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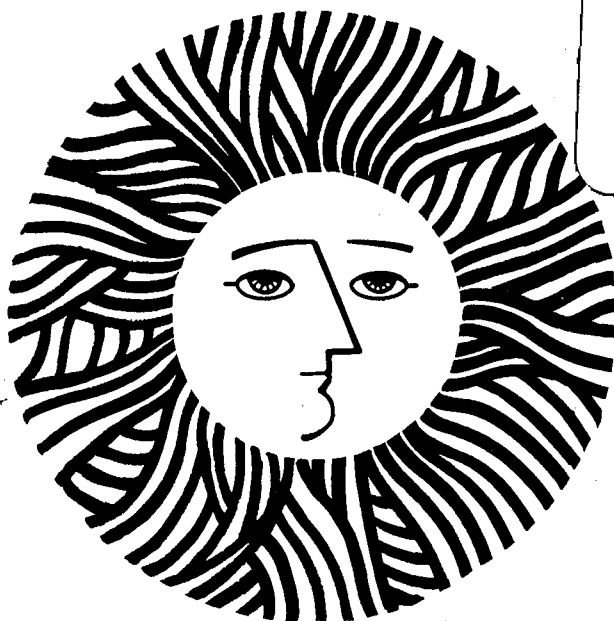
DIRECT MEASUREMENT OF THE ABSORPTION TAIL OF a-Si:H IN THE RANGE OF $2.1 \text{ eV} > h\nu > 0.6 \text{ eV}$

Warren B. Jackson and Nabil M. Amer

March 1981

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DIRECT MEASUREMENT OF THE ABSORPTION
TAIL OF a-Si:H IN THE RANGE OF
2.1 eV > hv > 0.6 eV

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ABSTRACT

The absorption edge of a-Si:H has been measured in the 0.6 - 2.1 eV (or $\alpha\ell = 5 \times 10^{-4}$) range using a sensitive technique of photo-thermal deflection spectroscopy which measures the optical absorption directly and is insensitive to scattering. Absorption edges were measured for films formed under a variety of deposition conditions. An absorption shoulder was found in materials with high defect densities and is strongly correlated with spin densities.

INTRODUCTION

The complete characterization of the shape of the optical absorption edge and tail of a-Si:H at and below the absorption edge yields information on the nature of the joint density of states. Furthermore, since the absorption tail in, for example, the chalcogenides has been attributed to transitions associated with defect centers, it would be of interest to investigate the applicability of this conclusion to a-Si:H films. However, published optical transmission measurements have been restricted to absorption coefficient values of $\alpha > 10 \text{ cm}^{-1}$. This limitation is set by the inability of conventional techniques to measure small values of $\alpha\ell$.

We have recently developed a new technique, photothermal deflection spectroscopy (PDS)⁽¹⁾, which enables us to extend the sensitivity of determining α by two orders of magnitude over published values. PDS is highly insensitive to scattering and does not involve the use of experimentally unverified assumptions.

EXPERIMENTAL CONSIDERATIONS

When an intensity-modulated light beam (pump beam) is absorbed by a medium, heating will ensue. This heating causes a periodic index of refraction gradient in a thin layer adjacent to the sample surface. A second beam (probe beam), propagating through this thin layer, will then experience a periodic deflection which can be quantitatively related to the optical absorption. We have shown that the magnitude of the deflection ϕ is related to optical absorption in the following manner

$$\phi \propto (1 - e^{-\alpha\ell}) \quad (1)$$

where ℓ is the film thickness. The experimental arrangement is

shown in Fig. (1). Our pump beam was the monochromatized output of Hg-Xe arc lamp (0.01 eV bandwidth), and the deflection of the He-Ne laser probe beam was monitored with a conventional position sensor whose output was detected with a lock-in amplifier and normalized for the intensity variations of the pump beam as the wavelength was changed. The absolute absorption coefficient was obtained by using measured values of reflection and transmission at 1.96 eV in the formulae for reflectance and transmittance for thin films. These equations were then solved for the absorption coefficient and the index of refraction using a numerical routine

To verify that PDS spectra are identical to those obtained by conventional techniques, we measured the absorption spectra of crystalline silicon, Nd³⁺ doped glasses, and graphite and found that our PDS results accurately reproduced those reported in the literature.

