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BAND-TAIL SHOCKLEY-READ-HALL RECOMBINATION IN HEAVILY DOPED SILICON

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Résumé - La densité des centres de recombinaison type Shockley-Read-Hall due aux états localisés situés dans le prolongement de la bande des porteurs minoritaires a été calculée pour le silicium fortement dopé. Nous prouvons que l'effet de ces états devient dominant pour des concentrations de dopage supérieur à 10^{17} cm^{-3} .

Abstract - Shockley-Read-Hall recombination center density due to the localized states in the minority carrier band tail has been calculated. It is shown that in heavily doped silicon, the effect of these band tail states is comparable to or more important than that due to deep states and modifies the lifetime of minority carriers significantly.

1 - INTRODUCTION

In the bulk of a semiconductor, Shockley-Read-Hall (SRH) recombination assumes the presence of all recombination centers at a single energy level in the energy band-gap. The recombination rate is given by

$$U_o = \frac{\sigma_n \sigma_p v_{th} N_t (pn - n_i^2)}{\sigma_n [n + n_i \exp(E_t - E_i)/kT] + \sigma_p [p + n_i \exp(E_i - E_t)/kT]} \quad (1)$$

where σ_n and σ_p represent the electron and hole capture cross sections, N_t is the recombination center density per unit volume, v_{th} is the carrier average thermal velocity, n and p are the electron and hole concentration respectively, n_i is the intrinsic carrier concentration, E_i is the intrinsic energy level and E_t is the recombination center energy level, k is Boltzman constant and finally T is the absolute temperature.

When a continuum of localized states is inserted in the energy band-gap a more generalized formula has to be used. In this case the density of the recombination centers N_t has to be modified to consider the continuous nature of the localized states. A per unit energy per unit volume density of states $D(E)$ now replaces N_t in equation (1) and the recombination rate equals the integral of the per energy rate over all the continuum levels. The resulting expression has the form

$$U = \int_{E_g} \frac{\sigma_n \sigma_p v_{th} D(E) (pn - n_i^2) dE}{\sigma_n [n + n_i \exp(E - E_i)/kT] + \sigma_p [p + n_i \exp(E_i - E)/kT]} = \int_{E_g} u(E) dE \quad (2)$$

This procedure has been followed for instance to describe the surface recombination rate U_s . In this case, however, $D(E)$ has a per unit energy per unit area dimension. In a heavily doped semiconductor, potential energy fluctuations result in energy tails that appear at the conduction and valence band edges and extend deeper in the band-gap. The localized states in these band tails act as recombination centers. Though they are situated far away from midgap, the density of these states might be so high such that they contribute significantly to U . The total recombination rate in the bulk of a heavily doped semiconductor should therefore be expressed by equation (2). The integration should be carried out starting from the lowest localized state level in the tail of the valence band up to the highest localized state level in the tail of the conduction band. This integral can therefore be splitted into three components. The first component represents the recombination rate caused by the centers situated at the discrete level near midgap which is responsible for the recombination process taking place in unperturbed-band material. The second and third components represent the recombination rates caused by the centers in the tail of the valence band and in the tail of the conduction band. In heavily doped semiconductors, equation (2) can therefore be written as

$$U = U_o + \int_{VBtail} u(E) dE + \int_{CBtail} u(E) dE \quad (3)$$

In terms of lifetime, equation (3) can be rewritten as

$$1/\tau_{eq} = 1/\tau_o + 1/\tau_{vbt} + 1/\tau_{cbt} \quad (4)$$

where τ_{eq} is the equivalent lifetime, τ_o represents the lifetime due to recombination at the discrete center near midgap, and τ_{vbt} and τ_{cvt} represent the lifetime due to recombination in the tail of the valence band and in the tail of the conduction band, respectively. Note that band tails are fundamental phenomena in heavily doped semiconductors and therefore the recombination taking place through the band tail centers is associated with a lifetime that represents a fundamental limit. We shall neglect here the recombination rate due to recombination via the localized states in the majority carrier band tail, if such states would exist. In such a situation equation (4) reduces to

$$1/\tau_{eq} = 1/\tau_o + 1/\tau_{bt} \quad (5)$$

where τ_{bt} represents the lifetime due to recombination via the centers located in the minority carrier band tail and is given by

$$1/\tau_{bt} = \sigma_{min} v_{th} N_{ibt} \quad (6)$$

where N_{ibt} represents the effective density of recombination centers in the band tail. By combining equations (2), (3), (5) and (6) N_{ibt} for n-type material can be expressed as

$$N_{ibt} = \int_{E_{min}}^{E_{max}} \frac{D(E).dE}{1 + (n_i/n).(\sigma_p/\sigma_n).exp(E_i - E)/kT} \quad (7)$$

