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Temperature Dependence of Effective Mass of Electrons & Holes and Intrinsic Concentration in Silicon

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From investigations on the temperature dependence of density-of-states effective mass of electrons in silicon, it is suggested that the ratio of density-of-states effective mass to that of energy band gap varies in direct proportion to the temperature. Assuming the same relationship to hold good for the density-of-states effective mass of holes as well, the intrinsic concentration in silicon has been computed in the middle and high temperature regions. Results of the calculations compare well with the available experimental data.

1 Introduction

In the past few years, several attempts[1-4] have been made to compute the intrinsic concentration (n_i) of silicon as a function of temperature. All of these computations require the temperature dependence of the density-of-states effective masses of electrons (m_e^*) and holes (m_h^*) to be known. Unfortunately, the available experimental and theoretical data in this regard is not sufficient and one has to normally depend on empirical relations to estimate m_e^* and m_h^* in the middle and high temperature regions. The published work shows that none of the previously suggested[2-4] empirical relations follows the trend of the known experimental and theoretical data satisfactorily. The purpose of the present paper is to report a new relation, which describes the temperature dependence of m_e^* and m_h^* much closer to the experimental and theoretical data. This relation has also been used to compute the variation of n_i with temperature; the values obtained compare well with the previously reported results.

2 Temperature Dependence of m_e^*

The available experimental data on the temperature dependence of m_e^* in silicon are limited only up to 600 K and have already been summarized well by Barber[1] and Jain[4]. It is shown by the continuous line curve in Fig. 1 and corresponds to the continuous line curve of Fig. 2 of Ref. 1 and curve 1 of Ref. 4.

Heasell[2] suggested the following relation to describe the dependence of m_e^* on temperature:

$$m_t(T) = \alpha^2 m_t(0) \qquad \ldots(1)$$

where α is defined as $E_g(0)/E_g(T)$, $E_g(0)$ is the intercept obtained by the extrapolation of high temperature band gap data to 0 K. The transverse effective mass, m_t, is related to m_e^* by the relation,

$$m_e^* = [6\{m_l m_t^2\}^{\frac{1}{2}}]^{2/3} \qquad \ldots(2)$$

where m_l is the longitudinal effective mass, whose value (0.9163) in silicon has been found to be nearly independent of temperature.

The results of the combination of Eqs (1) and (2) are shown by □ points in Fig. 1.

Based on the suggestion of Barber[1] that the density-of-states near the band edges must vary in a manner sympathetic with the temperature variation of the energy band gap (E_g), Jain and Overstraeten[3] assumed the following inverse dependence of m_e^* on E_g,

$$m_e^*(T) = m_e^*(300\,\mathrm{K})\left[\frac{E_g(300\,\mathrm{K})}{E_g(T)}\right]^{2/3} \qquad \ldots(3)$$

Jain[4] subsequently modified relation (3) to:

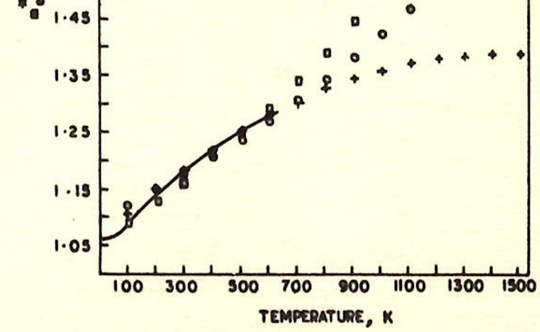

Fig. 1—Temperature dependence of m_e^* [—, Experimental; □, based on Eqs (1) and (2); ○, based on Eq. (4); +, based on Eq. (5) or (6)]

$$m_e^*(T) = m_e^*(300\,\mathrm{K})\frac{E_g(300\,\mathrm{K})}{E_g(T)} \qquad \ldots(4)$$

Relation (4) was shown[4] to follow the experimental data much better than relation (3). The results from relation (4) have been plotted as circles in Fig. 1.

It is observed from Fig. 1 that the relations (1) and (4) are in approximate agreement with the experimental results. None of these relations, however, appears to follow the trend of experimental data closely.

As regards the temperature dependence of m_e^* and E_g, it is worthwhile to note that E_g of silicon can be fairly well described[1,5] as a linear function of T ($T > 300$ K), independent of the variations in m_e^*. Should it not be then possible to relate the variation in m_e^* as an independent function of temperature irrespective of the variations in E_g? The answer seems to be in the affirmative as the known experimental data on m_e^* can be closely fitted to the following equation above 300 K:

$$m_e^*(T) = 1.062 + 4.714 \times 10^{-4} T - 16.688 \times 10^{-8} T^2 \qquad \ldots(5)$$

It is interesting to note that Eq. (5) can be rewritten as,

$$\frac{m_e^*(T)}{E_g(T)} - \frac{m_e^*(0)}{E_g(0)} = 5.960 \times 10^{-4} T \qquad \ldots(6)$$

where

$$m_e^*(0) = m_e^*(4.2\,\mathrm{K}) = 1.062 \,(\text{Ref. } 6)$$

$$E_g(T) = E_g(0) - 2.8 \times 10^{-4} T \qquad \ldots(7)$$

$$E_g(0) = 1.205\,\mathrm{eV}$$

Eq. (7) is the well known relation[1,6] describing the temperature dependence of the energy band gap in silicon and has already been used by earlier workers[1-4] to compute $E_g(T)$.

The present investigation thus suggests that the ratio of density-of-states effective mass to the energy band gap varies in direct proportion to the temperature.