One important advantage of PDS over conventional transmission measurements is its insensitivity to elastic scattering of light by imperfections in the sample. Using the one-dimensional equation for radiation transport in an isotropically scattering slab and the heat diffusion equation, we find that⁽²⁾

$$\phi \propto (1-R-T) \quad (2)$$

where R (T) is the reflection (transmission) coefficients for diffuse and specular beams. Fig. (2) shows that PDS signal is independent of scattering up to $\lambda\alpha\ell = 1$, where λ is the fraction of light scattered, α is the total extinction coefficient (scattering plus absorption), and ℓ is the film thickness. Hence, if the transmitted flux is reasonably collimated, PDS will be independent of scattering.

The a-Si:H samples used were obtained from the Xerox and RCA research groups. The RCA samples were produced by the d.c. discharge decomposition of silane and were deposited on SiO₂ substrate. Xerox samples were deposited by r.f. decomposition of silane on quartz and 7059 glass substrates. A summary of the characteristics and deposition parameters is given in Table I.

RESULTS AND DISCUSSION

Figs. 3-5 summarize our results for the absorption coefficient as a function of photon energy for films deposited at various substrate temperatures, r.f. powers, and for samples doped with phosphorous. Note in Fig. 3 that for low substrate temperature ($\sim 100^\circ\text{C}$), a pronounced shoulder appears at 1.3 - 1.4 eV which is not exhibited by samples deposited at higher temperatures. As one would expect, samples prepared at 230°C show the lowest tail absorption. The dependence of the absorption tail on deposition power is given in Fig. 4. Again, for deposition conditions known to produce large defect densities and columnar morphology, a discernable shoulder is observed. Similarly, the effect of doping (P) is to give rise to a clear shoulder at ~ 1.3 eV. In Fig. (5), we plot the absorption at 1.4 eV as a function of spin density.

From these results, the following tentative conclusions can be drawn:

1. Deposition parameters play a dominant role in the nature and number of states in the pseudo-gap. Furthermore, the tail absorption appears to be strongly correlated with unpaired spins.
2. By comparing luminescence data⁽³⁾ with our absorption results, it appears that strong luminescence is inversely related to the observation of a shoulder on the absorption tail. In fact, one can argue that such a structure on the absorption tail appears to compete with radiative transitions. Thus models of radiative recombination of carriers need not be based on the presence of such a shoulder.
3. Since the size of the shoulder shows significant variations with deposition parameters, this suggests that it is caused by defects rather than being an intrinsic property of the film.

We are currently measuring the photoconductivity as a function of photon energy and comparing these results with the absorption measurements to deduce the dependence of η_{ph} on photon energy.

Table I. Sample Parameters

Sample	Deposition Conditions	Substrate	Thickness (μm)
Xerox			
1	1 W rf 5% SiH_4 in Ar	100°C-7059 glass	2.27
2	1 W rf 100% SiH_4	230°C-Quartz	0.7
3	2 W rf 10^{-3} P	230°C	1.1
4	2 W rf 5% SiH_4 in Ar	230°C-Quartz	1.15
5	5 W rf 10% SiH_4 in Ar	230°C-Quartz	1.01
6	15 W rf 5% SiH_4 in Ar	230°C-Quartz	1.825
7	30 W rf 10% SiH_4 in Ar	230°C-Quartz	2.29
8	40 W rf 5% SiH_4 in Ar	230°C-Quartz	1.55
RCA			
9	DC Proximity discharge	250°C- SiO_2	2.8
10	DC Proximity discharge	330°C- SiO_2	.95

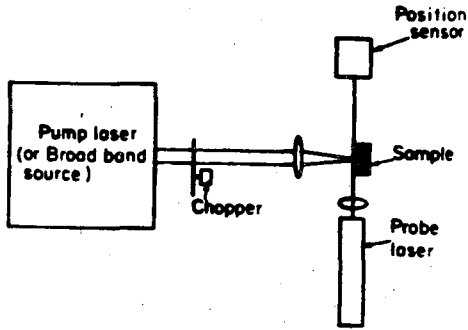


Fig. 1. Experimental configuration. The broad band output is passed through a monochromator before the chopper.