In order to calculate N_{ibt} , $D(E)$ should be known. In section 2 we introduce some functions that can be used to represent $D(E)$. Also, the limits of integration must be defined. Section 3 deals with the model followed to determine the localization edge in the minority carrier band tail. In section 4 the doping dependence of N_{ibt} (τ_{bt}) is discussed and in section 5 some numerical examples are presented and fitting of experimental data is carried out. Finally a short discussion followed by a conclusion is presented in section 6.

2 - DENSITY OF STATES IN THE BAND TAILS

In heavily doped semiconductors, energy band tails are created due to potential energy fluctuations as it is schematically represented in Fig.1. The parabolic representation of the energy band states does not hold anymore. A relatively simple model for the new density of state function was given by Kane [1]. In his model, the potential energy fluctuation is assumed gaussian with a standard deviation δ . The potential energy fluctuation arises from the Coulomb potential of the ionized impurities per unit volume that are randomly distributed on lattice sites. The rms potential energy fluctuation δ is therefore given by [2]

$$\delta = q^2/(4\pi\epsilon).[2\pi(N_D^+ + N_A^-)L_s]^{1/2} \quad (8)$$

where L_s is the screening length which depends on the carrier concentration and on temperature. The border between degenerate and non-degenerate material is controlled by a critical temperature T_c which for n-type material is given by [3]

$$T_c(K) = (3/\pi)^{2/3} (h^2/8km^*)n^{2/3} \quad (9)$$

where m^* represents the effective density of states electron mass. The material is non-degenerate when T is greater than T_c . In this case, the screening length L_s is quite accurately represented by the extrinsic Debye length [2]

$$L_s = (kT\epsilon/q^2n)^{1/2} \quad (10)$$

On the other hand, the material is degenerate when T is smaller than T_c . In this case, L_s can be satisfactorily represented by the Thomas-Fermi screening length [1,2]

$$L_s = (\pi\epsilon h^2/m^*q^2)^{1/2}.(\pi/3n)^{1/6} \quad (11)$$

For the valence band in an n-type material, Kane's density of states has the form

$$D(E) = (2\eta_v)^{1/2}.(m_p^{3/2}/\pi^2 h^3).y(E/\eta_v) \quad (12)$$

where m_p is the effective density of states mass for the valence band and $\eta_v = \sqrt{2}\delta$. The dimensionless variable y is represented in integral form by

$$y(x) = \pi^{-1/2} \int_x^\infty (z-x)^{1/2}.exp(-z^2)dz \quad (13)$$

Substituting some values for n-type silicon in the set of equations (8) to (13), we obtain $D(E)$ for the valence band (minority carrier band) which is displayed in Fig.2 together with the parabolic band.

Other models have been proposed to represent the band tail states. For comparison, the density of states

based on Halperin and Lax model [4] is plotted together with Kane's density of states in Fig.3 [5]. The model of Halperin and Lax takes into account the kinetic energy of the carriers when solving Schroedinger equation. This kinetic energy was neglected in Kane's model and therefore it results in a much larger density of states. The extent to which kinetic energy effects reduce band tailing depends on the kinetic energy $\hbar^2/2m^*L_z^2$ in relation to δ . Localized tail states have also been described by mobility edge models (e.g.[6]). We use Kane's model here merely to illustrate the importance of band tails in determining U . The effect can be evaluated for any other model of band tails in a similar way.

