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 f)
IBM Research Division, Almaden Research Center, 650 Harry Road, San Jose, California 95120-6099
(Received 25 November 1991; accepted for publication 24 February 1992)

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 were 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 (R) and transmittance (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 R and 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 R and 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 T decaying monotonically with temperature for 0.752 μm wavelength. 11

The measured values for R and 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=1.3×10^−4 °C−1, a situation similar to the case of c-Si, the behaviors for k(T) are quite different. At λ=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 λ=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=5.0×10−4 °C−1 at λ=0.752 μm. Figure 2(b) shows significant increase of k with temperature, both at 0.752 and 1.15 μm. While dk/dT=2.0×10−4 °C−1 for λ=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-
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.

Previous investigations simply because these previous studies were carried out in the highly transparent situation.

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.

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.

In addition, it is of interest to note that by applying the Mott–Davis (MD) formula, it is possible to deduce the 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 $E_g$, the MD formula is still found to have high accuracy for a-Si, both empirically and theoretically. 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 $C = 1.24 \times 10^4$ eV$^{-1/2}$ m$^{-1/2}$ for the 0.2 μm sample and $C = 1.25 \times 10^4$ 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. It turns out that all these curves can be fitted by the well known formula:

$$E_g(T) = E_{g0} - \left(\frac{\gamma T^2}{\beta + T}\right),$$

with $E_g$ in eV, $T$ in K, $\gamma$ in eV K$^{-1}$, and $\beta$ in K. The values for $E_{g0}$, $\gamma$, and $\beta$ for both a-Si and c-Si are given in Table I.

![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.](image)

![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, (O) 1.0 μm a-Si sample, (O) c-Si (from Ref. 17).](image)

<table>
<thead>
<tr>
<th>Sample</th>
<th>$E_{g0}$ (eV)</th>
<th>$\gamma$ (meV K$^{-1}$)</th>
<th>$\beta$ (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>c-Si</td>
<td>1.155</td>
<td>0.473</td>
<td>635.0</td>
</tr>
<tr>
<td>a-Si (1.0 μm)</td>
<td>1.508</td>
<td>0.665</td>
<td>669.7</td>
</tr>
<tr>
<td>a-Si (0.2 μm)</td>
<td>1.495</td>
<td>0.494</td>
<td>646.6</td>
</tr>
</tbody>
</table>

*Values from Ref. 17.
We should also remark that only the results for 0.752 
\(\mu\)m wavelength have been used to determine \(E_g(T)\) for 
a-Si, since for the 1.15 \(\mu\)m 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 de-
pendent (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 the-
oretical understanding of such behavior in contrast with 
that for c-Si.

We thank Professor Lui Lam of San Jose State Uni-
versity for advice and support of Nhan Do, and Professor 
Dr. Tschudi of the University of Darmstadt (Germany) 
for his kind support of Leander Klees. We would also like 
to acknowledge J. S. Logan, R. Guarneri, P. E. Green, V. 
Novotny, and I. Pour for useful discussions and support; 
and the Central Scientiﬁc Service of IBM Yorktown 
Heights for preparation of the samples.

\(^{1}\)See, e.g., H. G. Drexhage, C. Hartwich, J. H. Schaefer, and I. Uhlen-

\(^{2}\)See, e.g., the review article by G. E. Jellison, Jr., in Semiconductors and 
(Academic, New York, 1984), p. 95, and references therein; G. E. 
also, M. Bertolotti, V. Bogdanov, A. Ferrari, A. Jascow, N. Nazorova, 

\(^{3}\)See, e.g., M. E. Thomas, in Handbook of Optical Constants of Solids II, 
edited by E. D. Palik (Academic, New York, 1991), p. 177, and refer-
cences therein.

\(^{4}\)See, e.g., H. Piller, in Handbook of Optical Constants of Solids I, edited 
by E. D. Palik (Academic, New York, 1985), p. 571, and references 
therein.

45 (1979).

\(^{6}\)M. von Allmen, W. Lüthy, J. P. Thomas, M. Fallavier, J. M. Mack-
34, 82 (1979).


\(^{9}\)The nitridation of Si occurs at a much higher temperature. See, e.g., H. 
Nakamura, M. Kaneko, and S. Matsumoto, Appl. Phys. Lett. 43, 691 
(1983).

\(^{10}\)J. E. Fredrickson, C. N. Waddell, W. G. Spitter, and G. K. Hubler, 


\(^{12}\)N. F. Mott and E. A. Davis, Electronic Processes in Non-Crystalline 


\(^{14}\)See, e.g., R. H. Klazes, M. H. L. M. van den Broek, J. Bezemer, and S. 


\(^{16}\)A. R. Forouhi and I. Bloomer, Phys. Rev. B 34, 7018 (1986); S. Ada-

\(^{17}\)C. D. Thurmond, J. Electrochem. Soc. 122, 1133 (1975); and as quoted 
in G. E. Jellison, Jr. and D. H. Lowndes, Appl. Phys. Lett. 41, 594 
(1982).

\(^{18}\)Y. P. Varshni, Physica (Utrecht) 34, 149 (1967).