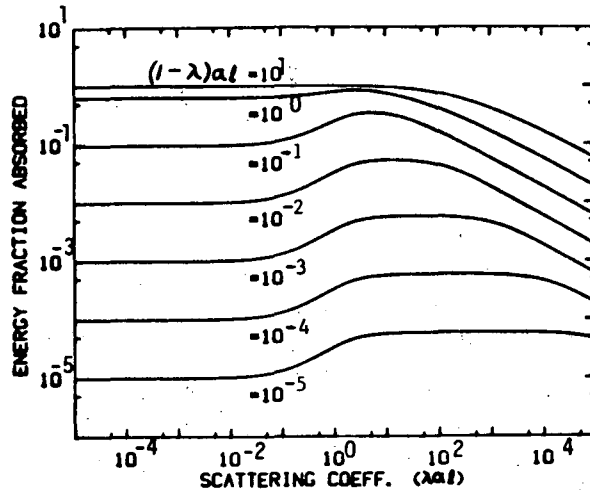


Fig. 2. Theoretical PDS signal vs. scattering ($\lambda\alpha l$) for different absorptions. λ is the fraction of light scattered and α is the total attenuation coefficient.

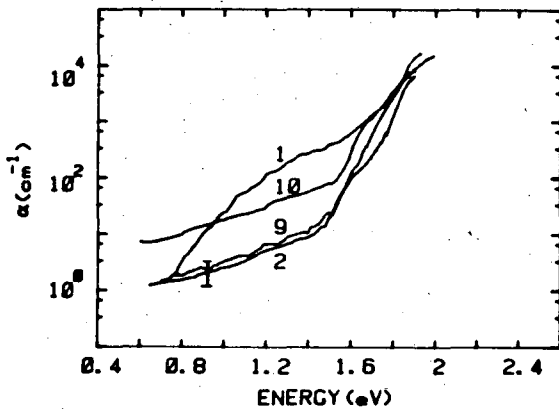


Fig. 3. Absorption vs. photon energy for various substrate temperatures.

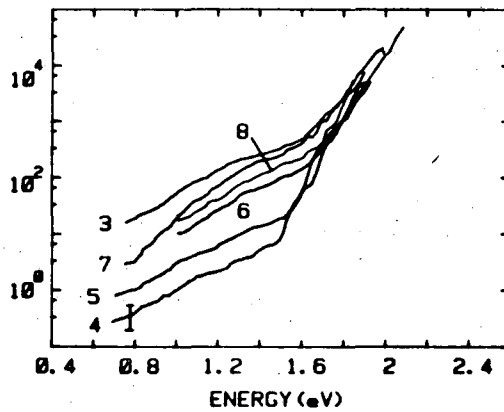


Fig. 4. Absorption vs. photon energy for various rf powers. 3 is phosphorous doped.

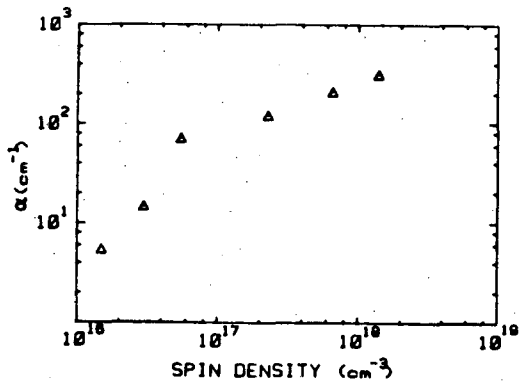


Fig. 5. Absorption vs. spin density (provided by the Xerox group).

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