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Optical properties of hydrogenated amorphous silicon[a)]

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A detailed study of the optical properties of sputtered hydrogenated amorphous silicon films with varying hydrogen concentration is presented here. The energy dependence of the absorption coefficient is looked into, in detail, from a point of view of understanding the well known Tauc rule and the alternate relations being proposed in recent years. Spectroscopic and band-structural models like Wemple–Didomenico and Penn are then utilized to analyze the optical parameters near the band-gap region of the wavelength spectra. Extensive comparisons of our results are made with those of sputtered *a*-Si:H films of other workers, glow discharge prepared *a*-Si:H, chemically vapor deposited and evaporated *a*-Si, and also crystalline silicon. The similarities in the variation of the optical properties of *a*-Si:H with increasing hydrogen concentration (or decreasing measurement temperature) to that of crystalline silicon with decreasing measurement temperature lead us to interesting conclusions. Thus, it seems that decreasing disorder (topological or thermal) in *a*-Si:H is equivalent to decreasing thermal disorder in *c*-Si, at least as far as the disorder-optical property relationships are concerned.

I. INTRODUCTION

Hydrogenated amorphous silicon continues to interest material scientists and device physicists from the point of view of (i) the possibility of having tailor made materials with made-to-order properties, (ii) highly technology-dependent varying material properties, (iii) an inexpensive technology, and (iv) the promise of replacing crystalline silicon in its utilization in the fabrication of solar cells. Recent reviews[1–5] have dealt with, in detail, the physics, chemistry, technology, and applications of this fascinating material. In spite of all this, quite a lot of work needs to be done to correlate precisely the technology–hydrogen content–property relationships.

With a view to understand and analyze such relationships, we present here our studies of the optical properties of a set of magnetron sputtered *a*-Si:H films prepared under very similar conditions with varying hydrogen concentrations. We then attempt to interpret these optical properties in terms of well-accepted models. Wherever relevant, comparisons are made with the results in the literature for *a*-Si:H films prepared by well-known methods, as also with crystalline silicon.

II. EXPERIMENTAL DETAILS

The samples were prepared by magnetron sputtering of two Czochralski grown monocrystalline silicon targets (of 120-cm diameter) of about 10 Ω cm resistivity. The targets were supplied with a constant power of 500 W. Power densities on the targets were typically in the range of 3–4 W/sq cm. The substrate temperature was maintained at 250 °C. The substrates were held at a floating potential in Ar-H_2 atmosphere at a total pressure of $(5–10)\times 10^{-3}$ mbar. Distance between the targets and the substrates was maintained at 41 mm. The substrates were mounted on a rotating table.

The systems total leak rate was less than 10^{-6} mbar l s^{-1}. Deposition rates were typically in the range of 1–2.5 Å/s. Hydrogen content in the sputtering gas was varied from 3–20% by volume in the Ar-H_2 atmosphere. Thus, the partial pressures of H_2 and Ar in the H_2-Ar mixture, p_H and p_{Ar} were the only variable parameters during the deposition of the films. Films were deposited on suprasil quartz, crystalline silicon, and hyperfine graphite substrates. Film thicknesses were determined[7] from stylus displacement measurements or by the method of Fizeau fringes viewed with a varian interferometer.

The hydrogen content in the films and the bonding configurations were determined, respectively, from resonant nuclear reaction method $^{15}N + {}^{1}H \rightarrow {}^{12}C + {}^{4}He + \gamma$ and infrared absorption measurements.[7,8] Transmittance and reflectance measurements were made in the wavelength range of 0.2–1.5 μm with a Beckman UV-visible-NIR spectrophotometer model UV 5240.[7] Resistivities were measured[7] under vacuum using a high sensitivity electrometer. Further details of the electrical, infrared, and nuclear measurements are reported elsewhere.[6–8]

[a)] This work is a result of the study carried out by the last author (N. M. R.) on samples prepared at Elettrorava (PR) and the experimental measurements and the optical constant (n, k) evaluations made at the Polytechnic (F. D. *et al.*).

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III. RESULTS, THEORY, AND DISCUSSION

Although the measurements of transmittance (T) and reflectance (R) have been made[7] in the wavelength range of 0.2–1.5 μm, most of the discussions will be centered around $\lambda = 0.4 - 1.15$ μm, that is near the band-gap region of aSi:H. The measured T, R, and the thickness of the films lead to an evaluation of the optical constants—the refractive index (n) and the extinction coefficient (k).[7] For details of the method, see Ref. 9. The absorption coefficient α hence follows ($\alpha = 4\pi k/\lambda$). In Fig. 1, log α is plotted vs E for the four samples under consideration. In Table I, the main features of these films are noted. As can be seen in the figure, the absorption coefficient decreases systematically with increasing hydrogen content C_H (for a given energy E).