3 - DETERMINATION OF THE LOCALIZED STATES IN THE BAND TAILS

In order to determine the recombination center levels in the band tail, one has to define sharply the localization edge which is the energy level that separates the localized states from the extended states in the tail. Using a carrier transport model based on effective medium theory [7] and percolation theory [8], one can determine accurately the edge of localization in the minority carrier band tail. This model assumes that, due to band edge distortion, the volume of a heavily doped silicon crystal is divided into potential wells and barriers of different height as shown in Fig.4. The barriers constitute non conductive regions and free carriers can move between the hills only. The fractional space f occupied by free holes of energy E is given by

$$f = 1/2 \operatorname{erfc}(E/\eta_v) \quad (14)$$

It is known that in a binary mixture of conducting (with conductivity g_1) and insulating particles, the effective conductivity in three dimensions is given by [9]

$$g = 1/2 \cdot g_1 \cdot (3f - 1) \quad (15)$$

Therefore, if f is smaller than the percolation threshold $f_{pc} = 1/3$ the conductivity g becomes zero. Putting $f = 1/3$ in equation (14) we get the percolation threshold energy

$$E = E_{pc} = 0.4306 \delta \quad (16)$$

which represents the localization edge and in the same time the lower integration limit E_{min} of equation (7).

All states with energy above E_{pc} are localized and act as recombination centers. Due to their high density, only those centers having energies within a few δ 's from E_{pc} are effective. Numerical results show that centers having energies greater than 6δ contribute to the band tail recombination by less than 0.01 %. Therefore, we substitute for the higher integration limit of equation (7) by $E_{max} = 6 \delta$.

4 - DOPING DEPENDENCE OF THE BAND TAIL LIFETIME

As discussed in the introduction, the recombination taking place via band tail centers is characterized by a lifetime τ_{bt} and an equivalent center density N_{tbt} . At low doping N_{tbt} is extremely small such that the band tail recombination is negligible. In this case, the lifetime τ_{eq} is totally governed by recombination via the centers situated at the discrete energy level near midgap. Assuming that the density of these centers is independent of the doping level, τ_{eq} will also be independent of the doping level and equals τ_o . At high doping levels the density of the band tail centers N_{tbt} becomes large such that τ_{eq} becomes much smaller than τ_o and approximately equal to τ_{bt} . Since N_{tbt} increases rapidly with the doping level, τ_{eq} will follow the inverse behavior. In a certain doping range results of numerical calculations show that

$$N_{tbt} = C N^a \quad (17)$$

where C and the exponent a are constants and N is the doping concentration. Combining equations (5) and (17), the equivalent lifetime τ_{eq} can be expressed as

$$\tau_{eq} = \frac{\tau_o}{1 + (N/N_o)^a} \quad (18)$$

Equation (18) states that at low doping concentration $(N/N_o)^a \ll 1$ and $\tau_{eq} = \tau_o$ while at high doping levels $(N/N_o)^a \gg 1$ such that $\tau_{eq} = \tau_o(N_o/N)^a$.

5 - NUMERICAL RESULTS AND COMPARISON WITH EXPERIMENTAL DATA

The band tail recombination center density N_{tbt} as expressed in equation (7) is plotted in Fig.5 versus doping level taking the electron to hole capture cross section ratio R as an independent parameter. At each doping level $D(E)$ is replaced by its corresponding Kane's function. E_{min} and E_{max} are determined in the way described in section 3. The intrinsic carrier concentration is modified to include band-gap narrowing [10]. As expected, a continuous increase in N_{tbt} with doping level is obtained. In the doping range $10^{16} - 10^{19} \text{ cm}^{-3}$ the exponent a of equation (17) is strongly dependent on R . In order to fit our theory to the reported experimental data representing the fundamental minority carrier lifetime in n-type and p-type material [11] we have to:

1) determine the constants τ_o , N_o and a of equation (18) from the experimental dependence. Indeed, τ_o is the constant lifetime of the low doping region, N_o is the doping level at which $\tau_{eq} = \tau_o/2$ and a is the slope of the high doping region.

2) use Fig.5 to relate the value of a to its corresponding R value (note that due to the difference in the effective mass of the minority carrier, $D(E)$ hence N_{tbt} are not equal for p-type and n-type silicon). Consequently the N_{tbt} curve that has to be considered is defined. Knowing N_{tbt} and τ_{bt} and using equation (6) we are able to extract the value of the minority capture cross section. Since R has been determined in a previous step, we can now obtain a value for the majority capture cross section.

