On the problem of type of deep recombination centres in InSb

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Abstract

Deep levels of structural defects in InSb, which are the main centres of recombination in this material, have been studied experimentally for a long time. However, neither clear understanding of the nature of these levels nor relevant information about their binding energy has been achieved until now, while the experimental data of different works are contradictory. In this paper a theoretical model of recombination processes in InSb is built that takes into account the Auger recombination, band-to-band radiative recombination, and the recombination via deep defect levels, the intensities of which depend in different ways on the uniaxial stresses applied. A comparison of experimental stress dependences of the photoconductivity in both *n*-InSb and *p*-InSb with the predictions of our theory allows identifying the deep recombination level with an *h*-centre of acceptor type, with the symmetry Γ_8 of the v-band top, which shifts together with the v-band edge under the uniaxial compression.

Keywords: recombination processes, photoconductivity, uniaxial stress, deep centres, lifetime

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1. Introduction

Together with mercury-cadmium-telluride compound MCT, narrow-gap InSb crystals still remain principal materials for different IR receivers and detectors (see, e.g., the review [1]). Recombination characteristics of InSb in the range of temperatures $T < 300$ K and under conditions of relatively low injection/generation of carriers are determined by the levels of structural defects (see [1] and references therein). In spite of a great number of experimental works, the origin and the type of these deep centres still remain unclear. Moreover, the data derived by different authors for the energy position of the levels contradict each other. The most specious results of the work [2] have yielded the characteristics of deep levels of InSb presented in Table 1.

These data correlate qualitatively with the results [3, 4], where the shift of the deep levels with pressure has been studied. It has been demonstrated in the latter works that the levels marked as 2 and 3 in Table 1 are shifted with pressure, together with the c-band bottom, though the binding energies presented in [4] differ from those of [2]. This corresponds to so-called *l*-*c*-centres, with Γ_6 symmetry of the c-band bottom [5, 6]. The centres mentioned above are doubly degenerate and so they do not split under uniaxial stress. On the contrary, the results of the work [7], where photoionization spectra have been carefully studied, assume the level 3 in InSb as an *h*-centre with Γ_8 symmetry of the v-band top. These fourfold degenerate levels should shift with stress, together with the v-band. Moreover, they should split into two levels. Notice that these results obviously contradict the experimental data [3, 4]. Therefore additional studies of the deep levels in InSb would be timely.

Table 1. Characteristics of deep levels in InSb.

Number of level	Type of level	Degeneracy g_j	Energy $E_j - E_V$ (77 K), meV	Concentration $N_j, 10^{13}\,\mathrm{cm}^{-3}$
1	Acceptor	4	68±2	3÷4
2	Donor	2	99±0.5	6÷8
3	Donor	2	132±3	2÷3

Our analysis is based on a selective effect of uniaxial compression on different recombination channels in semiconductors. The stress causes an increase in the interband radiative recombination rate in narrow-gap semiconductors, and a decrease in the nonradiative interband impact (Auger) recombination rate. As a result, the quantum yield of radiation can essentially increase. This is why studies of dependence of the carrier lifetime on the compression can elucidate the type of dominant recombination channel (see, e.g., [8, 9]).

2. Theory

It is necessary to emphasize that, to the best of our knowledge, no studies of the pressure effect on the rate of multi-phonon carrier capture by the deep centres have been performed until now. A strict and general numerical theory of this effect is hardly possible due to lack of general adequate model for the deep local centres. However, as we will demonstrate in this work, some important qualitative results may be obtained from a general examination within the model of adiabatic terms.

Below we will treat the three competing recombination mechanisms: a band-to-band Auger recombination, band-to-band radiative recombination, and a Shockley-Read recombination via deep defect levels. After standard procedure (see, e.g., [10]) one can get the following equation for the carrier concentration dynamics:

$$\frac{dn}{dt} = G - \left(np - n_i^2\right) \times \left[\beta_n n + \beta_p p + \nu_{np} + \frac{c_n c_p N}{c_n(n+n_1) + c_p(p+p_1)}\right]. \quad (1)$$