3 Temperature Dependence of m_h^*

The available data on the temperature dependence of m_h^* are far from satisfactory owing to the conflicting experimental results. The results shown in Fig. 2 are obtained from Barber's[1] calculations using Kane's valence band model[7] (dashed line) and corrected for the temperature dependence of the density-of-states (continuous line).

Jain[4] suggested the following empirical relation to describe the temperature dependence of m_h^*:

$$m_h^*(T) = m_h^*(300\,\mathrm{K})\frac{E_g(300\,\mathrm{K})}{E_g(T)} \qquad \ldots(8)$$

The results from Eq. (8) are shown by o points in Fig. 2.

In Sec. 2, the ratio of the electron density-of-states effective mass to the energy band gap was found to vary

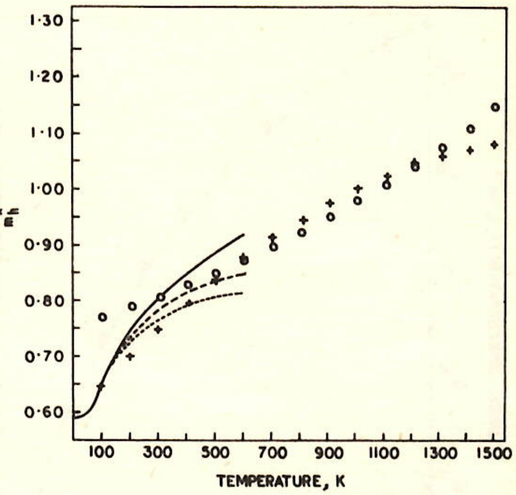

Fig. 2—Temperature dependence of m_h^* [O, based on Eq. (8); +, based on Eq. (9); remaining curves have the same meanings as in Fig. 4 of Ref. 1]

in direct proportion to the temperature. Since the density-of-states effective mass is in general defined as a scalar mass which accurately describes the density-of-states of bands which need not be ideal, it is proposed that the same effective mass-band gap proportionality relation should hold good for the hole density-of-states effective mass as well. In this case, Eq. (6) should, therefore, be rewritten as:

$$\frac{m_h^*(T)}{E_g(T)} - \frac{m_h^*(0)}{E_g(0)} = 5.960 \times 10^{-4} T \qquad \ldots(9)$$

The constant of proportionality has been assumed to be the characteristic of the material, i.e. Si. Using the value of $m_h^*(0)$ as 0.591 from Ref. 1, the calculated results from Eq. (9) are also shown in Fig. 2. It is observed that the present calculations of m_h^* follow the theoretical results of Barber[1] much better than those from relation (8).

4 Temperature Dependence of n_i

As a further check on the applicability of relations (6) and (9), we propose to calculate the n_i of silicon as a function of temperature in middle and high temperature regions, using the predicted temperature dependence of m_h^* and m_e^*. In theory, n_i is given by

$$n_i = (np)^{\frac{1}{2}} = 2\left[\frac{2\pi m_0 k}{h^2}\right]^{3/2} (m_e^* m_h^*)^{\frac{3}{4}} T^{3/2} \exp\left(-\frac{E_g}{2kT}\right) \qquad \ldots(10)$$

where m_0, k and h are physical constants.

Combination of Eqs (10), (6), (9) and (7) can straightaway be used to compute n_i of Si as a function of temperature at temperatures less than 500 K. At temperatures above 500 K, E_g depends[8] appreciably

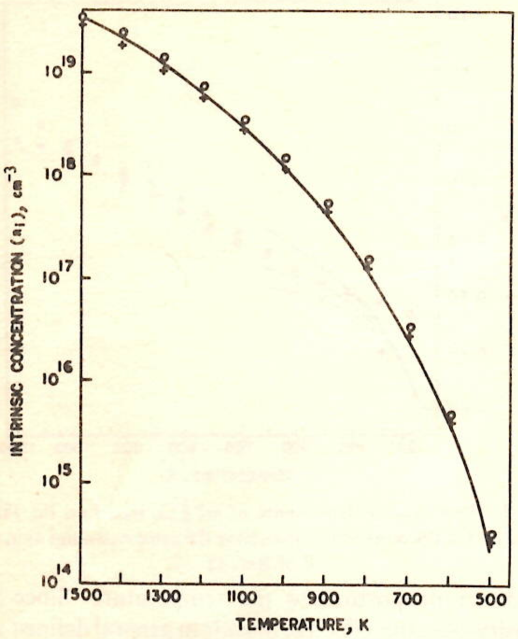

Fig. 3—Temperature dependence of n_i [—, Present calculations; O, based on the experimental data of Morin and Maita[9]; +, based on the extrapolated data of Putley and Mitchell[10]]

upon the electrostatic interaction of charge carriers. The effect of this dependence of E_g on np can be included by correcting E_g using the following relation[9]

$$\Delta E_g = -7.1 \times 10^{-10} (np)^{\frac{1}{4}} T^{-\frac{1}{2}} \quad \ldots (11)$$

The continuous line curve shown in Fig. 3 was generated using Eqs (6), (7), (9), (10) and (11). For comparison, the experimental data of Morin and Maita[9] have also been shown. We have also plotted in Fig. 3 the extrapolated data from Putley and Mitchell's measurements[10]. This extrapolated high temperature data were also corrected for the dependence of E_g on the electrostatic interaction of charge carriers by applying Eq. (11). A comparison of present calculations with the experimental results shows that our results compare well with the reported experimental results[9,10]. This supports the applicability of relations (6) and (9), suggesting thereby that the ratio of density-of-states effective mass to the energy band gap might vary, in general, in direct proportion to the temperature.

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