ABSORPTION COEFFICIENT OF SILICON FOR SOLAR CELL CALCULATIONS†

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Abstract—The optical absorption coefficient is an important parameter in calculating the performance charac-
teristics of solar cells. For silicon solar cells it is desirable to know the absorption coefficient over the range of
1.1–4.0 eV and over a wide range of temperature, particularly when evaluating the concentration type systems. An
analytical (empirical) expression has been developed for this purpose. We have interpreted the available experi-
mental data in terms of three bands of silicon. With our fit, the experimental data can be explained to within an
accuracy of 20% and its validity extends from 1.1 to 4.0 eV and over the temperature range of 20–500°K.

Silicon is one of the most extensively used semiconduc-
tors in the fabrication of solar cells. Most of the obser-
ved optical and electrical parameters of silicon (for
example, band gap and mobility variation with tem-
perature) are available in analytical forms based on
known theories. However, in our attempt to characterize
silicon based solar cells as a function of temperature, we
were not able to obtain from the literature an adequate
description of the variation of the absorption coefficient
in its fundamental absorption range (1.1–4.0 eV).
Experimental data exists at 77 and 300°K for the above
quoted absorption range[1–4]. Data at other tem-
peratures are available, but only for the limited spectral
range of 1.0–1.3 eV [5–6]. Interpolation or extrapolation
of these limited data in order to compute the charac-
teristics of solar cells as a function of temperature is an
unpalatable proposition because of the large inaccuracies
that would be involved. Thus, there is a need for a good
analytical expression for the silicon absorption
coefficient over a wide spectral and temperature range
founded on a fit to the best experimental data.

In a recent publication[7], experimental absorption
data at 300°K were fitted using a simple form of the
Bardeen–Blatt–Hall formula[8–10] in the photon energy
range of 1.175–3.0 eV. Using this formula we found that
the points generated in this range were on the average
(an average over 129 generated points) 39% off as com-
pared to an absorption curve supplied by NASA[4]; and
for the same temperature, when points were generated in
the range of 1.1–4.0 eV, they were on the average (an
average of 164 generated points) 53.6% off. The NASA
curve[4] is a weighted average of several experimental
data available in the literature[1–3] and is reproduced in
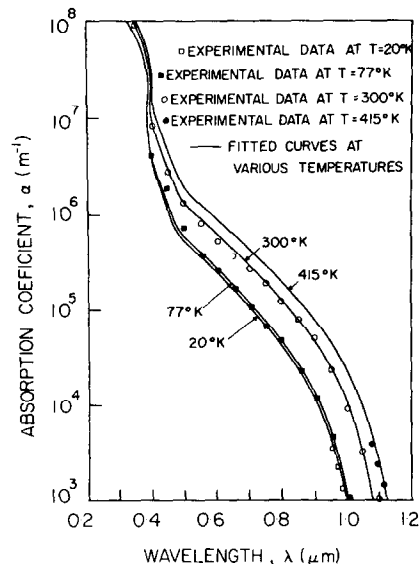Fig. 1. The averaging process is expected to minimize the

Fig. 1. Fitted absorption coefficient of silicon at $T = 20$, 77, 300
and 415°K. Experimental data at $T = 77$ and 300°K are from the
NASA absorption curve[4] and those at $T = 20$ and 415°K are
taken from Ref. [5].

effects of experimental errors. In this paper, we propose
a fit to the NASA curve by taking into consideration both
direct and indirect interband transitions in silicon.

The fundamental absorption coefficient, α, in a semi-
conductor at temperature T, can be written as

$$\alpha(T) = \alpha_v(T) + \alpha_n(T) \tag{1}$$

where $\alpha_v(T)$ is due to direct (vertical) transitions and is
proportional to $[\hbar\omega - E_{gd}(T)]^{1/2}$ for the parabolic band
approximation, with E_{gd} as the direct band gap
energy[8, 10]. $\alpha_n(T)$ is the indirect (non-vertical) tran-
sition component of the absorption coefficient.