Here $n = n^{(o)} + \delta n$ and $p = p^{(o)} + \delta p$ are respectively the electron and hole concentrations, $n_i^2 = n^{(o)} p^{(o)}$, G denotes the generation rate, N the concentration of recombination centres, β_n and β_p constants of respectively the Auger processes of cc-cv and cv-vv types (the recombination energy is then transferred to a free electron or a free hole, respectively), the constant parameter v_{np} describes the rate of band-to-band radiative recombination, c_n and c_p govern respectively the capture rates for electron and hole on the defect, and n_1 and p_1 define (with the accuracy of the factor of defect degeneration) respectively the concentrations of free electrons and free holes in the case if the Fermi level corresponded to the energy position of the defect level [10]. In case of the absence of pressure we have $\beta_n >> \beta_p$ because of an additional overlap integral between the orthogonal states of heavy and light holes in the transition matrix for the cv-vv process [9].

Now we examine the case of small generation rate, when the concentrations of excess carriers δn, δp are small in comparison with their equilibrium values $n^{(o)}, p^{(o)}$. We also treat the case of low temperatures, when kT is smaller than the Auger recombination threshold energy [10] (this approximation is good for InSb up to the temperatures of the order of 100 K). Then we obtain

$$\frac{dn}{dt} = G - \frac{\delta p}{\tau_p}, \qquad \frac{1}{\tau_p} = v_{np} n^{(o)} + c_p N \tag{2}$$

for the n-type crystal and

$$\frac{dp}{dt} = G - \frac{\delta n}{\tau_n}, \qquad \frac{1}{\tau_n} = v_{np} p^{(o)} + c_n N \tag{3}$$

for the p-type one.

Notice that in the case of donor centre we have $c_n >> c_p$, i.e. the rate of the capture of electrons by an ionized centre is much higher than that of the capture of holes by a neutral centre [10]. If the additional relation $v_{np} \approx c_n >> c_p$ is valid and the values of the N concentration presented in Table 1 are taken into account, we get that, for T > 40 K, the lifetime in the n-type crystal is determined by the rate of band-to-band radiative recombination, while in the case of the p-type crystal the two competing channels should be simultaneously considered.

On the contrary, the relationship $c_n << c_p$ holds true in the case of acceptor centre, i.e. the capture rate of holes by an ionized centre is much higher than that of the capture of electrons by a neutral one. In a similar manner, if the additional inequality $v_{np} \approx c_p >> c_n$ is satisfied, the lifetime in the p-type crystal is determined by the rate of band-to-band radiative recombination, while in the case of the n-type crystal the both competing channels should be accounted for.

In the stationary case Eqs. (2) and (3) result in the excess carrier concentrations

$$\delta p = \tau_p G, \;\; \delta n = \tau_n G \,. \tag{4}$$

These values can be measured experimentally, e.g., using a photoconductivity. Finally, in the opposite case of strong generation ($\delta n = \delta p >> n^{(o)}, p^{(0)}, N$) we arrive at

$$\frac{dn}{dt} = G - \frac{\delta n}{\tau}, \quad \frac{1}{\tau} = \delta n\left[\delta n(\beta_n + \beta_p) + v_{np}\right]. \tag{5}$$

Now let us examine the dependence of the lifetimes in Eqs. (2) and (3) on the uniaxial stress. The radiative recombination constant v_{np} increases with increasing compression due to renormalization of the hole density near the valence band top [8]. The scale of this increase in the range of stresses which can be obtained in practice (i.e., under conditions when the crystal is not yet mechanically destructed, $P < 5$ kbar for InSb [9]) is of the order of factor 1.5–2.0 only [8].

However, the dependences of c_n and c_p coefficients on the stress need a special treatment. It is known that, within the approximation of adiabatic terms, the temperature dependence

$$c_{n,p} = c_{n,p}^{(o)} \exp\left[-\frac{E_{n,p}^{act}}{kT}\right] \tag{6}$$

has an activation origin. In frame of the Huang-Rhys model the activation energies may be presented as

$$E_{n,p}^{act} = \frac{\left(E_T^{(n,p)} - \Delta\varepsilon^{(n,p)}\right)^2}{4\Delta\varepsilon^{(n,p)}}. \tag{7}$$

Here $E_T^{(n,p)}$ is the energy of thermal ionization of recombination level relatively to electrons and holes and $\Delta\varepsilon^{(n,p)}$ the corresponding thermal extinction energy [10]. Since one has generally $E_{n,p}^{act} \geq E_T^{(n,p)}$, the quantum tunnelling between the terms occurs in any real systems, and the activation energy in the exponent of Eq. (6) is somewhat smaller than that predicted by Eq. (7). Further corrections may be introduced into Eq. (6) when considering the deep centre in frame of the zero-radius potential model [10]. Anyway, the activation energy should represent some hyper-linear function of the thermal ionization energy $E_T^{(n,p)}$.

