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MULTIPHASES DESCRIPTION OF a-Si:H

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Abstract - Photoluminescence, thermally stimulated currents (TSC), optical absorption and electrical conductivity are reported versus deposition temperature and deposition rate of undoped a-Si:H. These results are coherent with a tentative model according to which the radiative recombination and thermal emission take place in a nearly constant and weakly disordered grain like zone, while optical absorption occurs mainly in a widely varying and largely disordered grain boundary like zone ; in this picture, the electrical conductivity involves both zones.

I. INTRODUCTION

Up to now, the electronic properties of amorphous hydrogenated silicon (a-Si:H) have been mainly described in the framework of a single distribution of localized states in an homogeneous material (1). Recently the Xerox group gave evidence (2) for the existence of two zones in a-Si:H, a grain like zone (GL) with few non interacting hydrogen (< 3 %) embedded in a grain boundary like zone (GBL) with a large concentration of interacting hydrogen (> 10 %). This quite naturally suggests that two different DOS have to originate from the GL and GBL zones. As a consequence, some signals might occur preferentially from one of these two zones which are expected to present very different electronic properties. Previous attempts to interpret the a-Si:H properties as those of an inhomogeneous material have been made by Brodsky (3) and Anderson and Paul (4). We choose here to study versus the deposition temperature (T_d) and the deposition rate (v), the optical absorption, the electrical conductivity, the photoluminescence and the thermally stimulated currents of a-Si:H.

II. PREPARATION AND CHARACTERISATION

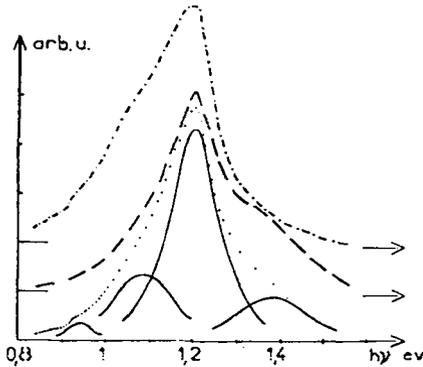
The films were prepared by RF diode sputtering of a C-Si target in a (constant) 80 % Ar / 20 % H₂ reactive mixture onto fused silica or C-Si substrates. We measure the total hydrogen content (5,6) and its distribution among the various sites (5), the Si and the Ar concentrations (6) within the films. The photoluminescence apparatus is described in another paper (7). Thermally stimulated currents are measured during a heating rate of 0.2 K/s by an electrometer Keithley 602B under sandwich configuration (with a-Si and Pd ohmic contacts (15)). Excitation is done at 120 K by a monochromatic light of 1.94 eV. The measurements of the optical absorption (5) and conductivity (15) were published previously.

III. RESULTS AND DISCUSSION

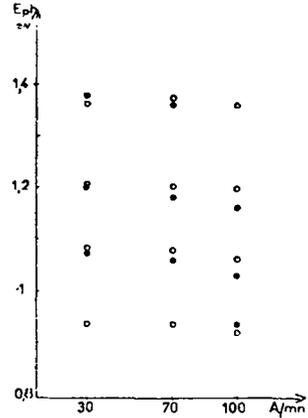
1. Photoluminescence

All the spectra exhibit structures at the same energies with various relative intensities (Fig. 1a). We look for the best fit of these spectra through the intensities and positions (around those of the structures) of four component lines of identical width. We discuss here the energy position of these lines versus the preparation parameters. Their relative intensities are discussed in another paper (7). Fig. 1b

Fig. 1. Photoluminescence in undoped a-Si:H.



1a. Three typical spectra and one example of decomposition.



1b. Energy position of the lines vs v at $T_s = 190^\circ\text{C}$ (o) a, d 250°C (●).

shows the energy of these lines versus v at $T_s = 190$ (o) and 250°C (●). There is a very slight systematic decrease as v increases around 1.36 eV, 1.2 eV, 1.08 eV and 0.93 eV. These lines are found in all the 20 undoped a-Si:H studied so far. For undoped glow discharge or sputtered a-Si:H all these lines (8) or some of them (9) have been found by other authors.

2. Thermally stimulated currents

Fig. 2 shows the TSC signals versus temperature for a heating rate of 0.2 K of undoped a-Si:H deposited at $v = 30 \text{ \AA}/\text{min}$, $70 \text{ \AA}/\text{min}$ and $100 \text{ \AA}/\text{min}$. We obtain current peaks at 210 and 278 K ($30 \text{ \AA}/\text{min}$), 275 and 315 K ($70 \text{ \AA}/\text{min}$) and a very large peak at 310 K ($100 \text{ \AA}/\text{min}$). These curves are typical of those obtained over a larger range of excitation, heating rates and samples which will be discussed elsewhere. The current peaks appear in all cases around the same temperatures 210 K, 275 K, 315 K. Similar TSC peak temperatures for similar heating rates were reported by other authors in both sputtered and glow discharge a-Si:H (10).