It may be noted here that the absorption coefficient α or the imaginary part ϵ_2 of the complex dielectric constant $\epsilon = \epsilon_1 + i\epsilon_2$ ($\alpha = 4\pi k/\lambda = \omega\epsilon_2/\text{cn}$) is proportional to the joint density of states at the considered frequency and to the square of the momentum matrix elements between initial and final states.[10] Such a decrease in α with increasing C_H reflects a decrease in ϵ_2 with increasing C_H. ϵ_2 has been looked into, in detail, by several workers for glow discharge prepared,[11–14] electron-gun evaporated,[15] and LPCVD-prepared[16–18] a-Si films. Comparisons of such studies of ϵ_2 have also been reported in the literature.[19,20] However, in spite of the tremendous amount of work on the optical properties of rf-sputtered a-Si:H,[21–24] to the best of our knowledge, no such studies of ϵ_2 on these films exist in the literature. Such studies have been made only near the region of the energy gap in the energy range 1–3 eV.

As we shall see later on during this study, reflectance spectra of our samples (Fig. 8) show none of the sharp features present in the crystalline silicon spectra. This is understandable by virtue of the absence of the long-range order present in the crystalline phase. But, most of the macroscopic features like the shape and the width of the ϵ_2 spectra and the energy corresponding to the peak which is comparable to the Penn gap[25] are almost the same. As can be seen in Table II, at least for CVD and evaporated films, at low values of the photon energy, ϵ_2 attains a maximum which is also lower than either crystalline or glow discharge prepared amorphous silicon. For glow-discharge films (prepared by rf discharge), with decrease in the substrate temperature T_s, C_H increases, ϵ_2 max decreases, and E' (the energy corresponding to ϵ_2 max) moves to higher energies. This shift of E' to higher energies with decreasing T_S reflects an increase in strong bonds. The Si-H bond is known to be stronger than the Si-Si bond and hence an increased C_H aids E' to increase.

Although similar effects are expected in sputtered a-Si:H films, no proof of these exists in the literature. After all,

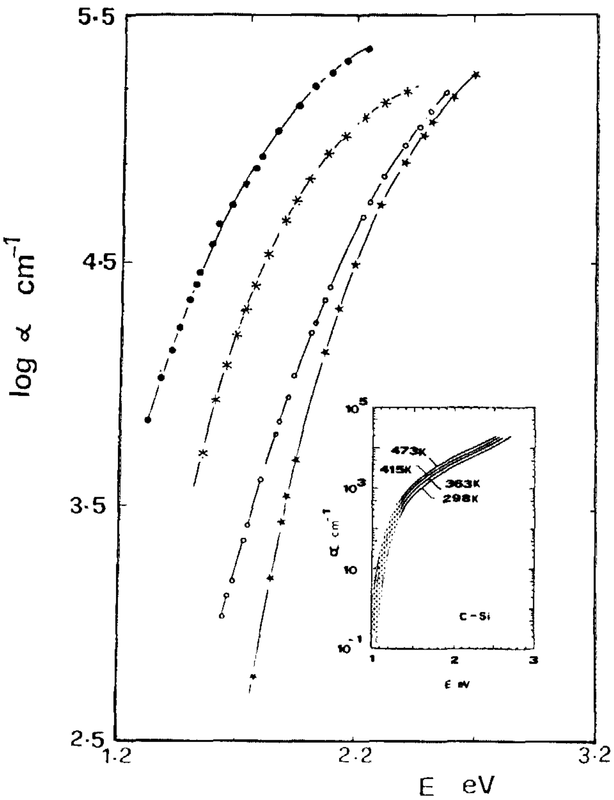

FIG. 1. The absorption coefficient vs energy near the region of the energy gap. The results have been compared with those for crystalline silicon measured at different temperatures (figure inset).[28] Symbols: in Figs. 1–5 and 8, the following symbols represent the samples: ● SIE 30, * SIE 31, ○ SIE 32, ⋆ SIE 33.

TABLE I. Some relevant characteristics of a-Si:H films.

Sample	SIE 30	SIE 31	SIE 32	SIE 33
% H_2 [a]	0	3	12	20
C_H at. % [b]	$\simeq 0$	9	23	29
Thickness μm	0.28	0.38	0.37	0.40
ρ (300 K) Ω cm	1.82×10^3	1.16×10^6	1.55×10^6	1.01×10^6
E_{GT} (eV) (Fig. 2)	1.31	1.47	1.76	1.90
C_T (eV cm)$^{-1/2}$	871.14	720	786.03	847.06
E_{GF} (eV) (Fig. 3)	1.01	1.23	1.54	1.64
C_F (eV^2 cm)$^{-1/3}$	69.90	65.69	71.93	76.84
E_{GC} (eV) (Fig. 4)	1.08	1.35	1.64	1.70
C_C (eV^3 cm)$^{-1/2}$	325.64	297.08	273.12	256.57
R_{max} % (Fig. 8)	62.33	61	55.66	53.33
E_{GTO}/E_{GTH}		0.9	0.75	0.7

[a] Percentage of hydrogen by volume in the sputtering atmosphere.
[b] Atomic percentage of hydrogen in a-Si:H films determined by resonant nuclear reaction method (see Refs. 7 and 8).
[c] $E_{GTO} = 1.31$ eV is the Tauc gap if SIE 30 (with minimum C_H). The ratios E_{GTO}/E_{GTH} are to be compared with n_H/n_0 in Fig. 7.