Let us analyse the behaviour of $E_T^{(n,p)}$ parameter for the centres of different symmetry types. The shifts of levels of these centres occurring under uniaxial stress have been examined in the studies [5, 6]. As demonstrated in the work [6], the level of an *h*-centre is split into two under the stress. However, the splitting value is an order of magnitude smaller than that for the valence band top, so that we can treat these two levels as a single one, when compare with all the other energy intervals of the problem. Considering the values of deformation potentials for InSb [4], we get the following deformation dependences of $E_T^{(n,p)}$:

(1) for the *l-c*-centre

$$E_T^{(n)}(P) = E_T^{(n)}(0) = \text{const},$$
$$E_T^{(p)}(P) = E_T^{(p)}(0) + 16.0\left[\frac{\text{meV}}{\text{kBar}}\right] \times P[\text{kbar}]. \tag{8}$$

(2) for the *h*-centre

$$E_T^{(n)}(P) = E_T^{(n)}(0) + 14.0\left[\frac{\text{meV}}{\text{kBar}}\right] \times P[\text{kBar}],$$
$$E_T^{(p)}(P) = E_T^{(p)}(0) - 4.0\left[\frac{\text{meV}}{\text{kBar}}\right] \times P[\text{kbar}]. \tag{9}$$

Let us mention that the decrease of $E_T^{(p)}(P)$ with increasing stress taking place in case of the *h*-centre is caused by comparatively large energy splitting of the valence band top.

After substitution of Eqs. (8) and (9) into Eqs. (6) and (7), and then into Eqs. (2) and (3), one can distinguish several possible cases for the low generation levels.

(1) *l-c*-centre:

The function $\tau_n(P)$ slowly decreases with increasing v_{np} (c_n being a constant), whereas $\tau_p(P)$ can be nonmonotonic due to essential decrease in c_p. However, if the *l-c*-centre is of a donor type (the majority of deep *l-c*-centres have this type of symmetry [5, 6]) and the inequality $v_{np} >> c_p$ is valid, one infers that $\tau_p(P)$ should decrease approximately two times in the *P* range from 0 to 4 kbar. In general we have

$$\tau_n(P) - \tau_n(0) < \tau_p(P) - \tau_p(0)\,. \tag{10}$$

This means that in the case of recombination via the *l-c*-centre the lifetime, and so the photoconductivity signal, decrease approximately two times in the *n*-type crystals subjected to the stresses in the range which could be obtained experimentally without destructing crystals. The decrease in the lifetime and the photoconductivity signal occurring for the *p*-type crystals is then smaller.

(2) *h*-centre:

The $\tau_n(P)$ dependence can be nonmonotonic due to essential decrease in c_n. However, if the *h*-centre is of an acceptor type (this type of symmetry is peculiar for the majority of deep *h*-centres [5,6]) and we have $v_{np} >> c_n$, the function $\tau_n(P)$ decreases approximately two times in the *P* range from 0 to 4 kbar. On the contrary, $\tau_p(P)$ decreases essentially when both v_{np} and c_p increase. In general, we have

$$\tau_n(P) - \tau_n(0) < \tau_p(P) - \tau_p(0)\,. \tag{11}$$

This means that, in the case of recombination via the *h*-centre, both the lifetime and the photoconductivity signal decrease approximately two times in the crystals of *p*-type in the range of stresses which could be obtained experimentally without destructing crystals.

The decrease in the lifetime and the photoconductivity can be essentially greater in the *n*-type crystals, being several times in the limiting case.

The inequalities (10) and (11) are qualitative because of a rough character of the Huang-Rhys model used for description of multi-phonon capture of carriers on the deep centre. Nonetheless, they give unambiguous information on the type of recombination centres.