The results of such procedure for n-type and p-type material are given in table 1 and the fit is displayed in Fig.6. The values of R seem reasonable and lie in the range reported in the literature. On the other hand, the values of σ_n and σ_p are very small compared to the values usually met. This result could have been expected since, as discussed earlier, Kane's density of states are overestimated and a more accurate model such as the one in [4] would reduce $D(E)$ by two orders of magnitude. Therefore, N_{tbt} would roughly be reduced also by the same amount which leads to an increase in the extracted capture cross section values by a factor of 100. On the other hand, the idea that the tail recombination centers have smaller capture cross sections than the deep level center is not totally rejected.

Table 1

	quantity	n-type	p-type
fitting param.	R	0.01	3
constants	τ_o (s)	4×10^{-4}	7×10^{-4}
	a	0.743	1.171
	N_o (cm $^{-3}$)	3×10^{15}	4×10^{16}
results	σ_p (cm 2)	1.334×10^{-20}	2.328×10^{-20}
	σ_n (cm 2)	1.334×10^{-18}	7.000×10^{-20}

6 - DISCUSSION

More generally, the reported experimental values of the fundamental minority carrier lifetime suggest values for the quantity σN_t between 10^{-4} and 10^{-1} /cm in the doping range 10^{16} - 10^{19} cm $^{-3}$ respectively. Considering that reasonable values of σ would lie between 10^{-13} and 10^{-17} cm 2 , the corresponding N_t values should be 10^9 - 10^{13} cm $^{-3}$ at a doping of 10^{16} cm $^{-3}$ and 10^{12} - 10^{16} cm $^{-3}$ at a doping of 10^{19} cm $^{-3}$. By consulting Fig.5 we clearly see that even if N_{tbt} is reduced by two order of magnitude its value could still easily lie in the range of values stated above. We therefore conclude that band tail SRH recombination is a phenomena that cannot be neglected in heavily doped silicon. One should be very carefull when trying to model the fundamental lifetime in silicon when the doping level exceeds 10^{17} cm $^{-3}$.

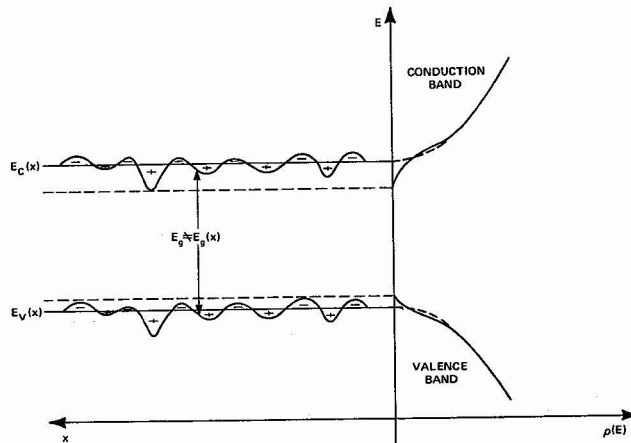


Fig. 1 - Schematic representation of the band tail formation resulting from random spatial variation of the electrostatic potential.

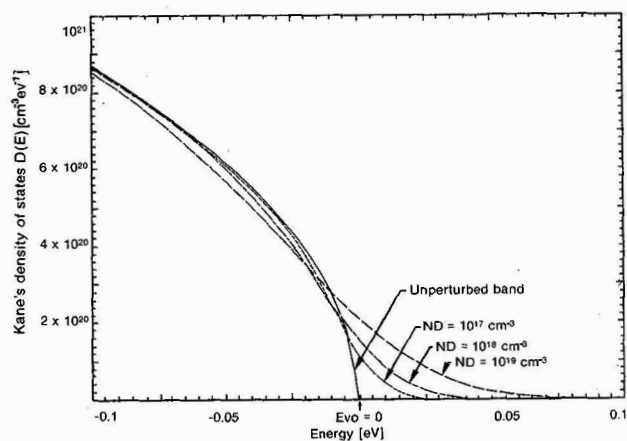


Fig. 2 - Density of states in the valence band of n-type silicon as calculated using Kane's model [1].