TABLE II. ϵ_2 peak values and the corresponding energy for c-Si and several types of amorphous silicon.[a]

Material	ϵ_2 max	E' (eV)	H (at. %)	T_S (°C)
c-Si	35.5;46.5	3.3;4.2	...	
Gd-a-SiH_x	31.5	3.7		
CVD a-Si	26	3.4		
evap. a-Si	20	2.9		
Gd-a-SiH_x	31.5	3.7	7.9	350
Gd-a-SiH_x	27.7	3.75	14.2	280
Gd-a-SiH_x	26.2	3.85	19.9	150
Gd-a-SiH_x	23.85	3.88	26.8	50

it is now well known that at a constant p_H, C_H increases with decrease in T_S (similar to glow-discharge films) for sputtered films.[22] Of course, increasing p_H at a constant T_S is another means to increase C_H. However, the results of Oguz and Paesler[26] indicate that C_H attains a maximum value of about 26 at. % ($T_S = 200$ °C) and decreases as p_H increases. Although a saturation value is preferred thermodynamically, the difficulties in appreciating such a decrease in C_H with increase in p_H remain.[27] At least for glow-discharge deposited films, no such behavior of a decrease in C_H (with decrease in T_S) is reported in the literature.[12]

In Fig. 1, with decrease in C_H, the absorption edge moves to lower energy. Such a red shift is similar to the shift of the absorption edge of crystalline silicon (c-Si) to lower energies with increasing temperature.[28,29] Our results in Fig. 1 are compared with those of Weakliem and Redfield[28] (figure inset). Figure 1 leads us to evaluate and examine the optical gap better known as the Tauc gap[30] and the alternate definitions being proposed in recent years.[20,31,32]

In early optical measurements on a-Ge[33] and a-Si,[34] it was found that in the energy range 1.2–2.2 eV [that is, $\alpha > (2–5) \times 10^4$ cm^{-1}], ϵ_2 varied as

$$\epsilon_2 E^2 = A(E - E_G)^2, \tag{1}$$

or

$$(\alpha E)^{1/2} = C_T(E - E_{GT}), \tag{2}$$

where E_{GT} is defined as the optical gap or the Tauc gap of the material. The above expression (2) is the well-known Tauc formula applicable to many amorphous semiconductors. E_{GT} is a measure of the optical transitions between extended states in the valence and conduction bands under the assumption of parabolic bands and constant matrix elements. These transitions do not involve conservation of momentum.

For a-Se, Davis[35] has reported that

$$(\alpha E) = C(E - E_G). \tag{3}$$

In multicomponent glasses, a relationship such as

$$(\alpha E)^{1/3} = C_F(E - E_{GF}) \tag{4}$$

has been reported by Fagen and Fritzsche.[36] Most of the variations in the $\alpha - E$ relationships have been attributed to (1) deviations from the parabolicity in the nature of the bands, and (2) the choice of matrix elements. Eventually, Mott and Davis[37] have attributed to the power N [where $\alpha E = C(E - E_G)^N$] a value ranging from 1 to 3.

Klazes et al.,[32] in agreement with Vorlicek et al.,[31] find that the exponent 1/3 fits the absorption data much better than 1/2 and therefore utilize $(\alpha E)^{1/3}$ vs E plot to evaluate the optical gap of glow-discharge and sputter-deposited a-Si:H films. Nitta et al.[14] and Cody et al.[20] find that the Tauc formula gives the best overall result in explaining the optical absorption for a-Si:H. Since the maximum energy E_{P1} in the photoluminescence spectra is known to be equal to or smaller than the optical gap, Nitta et al.[14] compare the optical gaps with E_{P1} and arrive at the above conclusion.

An alternative to all these expressions has been examined recently by Cody.[20] From analytical considerations of ϵ_2, based on a slightly different approach, Cody finds that

$$(\alpha/E)^{1/2} = C_C(E - E_{GC}). \tag{5}$$

It has further been concluded that one could distinguish between $(\alpha E)^{1/2}$ and $(\alpha/E)^{1/2}$ as a definition of the gap only while dealing with films of varying thicknesses.[20] Aspnes et al.[17] concur with Klazes and Cody [expressions (4) and (5), respectively] in their studies on LPCVD—a-Si films.

In Figs. 2, 3, and 4, $(\alpha E)^{1/2}$, $(\alpha E)^{1/3}$, and $(\alpha/E)^{1/2}$ are plotted vs E, respectively. In Fig. 2 the results are also compared with that of c-Si measured at different temperatures (figure inset). The values of the extrapolated gaps E_{GT}, E_{GF}, and E_{GC} and the respective slopes, C_T, C_F, and C_C are reported in Table I. While the usage of the 1/3 exponent decreases the Tauc gap by about 0.3 eV, in general, the gap increases with increase in C_H (or p_H). The gaps E_{GF} of our samples are comparable to those of Klazes et al.[32] for rf-sputtered a-Si:H films, but, the slopes C_F differ. Further, the