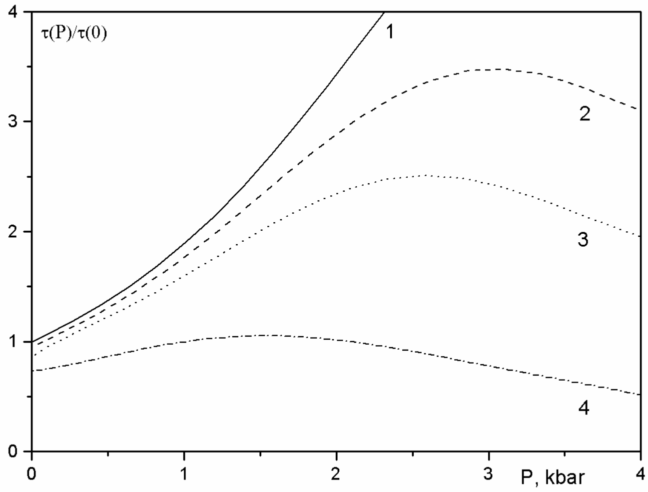

Fig 1. Calculated stress dependences of τ(*P*)/τ(0) for different values of quantum yield: curve 1 – 0.03, 2 – 0.06, 3 – 0.1, 4 – 0.4.

On the contrary, in the case of strong generation the Shockley-Read recombination via deep defects is not essential in comparison with the radiative and Auger band-to-band channels, which depend on the excess carrier concentration like $\propto \delta n$ and $\propto \delta n^2$, respectively. Then the lifetime given by Eq. (5) is not sensitive to the type of defects. The pressure dependences of τ(*P*)/τ(0) parameter calculated for different values of quantum yield under a zero stress, $\eta_0 = \dfrac{\tau_{Auger}(0)}{\tau_{Auger}(0) + \tau_{radiative}(0)} = \dfrac{\nu_{np}(0)}{\nu_{np}(0) + \delta n \beta_n(0)}$, are presented in Fig. 1. One can see that the scale of τ(*P*)/τ(0) changes is greater for smaller initial quantum yields (in general, the quantum yield decreases with increasing generation).

3. Discussion of experimental results

We have studied experimentally the crystals of *n*-InSb and *p*-InSb with the parameters $n^{(0)} = (2-3)\times 10^{13}\,\text{cm}^{-3}$ and $p^{(0)} = (4-6)\times 10^{14}\,\text{cm}^{-3}$. The InSb samples had the size of 1×2×6 mm^3. Especial attention was paid to preparation of samples and, in particular, we ensured their strictly parallel faces. The elastic stress *P* was applied along the crystallographic direction [100]. The photoconductivity of our samples was excited using a He-Ne laser operating in a continuous mode and a Nd^{3+} laser operating in a pulse mode. The stress dependences of the $\tau(P)/\tau(0)$ ratio obtained on the basis of photoconductivity measurements are presented in Fig. 2. Here the data of Fig. 2a refer to the *n*-type and those of Fig. 2b to the *p*-type crystals. In fact, these dependences represent the carrier lifetimes plotted in arbitrary units (see Eq. (4)). As seen from Fig. 2, one can derive $\frac{\tau_n(0)}{\tau_n(3\ \text{kbar})} = 1.5 \div 2$ and $\frac{\tau_p(0)}{\tau_p(3\ \text{kbar})} = 2.5 \div 5$ for the low generation levels. These values agree well with the inequality (11) for the *h*-centre of acceptor type.