Absorption due to indirect interband transitions, in-
volves phonons which can be either absorbed or emitted
to conserve the momentum of the electrons. $\alpha_n(T)$ can
be written for the parabolic band approximation as [6, 8–

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$$\alpha_n(T) = \sum_{i,j} C_i A_j(T) \left[\frac{\{\hbar\omega - E_{gj}(T) + E_{pi}\}^2}{\{\exp(E_{pi}/kT) - 1\}} \right.$$
$$\left. + \rho_i \frac{\{\hbar\omega - E_{gj}(T) - E_{pi}\}^2}{\{1 - \exp(-E_{pi}/kT)\}} \right] \qquad (2)$$

In the above expression, suffix i refers to various possible phonons of energy E_p and suffix j refers to different indirect bands E_g, which may be active in photon absorption. For $[E_{gj}(T) - E_{pi}] \leqslant \hbar\omega \leqslant [E_{gj}(T) + E_{pi}]$, only the transitions in which phonons of energy E_{pi} are absorbed, are allowed. In this case only the first term of (2) governs the indirect absorption. Below $[E_{gj}(T) - E_{pi}]$, the optical absorption is due to other mechanisms, like free carrier absorption etc. For $\hbar\omega \geqslant [E_{gj}(T) + E_{pi}]$ light can be absorbed either by absorption or emission of phonons, and then both terms of (2) have to be considered—the second term being for the phonon emission mechanism.

We would like to note that eqn (2) and the earlier expression for $\alpha_v(T)$ are not general expressions but ones which are valid only over regions where $E(k)$ varies as k^2 and may not be particularly accurate away from thresholds. However, as mentioned in the introduction, our objective is to find a simple analytic (empirical) expression, based on the basic physics of optical absorption, which yields an absorption coefficient of sufficient accuracy for solar cell or other opto-electronic device calculations. It is not our intention to provide a highly refined expression for the absorption coefficient which includes the particular $E(k)$ band properties of the material.

Because the indirect transitions are of second order, in order to calculate the transition probability, the matrix elements defining the interaction of the electrons with the electromagnetic field in the presence of suitable phonons have to be summed over intermediate quantized states. The factor ρ_i, appearing in (2), depends on the difference in the energy of intermediate and final states and defines the preference of absorption or emission of the ith phonon. Its maximum theoretical value for silicon is a little more than unity[6, 11]. For this reason, and to make the expression slightly simpler, we have set $\rho_i = 1$ in our calculations.

The answer to the question as to which phonons should be considered in the optical absorption process, is given by the phonon spectrum of silicon. The lattice vibration spectrum of silicon has been studied in detail by Brockhouse using neutron spectroscopy[12, 13]. Four branches of the lattice waves, LA, LO, TA and TO have been characterized in the $\langle 100 \rangle$ direction, the direction in which the minimum of the conduction band of silicon lies. In general, each branch should make two contributions: one for absorption and the other for emission of a phonon. LA and LO transitions are weak and overshadowed by very strong TO transitions. Therefore, for our purposes, only the TA and TO phonon energies are important. From the lattice vibration spectrum given by Brockhouse, these two energies should correspond to temperatures of about 212°K (TA) and 670°K (TO) res-

pectively. It should be noted that in the experiments of Macfarlane et al.[5, 6], these two temperatures were assigned erroneously to the TA and LA mode respectively[12, 13]. The temperatures of 1030 and 1420°K were assigned to LO and TO branches respectively, but as explained by Brockhouse, these two higher energies are inconsistent with the phonon spectrum and should be due to the double phonon processes, i.e. $TA + (L/T)O$ and $(L/T)O + (L/T)O$. It has been our experience, that for radiation of energy greater than 1.1 eV (minimum band gap in silicon) and for temperatures between 20 and 500°K, only the TA and TO phonons can adequately explain the absorption spectrum. Because in solar cell calculations, we are not much interested in absorption below the band gap, we have neglected the $TA + (L/T)O$ and $(L/T)O + (L/T)O$ phonons to keep the number of terms in (2) as small and simple as possible. Also the small temperature variation in phonon energies was neglected.

In expression (2), $A_j(T)$ has been treated as a proportionality constant. To describe the effect of different electron–phonon interactions for different phonons, a coupling constant C_i has been introduced. For silicon, C_{TA}/C_{TO} is 5.5/4.0[5]. $A_j(T)$ is then found by numerical fitting of experimental data. We found that for the temperature range of 20–500°K, a constant value of $A_j(T)$ was good enough for silicon.