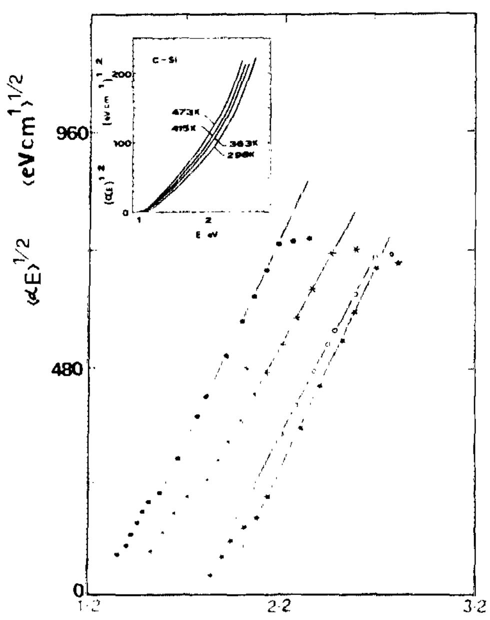

FIG. 2. $(\alpha E)^{1/2}$ vs E extrapolated to zero absorption to obtain the energy gap in accordance with the Tauc rule. Figure inset: the spectral region showing the slope changes associated with the fundamental indirect transition at several temperatures for crystalline silicon.

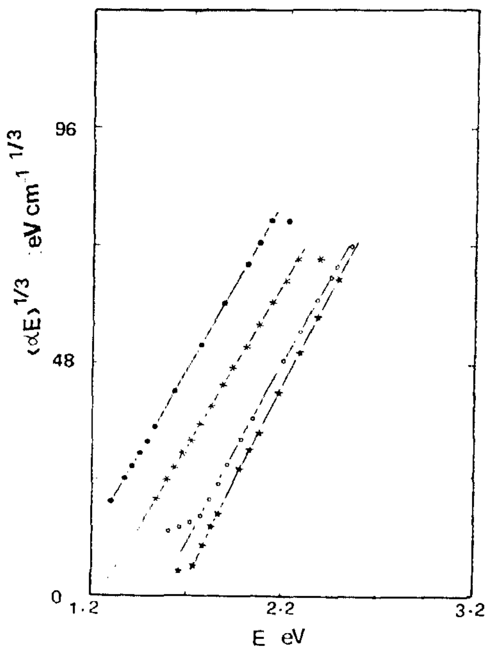

FIG. 3. $(\alpha E)^{1/3}$ vs E in order to examine the (1/3) exponent law.

increase in the gap E_{GT} with C_H for our samples is very similar to those of Moustakas for sputtered films.[38] However, unlike the results of Cody *et al.*[39] (for sputtered films), our results of the slope C_T-gap E_{GT} variations are nonlinear (see Table I). As C_H increases from 0 to 29 at. % for our films, C_T varies between 720 to 870 $(\text{eV cm})^{-1/2}$, that is in the range of values of C_T of Cody *et al.*[39]

While the slope C_T of $(\alpha E)^{1/2}$ vs E plot has a fundamental role in the optical matrix elements, it also has importance in photovoltaic applications. An optical gap of $E_{GT} < 1.6$ eV and $C_T > 320$ $(\text{eV cm})^{-1/2}$ would be suited for solar cell applications.[40,41] C_T is an extremely preparation-sensitive parameter. It has been seen earlier that, for *a*-Si:H films, C_T takes values from 640 to 780 $(\text{eV cm})^{-1/2}$.[42] For vacuum deposited films, C_T is about 540 $(\text{eV cm})^{-1/2}$, while for sputtered *a*-Si,[22] it is known to be about 650 $(\text{eV cm})^{-1/2}$. However, for films deposited chemically, at 650 °C, $C_T = 980$ $(\text{eV cm})^{-1/2}$.[43] For *c*-Si, $C_T = 133$ $(\text{eV cm})^{-1/2}$.[44]

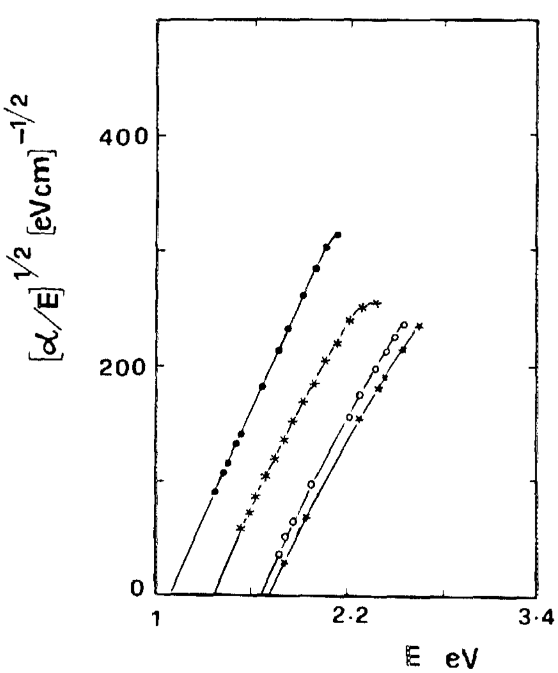

FIG. 4. $(\alpha/E)^{1/2}$ vs E in an attempt to investigate the interpretations of Cody.[20]

