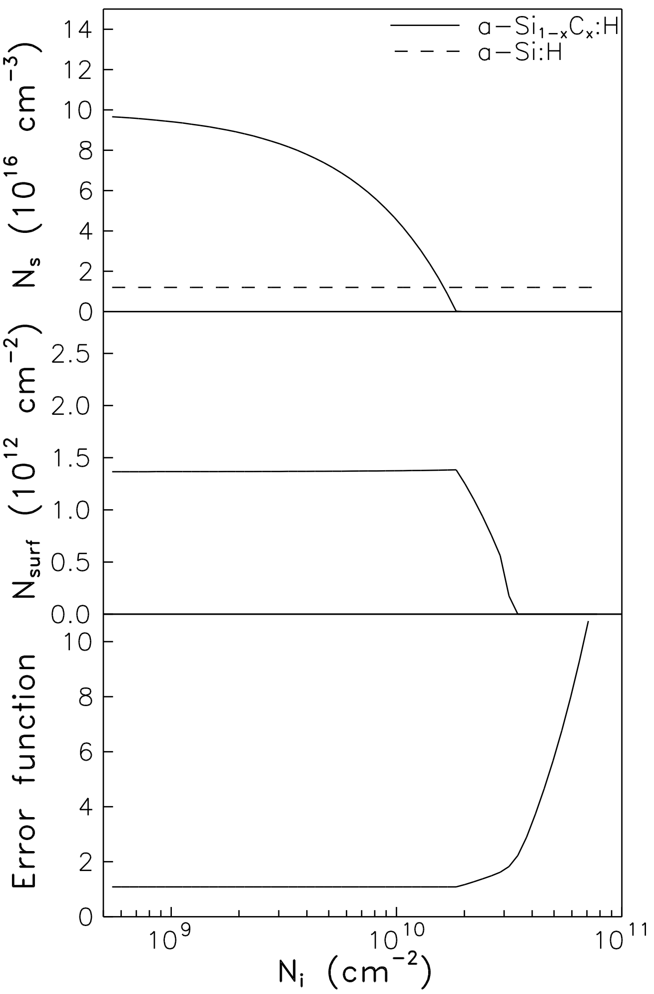

Figure 2. Volume and surface density of states and error function obtained from the fit of the measured total density of states of the series with constant a-Si$_{1-x}$C$_x$:H layer thickness.

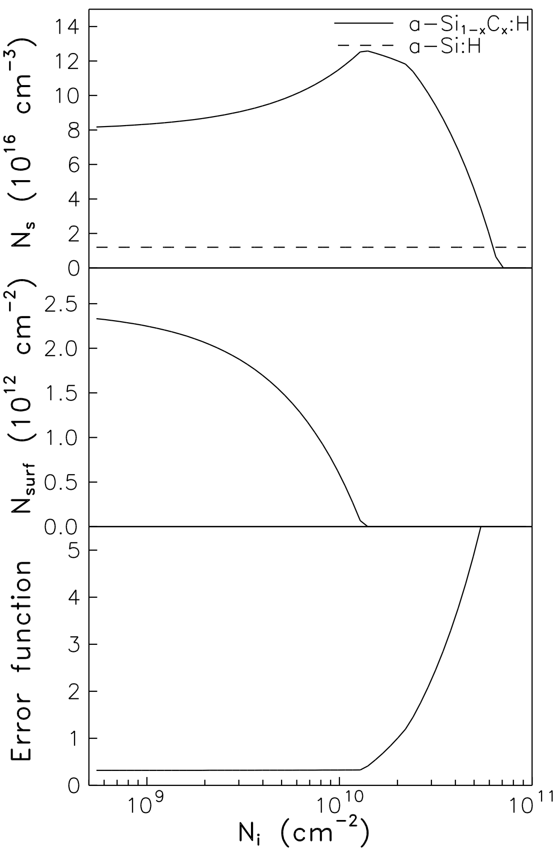

Figure 3. Volume and surface density of states and error function obtained from the fit of the measured total density of states of the series with constant a-Si:H layer thickness.