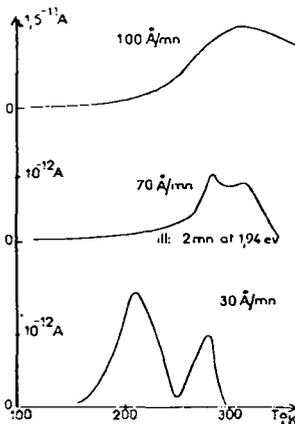
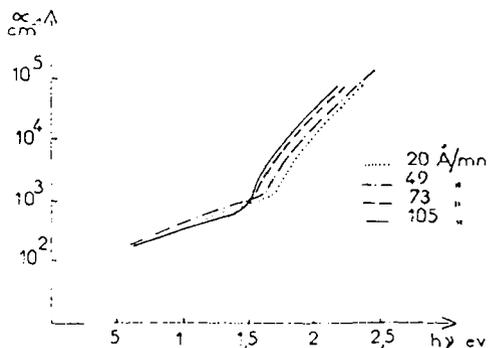


Fig. 2. Thermally absorption coefficient versus photon energy. $T_s = 190^\circ\text{C}$, $v = 20, 49, 73$ and $105 \text{ \AA}/\text{min}$.

3. Optical absorption $\alpha(h\nu)$

$\alpha(h\nu)$ is shown on Fig. 3 for $T_s = 190^\circ\text{C}$ and $v = 20, 49, 73$ and $105 \text{ \AA}/\text{mn}$. They exhibit a main component (which defines the optical gap) which is strongly dependent on v (5,7) and a low energy tail which on the contrary is nearly constant (11).

Fig. 3. Optical absorption coefficient versus photon energy. $T_s = 190^\circ\text{C}$, $v = 20, 49, 73$ and $105 \text{ \AA}/\text{mn}$.



4. Electrical conductivity versus temperature

The activation energy of the conductivity for coplanar measurements decreases from 0.69 eV to 0.62 eV as v increases (8), while it decreases from 0.9 eV to 0.7 eV in sandwich configuration on similar samples.

5. Discussion

We have obviously two sets of behaviours for the electronic properties of a-Si:H. The optical absorption and the electrical conductivity depend strongly on v and T_s , while the energy of the peaks of photoluminescence or thermally stimulated currents are independent of v and T_s . This suggests that each set takes place in a different zone of the material.

If the hydrogen atoms are mainly linked to Si structural defects (12), there is a weak disorder and so few localized defects in the grain like zone. The corresponding localized levels appear almost discrete and give well defined peaks in photoluminescence and TSC. Their energies give respectively their distances from the valence band edge (or from a large density of hole traps near it) and from the conduction band edge. For the three upper levels we find their sum nearly constant around 1.7 eV which would be the gap of the GL zone. It was suggested that this energy corresponds to a gap associated with the tetrahedral bonding symmetry, which is observed preferentially in disordered silicon (13). The constancy of all these energies indicates that the GL zone is weakly dependent on v in the undoped a-Si:H.

As a consequence, the optical absorption would occur preferentially in the more disordered GBL zone where the selection rules have been completely lost. This gives a main absorption component very sensitive to the preparation conditions as the GBL zone (2). On the contrary some short range order remains and so the selection rules are not completely removed in the GL zone. This results in a weak absorption component nearly constant with v and T_s (11).

Finally electrical conductivity needs thermal generation of carrier in the GL zone, then thermal emission in (or over) the GBL zone which introduce additional energy on E_G and a loss coefficient on σ_0 . In particular, the different hydrogen sites in the vicinity of the substrate or of the metal contact (14) result in different GBL zone which might explain the differences in electrical conductivity between coplanar and sandwich configurations (8).

Our tentative picture of the two zones behaviour of the material is summarized on Fig. 4. Actually, while the GL zone would have smooth variations, the GBL zone is very sensitive to the preparation parameters and to the boundary materials. So a-Si:H is rather a multiphase than a two phase material.

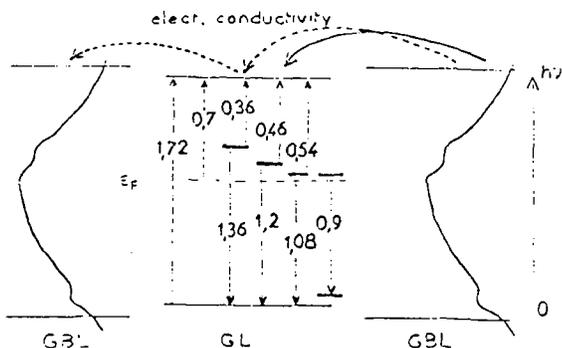


Fig. 4. Schematic energy band diagram for the grain like zone (GL) and the grain boundary like zone (GBL).

IV. CONCLUSION

We have described photoluminescence, thermally stimulated currents, optical absorption and conductivity-temperature measurements of sputtered a-Si:H films. Their interpretation is coherent with a model according to which there are two different distributions of states in the two zones description of the material originally proposed by the Xerox group.

The grain like zone exhibiting weak disorder would have smooth dependence with the preparation conditions. Photoluminescence and thermally stimulated current whose peak positions are very similar with very different a-Si:H preparation will originate from this region. The grain boundary like zone exhibiting a large disorder would be very dependent on the condition preparation. Optical absorption would occur mainly in this region. Conductivity would need carrier transfer between these two regions which would be very dependent on the preparation through the connection of the bands between these two regions.

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