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CALCULATION OF AUGER COEFFICIENTS FOR SILICON WITH EVALUATION OF THE OVERLAP INTEGRALS

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Proceeding from phonon-assisted Auger recombination the overlap integrals are calculated for Si by means of the full zone double group k·p-method. The results confirm that this recombination mechanism is predominating, both for highly doped as well as for highly excited Si where electron-hole drops appear.

I. Introduction

Phonon-assisted Auger recombination is suggested to be an important recombination process in indirect band gap semiconductors. To confirm this by quantitative calculations one has two difficulties: (i) Being a second order process there are several contributions of the different intermediate states where usually only one is regarded as predominating [1,2]. (ii) The overlap integrals arising from the matrix elements of the electron-electron interaction are generally roughly estimated [3]. In contrast, these integrals are calculated here for Si from first principles using the full zone double group k.p-method. Moreover, the second order process is investigated in more detail with the result that several contributions are of the same order of magnitude and must be taken into account. The Auger coefficients for Si calculated in this way are in good agreement with experimental values.

II. Phonon-assisted Auger Recombination

Phonon-assisted Auger recombination is a second order process involving two electrons and a hole (eeh-process) or one electron and two holes (ehh-process) and in addition one phonon. The transition probability is given by second order perturbation theory. Therefore the recombination process goes over intermediate states which are selected as follows: (i) Interband phonon scattering is omitted as usual. (ii) Coulomb terms are neglected in comparison with exchange terms because they are smaller by the dielectric constant ε [4], ε being 10 to 20 for the semiconductors in question. (iii) The large wave vector K between the band edges of the conduction band and the valence band can occur in the denominator; such terms are negligible. (iv) The initial states shall be near the corresponding band edges because there is the highest occupation probability.

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The total recombination probability is obtained by summing over all transition possibilities multipled by their statistical weight. The sums run over all electron and phonon states including the different valence bands and phonon branches as well as phonon emission and phonon absorption. Most of the sums can be evaluated immediately. The results are described by the lifetime τ or the Auger coefficient C_n where

$$\frac{1}{\tau} = C_n n^2 \quad (n = \text{electron concentration}). \tag{1}$$

C_n is essential for n-type material, the analogous coefficient C_p for p-type material. Details of the calculation are given in another paper [5].

III. Overlap Integrals

The evaluation of the Auger coefficients requires the knowledge of the overlap integrals

$$I_{n'n} = \int u^*_{n'} u_n d\tau \,, \tag{2}$$

which follow from the matrix elements of the electron-electron interaction; u_n are the lattice periodic Bloch factors, n includes all electronic quantum numbers. These integrals are calculated by means of the full zone double group k·p-method which is described in some papers [6,7]. The method proceeds from a transformation of the Schrödinger equation into the k-space where the eigenvalue problem is given by a matrix. This matrix contains the eigenvalues and momentum matrix elements for k=0 as parameters. The energy values are taken partly from experiments, partly from band calculations [6]. The momentum matrix elements can be reduced by symmetry conditions to ten independent values which are used as fitting parameters for the band structure. Then the problem is restricted to a 30x30 matrix and solved by numerical methods. The solution yields immediately the overlap integrals.

IV. Results

The Auger coefficients of Si are calculated for different temperatures and compared with the experimental values of Dziewior and Schmid [8] (Table 1).

T	77K	300K	400K
C_n (theor)	0.53	0.72	0.87
C_n (exp)	2.3	2.8	2.8
C_p (theor)	0.75	1.03	1.25
C_p (exp)	0.78	0.99	1.2

Table 1 Auger coefficients for Si (in units $10^{-31} cm^6 sec^{-1}$)

The agreement is very good, particularly for C_p whereas the values of C_n differ a little. This may be due to uncertainties of the deformation potentials or due to uncertainties in the measure of the electron concentration.

As mentioned above the results are also valid for electron-hole drops. Here the measurements give usually $C = C_n+C_p$ and the temperature is $T \approx 4K$. Moreover, the experimental value must be corrected by the enhancement factor g where $g \approx 3.5$ for Si [9,10]. Then the experimental value is C=1.91, the theoretical one C=1.28 (in units $10^{-31} cm^6 sec^{-1}$). The agreement is again fairly good. The small discrepancy corresponds to the difference in the results for C_n.

As a summary, our calculations confirm that phonon-assisted Auger recombination is the essential non-radiative recombination mechanism in highly doped and highly excited Si. Obviously these results hold also for other indirect band gap semiconductors.

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