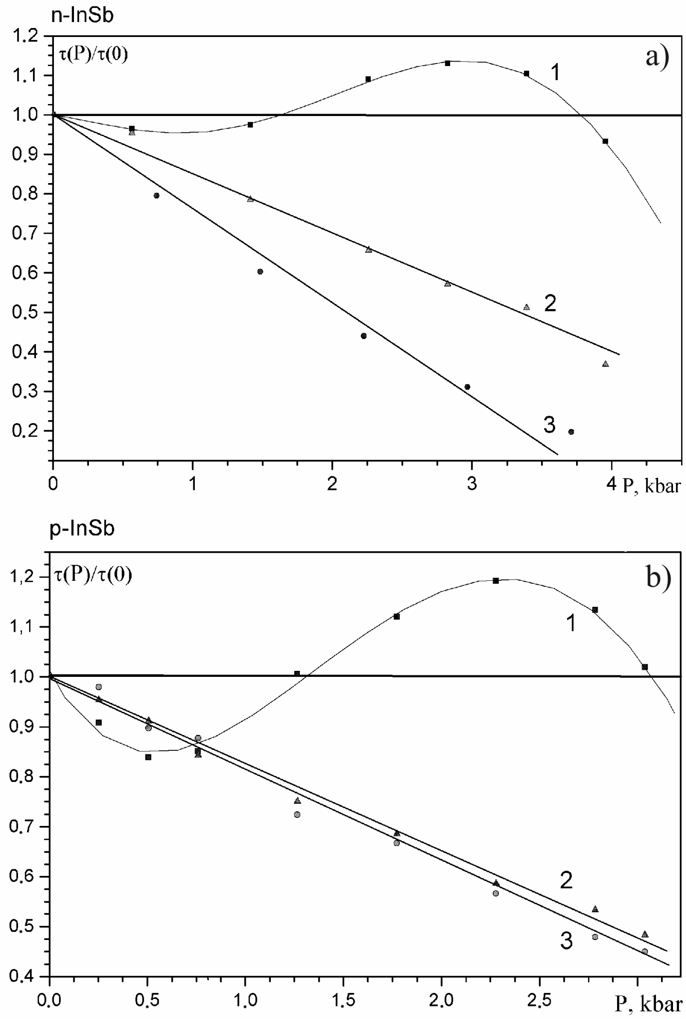

Fig. 2. Experimental stress dependences of lifetime for (a) *n*-type (1 – I_{max}, 2 – 0.01I_{max}, 3 – 0.0001I_{max}) and (b) *p*-type (1 – I_{max}, 2 – 0.01I_{max}, 3 – 0.001I_{max}) InSb crystals.

If a strong generation is dealt with ($I = 10^{23}\,\frac{\text{quanta}}{\text{cm}^2\times\text{s}}$, the case corresponding to $\delta n = 10^{16} - 10^{17}\,\text{cm}^{-3}$), the experimental dependences for the *n*- and *p*-type crystals are similar. They have characteristic maximums in the range of P = 2–3 kbar predicted by the theory (see Fig. 1). A decrease in the τ value at low stresses for some samples may be explained by competing recombination channels (e.g., via shallow levels), which have been neglected in the simple model given by Eq. (1).

Finally, we remark that the studies of stress dependences of the photoconductivity in InSb have allowed us to identify deep recombination centres in this crystal as the *h*-centres of acceptor type with the symmetry Γ_8 of the v-band top. The appropriate fourfold degenerate levels are shifted together with the v-band edge under the uniaxial stress and split into two levels.

Our results correlate with the data [7] obtained for the deep centres with the activation energy $E_j - E_V$, which are based on careful examination of the photoconductivity spectra. At the same time, they contradict the data for the same type of centres obtained from the Hall measurements [2–4].

There may be two possible explanations of this contradiction. The first is that the Hall measurements have been not accurate enough, while the second should imply that we deal in this work with some other type of recombination level (e.g., that of the type 1 from Table 1, with $E_j - E_V = 68$ meV). In any case, it is evident that the results concerned with the deep levels in InSb need especially careful re-examination.

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Анотація. *Глибокі рівні структурних дефектів в InSb, які є основними рекомбінаційними центрами в цьому матеріалі, експериментально вивчають упродовж тривалого часу. Однак досі немає чіткого розуміння природи й типу цих рівнів, відсутня надійна інформація щодо їхньої енергії зв'язку, а експериментальні дані різних робіт суперечливі. У цій роботі побудовано теоретичну модель рекомбінаційних процесів в InSb з урахуванням конкурентних механізмів оже-рекомбінації, випромінювальної зона-зонної рекомбінації та рекомбінації через глибокий домішковий рівень, інтенсивності яких по різному залежать від прикладеного одновісного тиску. Зіставлення одержаних експериментальних залежностей фотопровідності в електронному та дірковому InSb від величини одновісного стиску з прогнозами теорії дає змогу зробити висновок про те, що глибокий рекомбінаційний центр є h-центром акцепторного типу з симетрією вершини валентної зони* Γ_8*, який зміщується разом з вершиною валентної зони за умови прикладення одновісного стиску.*