Temperature dependence of optical constants for amorphous silicon

Nhan Do,[a] Leander Klees,[b] P. T. Leung,[c] Frank Tong,[d] Wing P. Leung,[e] and Andrew C. Tam

IBM Research Division, Almaden Research Center, 650 Harry Road, San Jose, California 95120-6099

The temperature dependence of the optical constants for amorphous silicon (a-Si) is studied for two different sample thicknesses at two infrared wavelengths. It is observed that the extinction coefficient of a-Si can increase significantly with temperature in the strong absorption regime. In addition, using the Mott–Davis formula, results are obtained for the variation of the optical gap energy for a-Si with temperature, with similar feature observed for both amorphous and crystal silicon.

The temperature dependence of optical properties for crystalline solids has been studied extensively.[1-3] Such knowledge is important in any photothermal processing of the material, such as laser annealing. On the contrary, amorphous substances such as silicon (a-Si) are much less studied in this aspect, although there is an extensive literature on room-temperature measurements[4] of optical constants at different wavelengths. Previous studies have reported that there is almost no temperature variation of the absorption coefficient for submicron thick a-Si samples at the Nd:YAG laser wavelength (1.06 μm).[5-7] It has then been sometimes assumed that unlike crystalline silicon (c-Si),[2] the optical constants of a-Si can indeed be taken as independent of temperature.[8]

In this letter, we present a thorough study on the dependence of the optical constants $n(T)$ and $k(T)$ as functions of temperature T for a-Si. We shall see that such dependence manifests itself significantly in a stronger absorption regime.

The a-Si samples for our experiment are prepared by e-beam evaporation of c-Si in vacuum (10^{-7} Torr) onto fused quartz substrates (250 μm thick). The substrate temperature is kept at 140 °C and the deposition rate at 10 Å/s. Different thicknesses of a-Si are prepared by controlling the deposition time, the uniformity and accuracy of these thicknesses are confirmed using the Tencor Alpha-Step 200 surface profilometer. The samples are then annealed at a temperature of 380 °C in a nitrogen chamber for about 5 h until optical measurements (reflectance and transmittance) versus change of temperature are reproducible for these samples. Under these conditions, the formation of oxide or nitride is kept at a minimum.[9] Stress relaxation of the sample is observed after the above heat treatment.

We have followed the standard reflectance ($\mathscr{R}$) and transmittance ($\mathscr{T}$) measurements for the determination of $n(T)$ and $k(T)$ for our a-Si samples.[10] Two different wavelengths of light are incident at a small angle (5°) onto the sample which is mounted on a heated aluminum block. The heater-thermal couple system can vary the sample temperature from room temperature to about 400 °C. The $\mathscr{R}$ and $\mathscr{T}$ signals at each temperature are detected by photodiodes which are connected to an oscilloscope. It is observed that for the 0.2 μm a-Si sample, both $\mathscr{R}$ and $\mathscr{T}$ are in the "interference region"[10,11] at the two wavelengths (0.752 and 1.15 μm) we studied. For the 1.0 μm sample, clear interference patterns only show up for 1.15 μm, with $\mathscr{T}$ decaying monotonically with temperature for 0.752 μm wavelength.[11]

The measured values for $\mathscr{R}$ and $\mathscr{T}$ are then fed into a computer iteration program to obtain values for n and k using Fresnel formula for a multilayer system. The results are shown in Figs. 1 and 2. We have taken into account the expansion of the layers by assuming the linear expansivity for a-Si and fused quartz to be 3×10^{-6} and 5×10^{-7} °C^{-1}, respectively. Figures 1(a) and 1(b) show the results for the 0.2 μm sample. While we see a slow linear rise of $n(T)$ with $dn/dT = 1.3 \times 10^{-4}$ °C^{-1}, a situation similar to the case of c-Si, the behaviors for $k(T)$ are quite different. At $\lambda = 1.15$ μm, we do find that the average dk/dT ($< 10^{-5}$ °C^{-1}) is totally insignificant, in agreement with previous observations at 1.06 μm.[5-7] However, $k(T)$ shows a significant increase at $\lambda = 0.752$ μm which is approximately linear with a slope equal to 2.3×10^{-4} °C^{-1}. For the 1.0 μm sample, Fig. 2(a) shows the same linear behavior with $dn/dT = 5.0 \times 10^{-4}$ °C^{-1} at $\lambda = 0.752$ μm. Figure 2(b) shows significant increase of k with temperature, both at 0.752 and 1.15 μm. While $dk/dT = 2.0 \times 10^{-4}$ °C^{-1} for $\lambda = 1.15$ μm, $k(T)$ for 0.752 μm is obviously nonlinear and can be fitted by the following expression:

$$k(T) = 5.48 \times 10^{-2} + 1.46 \times 10^{-4}T + 3.30 \times 10^{-7}T^2,$$

with temperature T expressed in °C. The dependence of the optical constants on sample thickness for a-Si has been previously observed.[5] This probably has to do with the different residual stress remained in the sample after heat treatment.

Thus we conclude that in the strong absorption regime, i.e., thick sample and absorptive wavelength, the absorption coefficient of a-Si can have a relatively strong temperature dependence. This could not be observed in the pre-

[a] Permanent address: Physics Department, San Jose State University, CA 95192-0106.
[b] Permanent address: Institut fur Angewandte Physik, Technische Hochschule Darmstadt, Hochschulstr. 6, 6100 Darmstadt, Germany.
[c] Permanent address: Department of Physics, Portland State University, OR 97207-0751.
[d] Permanent address: IBM Research Division, T. J. Watson Research Center, Yorktown Heights, NY 10598.
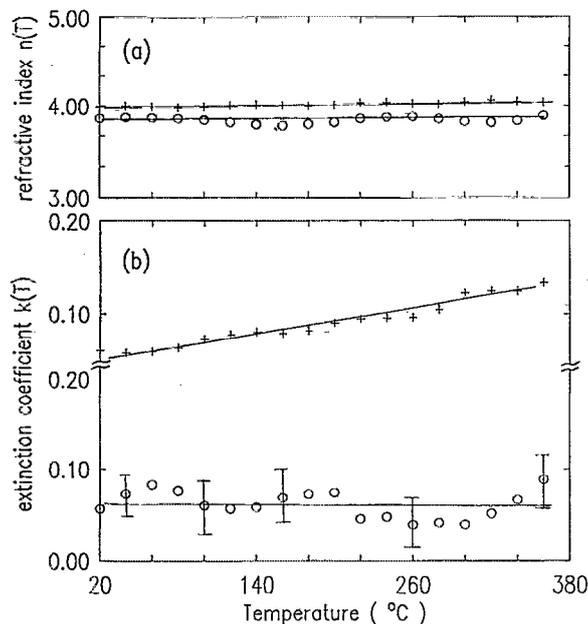[e] Permanent address: IBM, F12A/013, 5600 Cottle Road, San Jose, CA 95193.

FIG. 1. 0.2 μm a-Si sample: (a) Refractive index as a function of temperature; (+) $\lambda=0.752\,\mu m$; (O) $\lambda=1.15\,\mu m$, (b) Extinction coefficient as a function of temperature; (+) $\lambda=0.752\,\mu m$, (O) $\lambda=1.15\,\mu m$. The solid lines are from empirical fitting of the data; see text for details.

vious investigations simply because these previous studies were carried out in the highly transparent situation.[5-7]

Furthermore, if we compare our results with those for c-Si, we observe that while dn/dT is comparable in both the a-Si and c-Si cases, $k(T)$ generally increases much slower in the a-Si case compared to those in the c-Si case.[2] This may have to do with the very low mobility of the electrons in both the valence and conduction bands in a-Si as compared to those in c-Si.[12]

In addition, it is of interest to note that by applying the Mott–Davis (MD) formula,[12,13] it is possible to deduce the

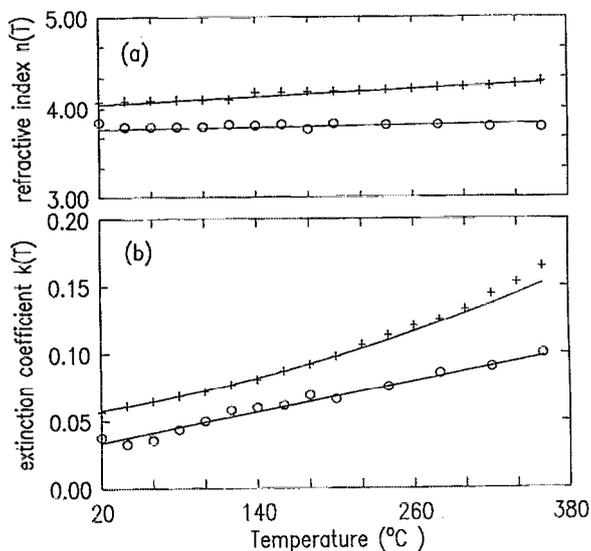FIG. 2. 1.0 μm a-Si sample: (a) Refractive index as a function of temperature; (+) $\lambda=0.752\,\mu m$, (O) $\lambda=1.15\,\mu m$. (b) Extinction coefficient as a function of temperature; (+) $\lambda=0.752\,\mu m$, (O) $\lambda=1.15\,\mu m$. The solid lines are from empirical fitting of the data; see text for details.