Thus, this small value of C_T for *c*-Si compared to that of *a*-Si:H reflects the deviation of the structure of *a*-Si:H from that of *c*-Si. In Fig. 4 we demonstrate the definition of Cody [Eq. (5)] for the gap E_{GC}. As can be seen in the figure, although the thicknesses of our films are in the range of only 0.28–0.40 μm,[7] the gaps E_{GC} obtained from the plot 4 are in better agreement with E_{GF} (differing by only 0.1 eV), than with the Tauc gap E_{GT} (see Table I). However, what remains interesting is a systematic decrease in the slope C_C with increasing C_H (Table I). We shall see later that our values of the refractive indices (n) and their dependencies on wavelength (λ) are in good accord with the Tauc gap E_{GT} and its variation with C_H, thus reiterating our faith in the Tauc formula.

The Si-Si bond strength is known to be 1.94 eV compared to the Si-H bond strength of 3.06 eV.[45] Thus, at high C_H, the optical gap is essentially controlled by the bonding configuration. The upper limit of the gap of *a*-Si:H is 2.4 eV characteristic of polysilane.[46] This has been confirmed by the recent work of Furukawa and Matsumoto[47] in their studies of optical and electrical properties of wide E_G (up to 2.4 eV) *a*-Si:H alloys containing many $(SiH_2)_n$ groups prepared by rf-glow discharge of disilane. Their studies indicate an increase in E_G with decrease in T_S.

Freeman and Paul[48] found different optical gaps for the same C_H within the films prepared by rf cathodic sputtering. They reported a monotonic increase of the gap with SiH_2 content in the material. Thus, it seems that the SiH_2 content is controlled not only by C_H. Bruyere *et al.*[49] attributed this to the deposition rate. They[49] were able to decrease E_G from 1.97 to 1.56 eV (at $T_S = 250$ °C) by increasing only the deposition rate from 15 to 100 Å/min, with the same reactive mixture of 20% H_2-80% Ar. However, at least the quality of the sputtered *a*-Si:H, that is, the density of states in the middle of the gap and the recombination properties, do not depend on the Si-H configuration, but on the total C_H in the film.[50] Our studies here consistently show that, at least as far as the optical quality is concerned, it is sufficient to vary p_H alone, with other experimental parameters fixed at values as mentioned earlier, to obtain good optical quality films.

In Table III values of E_{GT} for our samples are compared with those of Morel and Moustakas[51] (for sputtered films). As can be seen in the Table, our results are in good agreement with those of Morel and Moustakas.[51] The slight difference of about 0.1 eV may be attributed to variations in the deposition conditions. This difference is, however, negligible.

In Fig. 5, our results of the refractive indices are plotted as function of wavelength for varying C_H. The results are also compared with *c*-Si (figure inset; also, as function of temperature). With increasing C_H, n approaches a value of *c*-Si at about 0.45 eV but decreases further at longer wavelengths. This variation is generally in agreement with those

TABLE III. Variation of E_G with C_H for the samples studied compared to those Morel and Moustakas[51] for sputtered films.

Sample[2]	C_H (at. %)	E_G (eV)
SIE 30	0	1.31
248	8	1.58
SIE 31	9	1.47
245[a]	13.8	1.68
246	19.5	1.81
247	19.8	1.83
273	21.5	1.86
SIE 32	23	1.76
258	23.8	1.89
251	25	1.92
SIE 33	29	1.9

[a] Samples 245–273 are prepared by rf sputtering of a polycrystalline target at $T_S = 275\,°C$ (see Ref. 51 for details). For details of nuclear measurements, see Demichelis *et al.* (Refs. 7 and 8).

of Zanzucchi *et al.*[52] They[52] have reported their studies of the optical and photoconductive properties of rf discharge produced *a*-Si films prepared at various substrate temperatures of 195, 325, and 420 °C. It is generally expected that C_H decreases with increase in T_S.[12] In Fig. 6 their results are plotted and compared with that of *c*-Si.[53] As can be seen in the figure, while for our films n decreases over all λ in the range 0.4–1.00 μm, the behavior of discharge produced films (Fig. 6) is not so systematic. This leads us to believe that the sputtering technique has an inherent advantage over glow discharge in the fact that the hydrogen content in the films can be varied simply by adjusting p_H in the argon sputtering atmosphere with all other parameters remaining fixed. This study will naturally lead to (a) a knowledge of the influence of hydrogen alone on eliminating or creating defects in *a*-Si,[27] (b) good reproducibility of the films, and (c) an easy control over the optical/electronic quality of the films. Further, as can be seen in Fig. 5, there is a one-to-one resemblance between the hydrogen incorporation into *a*-Si and temperature effects on *c*-Si, with respect to the n-λ variations.