Finally, to assign proper band gap energies, we have to look at the electronic band structure of silicon. It is well established that silicon has one indirect band gap at about 1.1 eV corresponding to the $\Delta_1 - \Gamma_{25'}$ transition. Near the absorption edge, this is the only band gap which participates in the absorption process. Therefore fitted absorption data based on this band gap alone, works only near the absorption edge, and gives erroneous results for higher energies. Based on a small rise in the absorption spectrum at about 2.5 eV for measurements at 77°K, Dash and Newman suggested a direct band gap at 2.5 eV[1]. However, more recent measurements using higher optical resolution, show no sign of this rise until about 3.2 eV[3, 4]. The band structure of silicon has been investigated in detail using the pseudopotential method by Cohen and Bergstresser[14] and by Herman and Co-workers using empirically perturbed self consistent field theory[15]. The pseudopotential method predicts a direct band gap of 3.4 eV for the $\Gamma_{15} - \Gamma_{25'}$ allowed direct transition and another of 3.1 eV for $L_1 - L_3$ forbidden direct transition. From perturbation methods, these energies are 2.7–2.8 eV and 3.0–3.4 eV respectively using two parameter adjustments. Our most satisfactory fit to the NASA absorption curve[4] was obtained for an allowed direct transition at 3.2 eV although we cannot unambiguously label this transition. Even after using a direct allowed transition at 3.2 eV, the whole absorption spectrum could not be explained, particularly near the energy of 2.5 eV. Theoretically the only possibility was a $L_1 - \Gamma_{25'}$ indirect transition at 2.25 eV[15]. We noticed that instead of an indirect transition at 2.25 eV, an indirect transition at 2.5 eV using the same phonons as for the $\Delta_1 - \Gamma_{25'}$ transition gave the most reasonable fit to the NASA absorption curve.

The variation of band gap energy is important in finding the variation of absorption coefficient with temperature. Varshni[16] has studied this variation and proposed the following expression

$$E_g(T) = E_g(O) - [\beta T^2/(T + \gamma)]. \qquad (3)$$

For silicon, β is 7.021×10^{-4} eV °K^{-1} and γ is 1108°K. $E_g(O)$ for $\Delta_1 - \Gamma_{25'}$ transition is 1.1557 eV. We have assumed the same values for β and γ for two other transitions at 2.5 and 3.2 eV also. The final form of the absorption coefficient, α, is as follows:

$$\alpha(T) = \sum_{\substack{i=1,2 \\ j=1,2}} C_i A_i \left[\frac{\{\hbar\omega - E_{gj}(T) + E_{pi}\}^2}{\{\exp(E_{pi}/kT) - 1\}} \right.$$
$$\left. + \frac{\{\hbar\omega - E_{gj}(T) - E_{pi}\}^2}{\{1 - \exp(-E_{pi}/kT)\}} \right] + A_d [\hbar\omega - E_{gd}(T)]^{1/2}.$$
$$(4)$$

In this expression $E_{gj}(T)$ and $E_{gd}(T)$ are calculated by (3). Values of different constants for (4) are given in Table 1. Values of A_1, A_2 and A_d given in this table were obtained using the least square method to fit the NASA absorption data.

Using the values given in Table 1, NASA absorption data is fitted to within an accuracy of 20%. This fit is valid for the photon energy range of 1.1–4.0 eV and for

the temperature range of 20–500°K. Results for 20, 77, 300 and 415°K are shown in Fig. 1. We tried to fit the experimental data using several combinations of band gaps, but for a three band gap picture, the best accuracy was obtained with indirect band gaps at 1.1557 and 2.5 eV and a direct allowed gap at 3.2 eV. The first band gap is obviously the $\Delta_1 - \Gamma_{25'}$ transition, but the assignment of other two gaps is difficult, particularly in the case of the 3.2 eV gap. It seems that there are several interband transitions in an extended region around the centre of reduced zone, possibly from L- to Δ-region, which makes it difficult to fit the absorption data in the entire range of 1.1–4.0 eV in a reasonably simple form. Still, expression (4) is good enough for solar cell calculations because variations within 20% do not give any significant change in short-circuit current density. It is not surprising that such an accuracy has been obtained, considering our earlier comments on the use of the parabolic band approximation, because three well distributed energy bands (1.16, 2.5 and 3.2 eV) were used in the fitting process. This allowed the inaccuracies of the approximation to be smoothed out over the 1.1–4.0 eV range.

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Table 1.

Quantity	Value	Comment
$E_{g1}(0)$	1.1557 eV	Indirect gap
$E_{g2}(0)$	2.5 eV	Indirect gap
$E_{gd}(0)$	3.2 eV	Direct allowed gap
E_{p1}	1.827×10^{-2} eV	TA, $\theta = 212$°K
E_{p2}	5.773×10^{-2} eV	TO, $\theta = 670$°K
C_1	5.5	
C_2	4.0	
A_1	3.231×10^2 cm^{-1} eV^{-2}	
A_2	7.237×10^3 cm^{-1} eV^{-2}	
A_d	1.052×10^6 cm^{-1} eV^{-2}	
$\hbar$	6.582×10^{-16} eV-s	Planck's constant
k	8.617×10^{-5} eV °K^{-1}	Boltzmann constant