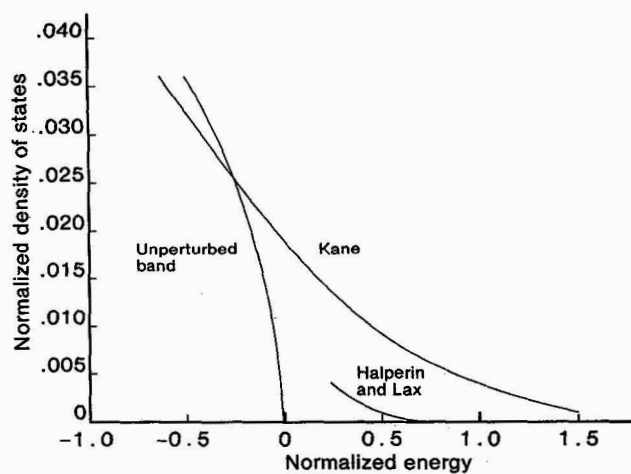


Fig. 3 - Comparison between the density of states calculated using Kane's model [1] and Halperin and Lax model [4].

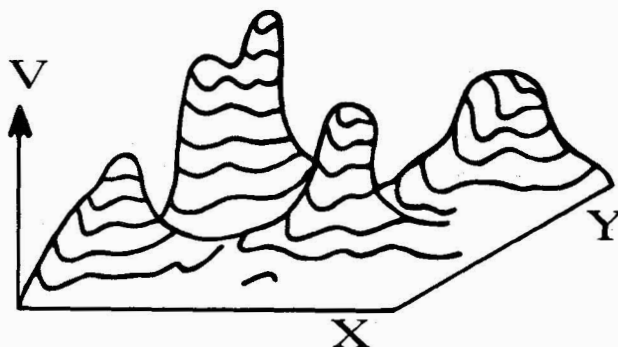


Fig. 4 - Schematic representation of the three dimension spatial variations of the valence band edge forming potential barriers and wells due to inhomogeneous impurity distribution in heavily doped n-type silicon.

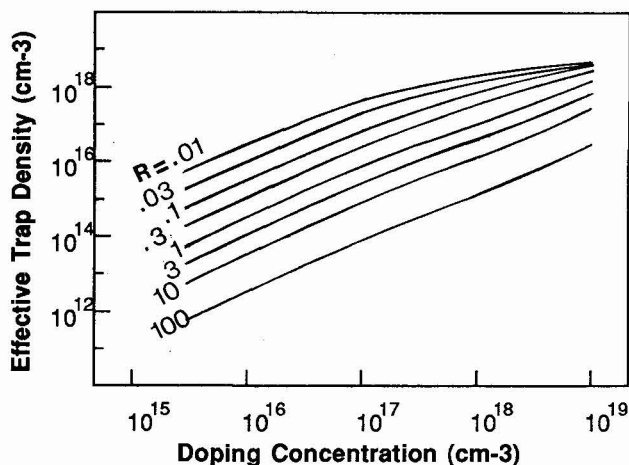


Fig. 5 - Equivalent recombination center density in the band tail of n-type silicon ($D(E)$ =Kane's) versus doping concentration. R represents the hole to electron capture cross section ratio.

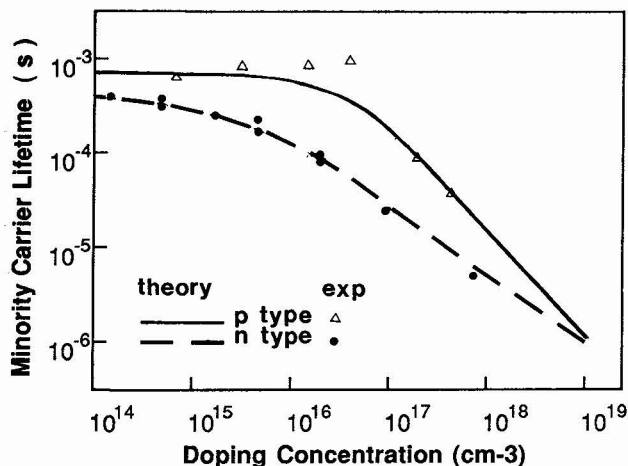


Fig. 6 - Fitting of the experimental data [11] concerning the fundamental lifetime versus doping for n-type and p-type silicon using a combined SRH lifetime that includes band tail recombination.

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