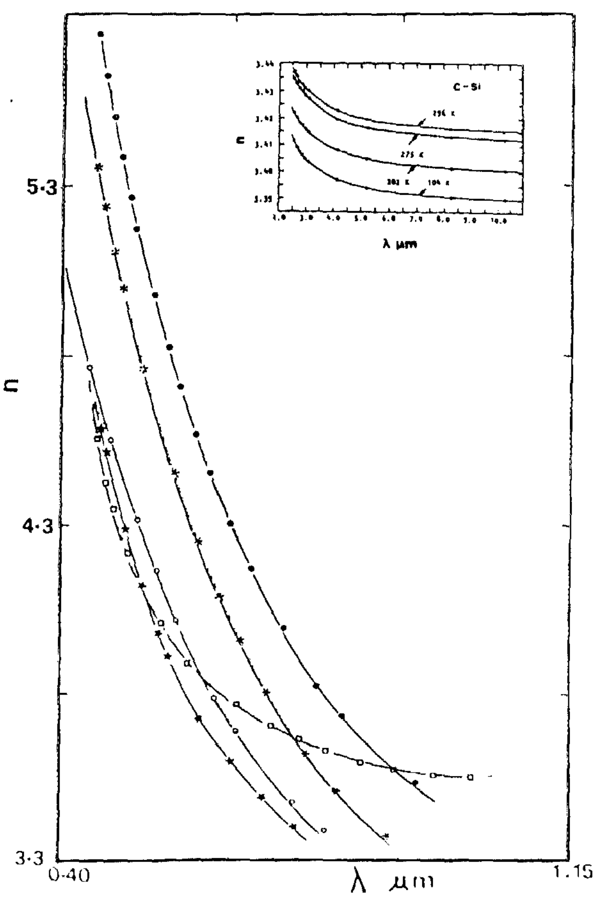

FIG. 5. Refractive index n vs wavelength λ for *a*-Si:H samples compared with crystalline silicon. Figure inset: refractive index of crystalline silicon at four temperatures in the long wavelength range. Symbols: □ crystalline silicon; rest of the symbols as explained in caption of Fig. 1.

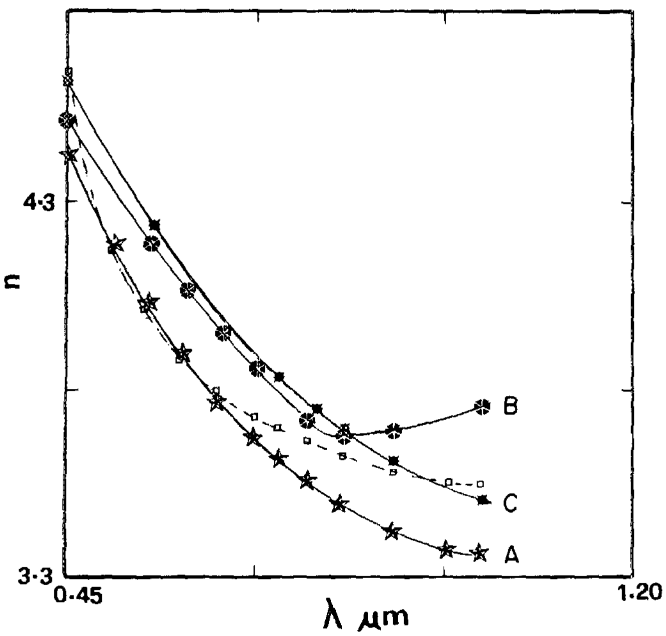

FIG. 6. n vs λ for *a*-Si:H films prepared by glow discharge compared with crystalline silicon (data taken from Ref. 52). Symbols: ✯A ($T_S = 195\,°C$); ✱B ($T_S = 325\,°C$); ■C ($T_S = 420\,°C$).

The monotonic decrease in n with T over all λ (figure inset) for *c*-Si[54] is similar to that of n with increasing C_H over all λ for *a*-Si:H. Moustakas[50] finds a decrease in n with increase in p_{Ar} at $\lambda = 2\,\mu m$ for sputtered films.

At this stage, it would be worthwhile to look into the $n - \lambda$ variations. The well-known Wemple–Didomenico model[55,56] explains the $n - \lambda$ behavior in the form

$$n^2(E) - 1 = \frac{E_d E_0}{E^2 - E_0^2}, \tag{6}$$

where E_d is the dispersion energy and is proportional to the volume density of valence electrons involved in the transitions at E_0, E_0 is an average excitation energy or an interband transition energy (almost equal to the Penn gap[25]) coinciding with the energy corresponding to ϵ_2 max in the ϵ_2-E spectra. Thus, a plot of $1/[n^2(E) - 1]$ vs E^2 will be a straight line and yields values of E_d and E_0. Wemple[56] has argued that E_d (corrected for differences in the densities) depends on the short-range order only and is the same in the crystalline and amorphous forms if the short-range order (the first coordination number) is the same.

TABLE IV. Derived spectroscopic parameters with relevance to Wemple–Didomenico model compared with glow-discharge prepared films of Zanzucchi *et al.*[52]

Sample [a]	E_d (eV)	E_0 (eV)	T_S (°C)
SIE 30	47.82	2.63	250
SIE 31	32.87	2.63	250
SIE 32	29.54	2.69	250
SIE 33	30.51	2.80	250
A[a]	30.64	2.18	195
B	49.42	2.20	325
C	47.49	2.26	420
c-Si	48.38	2.52	—

[a] Samples A, B, and C are prepared by the glow-discharge decomposition of silane.