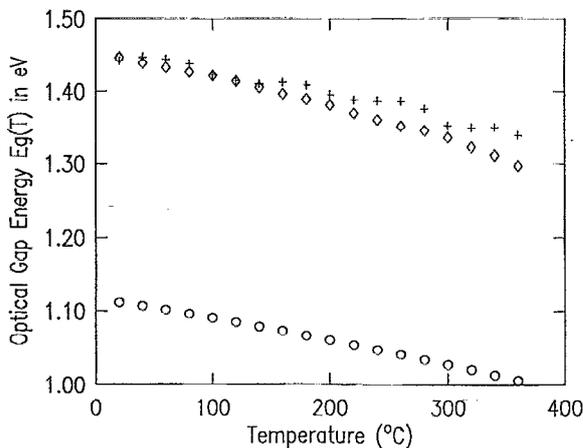FIG. 3. Optical gap energy E_g as a function of temperature for Si at $\lambda=0.752\,\mu m$: (+) 0.2 μm a-Si sample, (◊) 1.0 μm a-Si sample, (O) c-Si (from Ref. 17).

variation of the optical gap energy (E_g) for a-Si with temperature. Although there have been other alternative forms put forward in the literature relating the quantities n, k, and E_g,[14] the MD formula is still found to have high accuracy for a-Si, both empirically[15] and theoretically.[16] Furthermore, as long as the temperature is much below the Fermi temperature of the substance, the MD formula should have good validity. In this approach, we have:

$$(n\alpha E)^{1/2}=C(E-E_g),$$

where $\alpha=4\pi k/\lambda$ is the absorption coefficient, E is the photon energy, and C is a strength parameter. By plotting $(n\alpha E)^{1/2}$ vs E at room temperature for different wavelengths (measured by conventional transmission spectroscopy), the values for C and E_g could be determined at room temperature. We found that $C=1.24\times10^4$ eV$^{-1/2}$ m$^{-1/2}$ for the 0.2 μm sample and $C=1.25\times10^4$ eV$^{-1/2}$ m$^{-1/2}$ for the 1.0 μm sample, respectively. By assuming C stays roughly constant as the sample is being heated up, we can then use the results for $n(T)$ and $k(T)$ to determine $E_g(T)$.

Figure 3 shows the result for $E_g(T)$ and the comparison with that for c-Si.[17] It turns out that all these curves can be fitted by the well known formula:[18]

$$E_g(T)=E_{g_0}-\frac{\gamma T^2}{\beta+T},$$

with E_g in eV, T in K, γ in eV K^{-1}, and β in K. The values for E_{g_0}, γ, and β for both a-Si and c-Si are given in Table I.

TABLE I. Parameters for fitting E_g for both a-Si and c-Si.

Sample	E_{g_0} (eV)	γ (meV K^{-1})	β (K)
c-Si[a]	1.155	0.473	635.0
a-Si (1.0 μm)	1.508	0.665	669.7
a-Si (0.2 μm)	1.495	0.494	646.6

[a]Values from Ref. 17.

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We should also remark that only the results for 0.752 μm wavelength have been used to determine $E_g(T)$ for a-Si, since for the 1.15 μm case, the photon energy falls within the "absorption tail" in which the MD formula is no longer valid.[12,15]

In summary, we have been able to measure the temperature dependence of the optical constants as well as the optical energy gap for a-Si up to 360 °C. While we are aware that results for a-Si are in general very sample dependent (i.e., depending on the deposition conditions, the thickness,...,etc.), we expect that the qualitative temperature behavior for such physical quantities should have some general validity. This should stimulate a deeper theoretical understanding of such behavior in contrast with that for c-Si.

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