The data in Figs. 5 and 6 lead us to evaluate E_d and E_0. The results are presented in Table IV. As can be seen in the Table, E_d for sample SIE 30 ($C_H \simeq 0$ at. %) is comparable to the crystalline silicon value. Similarly, samples B and C of Zanzucchi *et al.*[52] which are prepared at high T_S have values of E_d comparable to that of *c*-Si. Tables III and IV permit us to compare E_0 with E'—the energy corresponding to ϵ_2 max in the ϵ_2-E spectra. As is evident from the tables, the evaporated *a*-Si value of 2.9 eV for E' is comparable to E_0 of sputtered films.

While the E_d values of our samples are comparable to those of de Neufville *et al.*[57] for reactively sputtered *a*-SiH_x films, the values of E_0 are however smaller. A nearly systematic decrease in E_d and an increase in E_0 with increasing C_H for our samples is almost similar to those of Zanzucchi *et al.* (see Table IV). A monotonic increase of E_0 with C_H is expected because of the higher oscillator strength or the binding energy of the Si-H bond over the Si-Si bond. Such an increase is similar to the shift of E' to higher energies with increasing C_H^{12}, for *a*-Si:H films prepared by rf glow discharge (see Table II). Our results of E_d in Table IV are in accord with Wemples' contention[56] of the dependence of E_d on the short-range order.

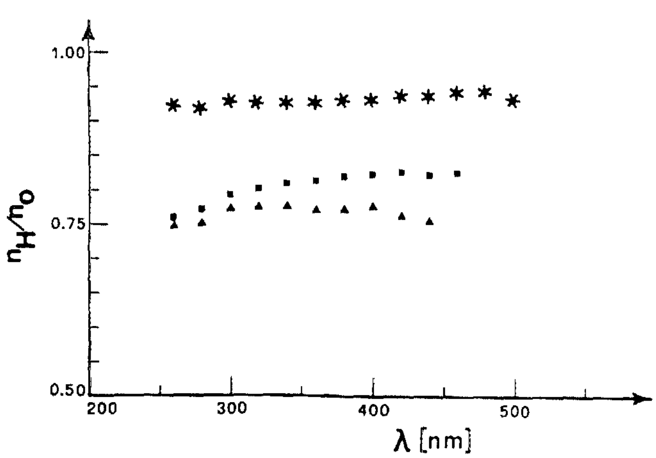

FIG. 7. Ratio of the index of refraction of film with different hydrogen concentrations (n_H) to the index of refraction of film with almost no hydrogen (n_0) vs wavelength.[7] Symbols: * n_{31}/n_{30}; ■ n_{32}/n_{30}; ▲ n_{33}/n_{30}.

In Fig. 7, the ratios of the indices of refraction (n_H) of samples SIE 33, SIE 32, and SIE 31 to SIE 30 (n_0) are plotted as functions of λ.[7] As can be seen in the figure, the ratios decrease with increasing C_H, over all λ. From Figs. 2 and 5, we have seen earlier that, with increase in C_H, E_G increases while n decreases. Such a decrease in n with increasing E_G is consistent with many general models.[25,55,58,59] For a model semiconductor, the high-frequency dielectric constant is given by[25]

$$\epsilon_\infty \simeq n^2 \simeq 1 + (\hbar\omega_p/E_P)^2, \tag{7}$$

where $\hbar\omega_p$ is the valence electron plasmon energy, and E_P is an average gap referred as the Penn gap (comparable to E_0, as also E'). The Penn model has been employed successfully by several workers to explain the optical properties of *a*-Si.[10,12,20,22,30,42] Since typical values of $\hbar\omega_p$ for *a*-Si:H films are ~ 15 eV and $E_P = 3.5$ eV,[12] Eq. (7) may be approximated as

$$n \simeq \hbar\omega_p/E_p,$$

or

$$n_2/n_1 \simeq E_{P1}/E_{P2},$$

neglecting the small changes in $\hbar\omega_p$. One feature common to most of the semiconductor band structures is that the valence and conduction bands are more or less parallel to one another, at least along the symmetry directions.[59,60] Thus, the energy gap or the optical gap varies linearly with the Penn gap. Thus,

$$n_1/n_2 \simeq E_{G2}/E_{G1}. \tag{8}$$

Results in Fig. 7[7] for our samples are consistent with Eq. (8) (see Table I). In Fig. 8, reflectance R is plotted versus energy for the films. The results have been compared with those of Pierce and Spicer[15] for pure *a*-Si prepared by vacuum deposition, as also, with *c*-Si[28] (figures inset). As can be seen in the figure, none of the sharp features in the *c*-Si spectra are visible in the *a*-Si spectra. A broad peak occurs with R_{max} decreasing from $\sim 63\%$ to $\sim 53\%$ with increasing C_H. Such a decrease in R_{max} with increasing C_H is in accord with the results for glow-discharge deposited films of *a*-Si:H of similar thicknesses.[11,13,14] Increasing T has similar effects on *c*-Si[28] (see figure inset). These studies are useful because *a*-Si films are known to become transparent rapidly at low photon energies.

Last but not least, values of the resistivity of our films[7] are in accord with those of Moustakas[27] and Brodsky *et al.*[23] for sputtered films. Although incorporation of hydrogen has increased the resistivity by three orders of magnitude (see Table I), the values are still lesser than those of Chittick[61] for glow-discharge prepared films. However, the general trend in the variation of ρ with C_H (increasing, attaining a maximum and then decreasing) is similar to that of Chittick (Table I).

IV. CONCLUSIONS

An investigation into the optical properties of sputtered hydrogenated amorphous silicon films has been reported in the above study. While all the preparation parameters have been maintained constant, only the partial pressures of hy-

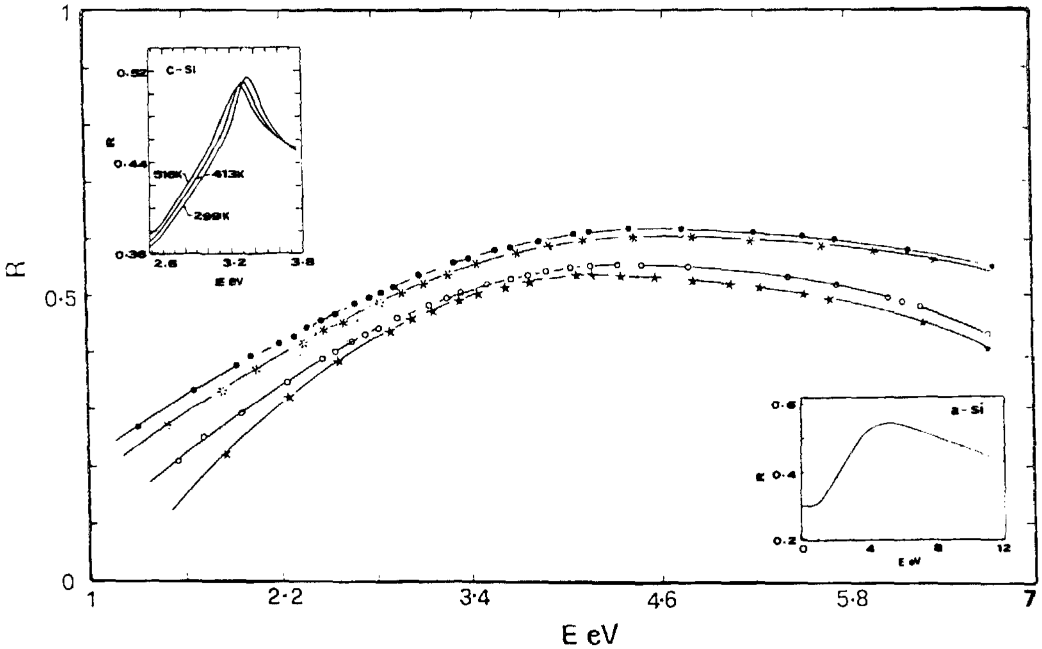

FIG. 8. Reflectance R vs energy for a-Si:H films. The results are compared with those of Pierce and Spicer[15] for pure a-Si films prepared by evaporation (figure inset; bottom right). Comparisons are also made with that of crystalline silicon measured at different temperatures (figure inset; top left).[54]

drogen and argon have been changed in order to obtain detailed informations on the influence of hydrogen content on the optical properties. Various possible alternatives to the Tauc rule to explain the variation of the absorption coefficient with energy, and their implications were discussed. Interpretation of our data and comparisons with the data in the literature were sought in terms of well-known models like those of Wemple–Didomenico and Penn. Detailed comparisons with amorphous silicon films prepared by sputtering and also by other methods, of other workers, were made above. Wherever relevant, comparisons with crystalline silicon were also looked into. These studies have shown that similarities in the optical property variations outweigh the differences. In particular, with increase in hydrogen concentration (or decrease in measurement temperature) for a-Si:H and, with decrease in measurement temperature for crystalline silicon, (i) the magnitude of the absorption coefficient at a wavelength decreased, (ii) the energy gap increased, and (iii) the refractive indices decreased systematically over all wavelengths.

Thus, generally, the influence of hydrogen (or temperature) on a-Si:H and the temperature effects in c-Si, on their optical properties appear to be similar. In conclusion, at least as far as the optical properties are concerned, the decrease in disorder (topological or thermal) in a-Si:H and the decrease in thermal disorder in c-Si on lowering measurement temperature have similar effects on their optical properties. This conclusion could go a long way in a better understanding of the disorder—optical property relationships in crystalline and noncrystalline solids such as those of Cody. Detailed theoretical calculations are being taken up to understand these variations.

However, from the technology point of view, a lot of work remains to be done. The role of substrate potential and its influence on the optoelectronic properties of sputtered a-Si:H films forms our work for the immediate future.

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