ASPECTS OF SILICON BULK LIFETIMES

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Abstract

Following some general remarks about (a) high efficiencies and (b) recombination lifetimes, two specific questions are considered. First, an analysis is made of the best lifetimes which have been attained for bulk crystalline silicon as a function of doping concentrations. This is done by adopting a separability assumption that the dopants which set the Fermi level do not contribute to the recombination traffic which is due to the unknown defect. This defect is assumed to have two charge states: neutral and negative, the neutral defect concentration being frozen-in at some temperature $T_f$. It is essential for the higher doping concentrations to include the band-band Auger effect by using a generalisation of the Shockley-Read-Hall (S.R.H.) mechanism. We infer single-electron band trap recombination coefficients of order $10^{-9}$ cm$^3$ s$^{-1}$ and an unknown defect level near mid-gap. Some speculations concerning its nature are also offered. Secondly, the above-mentioned generalisation of the SRH mechanism is discussed in detail by giving relevant formulae and quoting recent comparisons with experiment. This formulation gives a straightforward procedure for incorporating both band-band and band-trap Auger effects in the SRH procedure. There are two related questions which arise in this context: (a) It may sometimes be useful to write the steady-state occupation probability of the traps implied by SRH procedure in a form which approximates to the Fermi-Dirac distribution. It is shown how this can be done. (b) Some brief remarks about the effect on the SRH mechanism of spreading $N_t$ levels at one energy uniformly over a range of energies will also be made.
1. Introduction

In this talk I want to discuss two topics of importance for the improvement of silicon solar cells. The first (§4), relates to the problem of the residual defect in silicon. Working backwards from the measured lifetime-doping relationship, we shall ask if there is some single level with some capture probabilities which can account for the best lifetimes. The answer turns out that there seems to be such a level, but to identify its precise nature requires more experiments. The second topic is the identification of Auger trap and/or Auger band coefficients by an analysis which closely resembles that familiar from the Shockley-Read-Hall (SRH) statistics. With the increasing importance of heavy doping in devices, this rarely used procedure is worth noting and it will be described in some detail. Although not new it has been used only once or twice, and it ought to be more widely known.

As this is an "overview" talk, the work indicated above is preceded by general remarks on high efficiencies (§2) and lifetimes (§3).

2. General remarks: efficiencies

The achievement of 18% efficient solar cells based on terrestrial conditions and single crystal silicon has recently been reported. A key element in the design is a thin (20-50 Å) SiO₂ layer to passivate those n⁺ silicon surface regions which are without a contact (1). A first question to be raised is if one knows that SiO₂ is the ideal layer. One knows that other layers can be used, for example in MIS structures(2); it would be interesting and important to know their effect on device performance. [There are of course other ways of attaining high efficiencies, for example by the use of ion implantation, high resistivity silicon and using surface passivation(3)]. This is the first problem to which I want to direct attention.

A second potential method of obtaining high efficiencies is to employ several cells of different energy gaps in one unit (or even in separate units so that there are four or more terminals). If one envisages black-body radiation at 6000K and a very idealised model, a two gap tandem cell might push the efficiency up from a theoretical one-gap value of 31% to a two-gap value of 42.9%(4,5). Some idea of the fall-off of efficiencies for non-optimal band gaps is obtained from Figure 1(5). More realistically, one can study tandem cells based on, for example, a combination of amorphous and crystalline silicon as has been done at M.I.T. Figure 2 shows the results of such a calculation assuming optimised gaps, silicon properties for all gaps, one sun and room temperature operation. A four-terminal arrangement is seen to be best, but in this calculation, one finds only a modest improvement of 30% efficiency over the ideal 27.5% for a single junction crystalline cell. This makes the additional complication arising from a second junction of doubtful benefit(6). An additional problem with tandem cells is that an optimal adjustment of a tandem cell for one spectrum is upset if the incident spectrum is changed by cloudiness. The investigation of such matters represents a second problem to which I want to direct attention. Note that these high theoretical efficiencies for tandem cells have not even been
Figure 1. Maximum iso-efficiency curves for a two-band gap cell at 1 sun assuming a black-body spectrum at a black-body temperature twenty times the ambient temperature.\(^5\)

Figure 2. Maximum AMI, 1 sun conversion efficiencies of crystalline-on-amorphous silicon tandem structures at room temperature if separately connected (4 terminals) or in series (2 terminals).\(^6\)
realised approximately in practice. Presumably surface problems and recombination at surfaces are among the difficulties which have impeded progress.

Multi-gap structures entirely based on amorphous silicon have also been considered. For a three-gap structure in series ($E_g = 2.0, 1.7, 1.45$ eV) a 7% efficiency was attained, compared with a theoretical 24% (7). Our main interest here is, however, in crystalline silicon.

There is an additional step which can be taken, namely to raise the mobility of the current carriers by confining them to a well in the conduction band produced by growing different materials on top of each other. In this kind of multi-hetero junction scheme the electrons travel in a two-dimensional well. They have dropped into it from a region containing the original dopants. These are thus left behind leaving to the electrons a region relatively free of ionised impurity scattering. The need to pursue these ideas, is my third problem. A start has been made with it at the Sandia National Laboratory (8).

3. General remarks: Lifetimes

Properties of a silicon wafer may be specified by giving details concerning:

- Electrical properties (resistivity, conductivity type, lifetime, etc.)
- Mechanical properties (thickness, vacancy and interstitial densities, etc.)
- Chemical properties (chemical impurity concentrations, stoichiometry, etc.)
- Surface properties (surface scratches and roughness, etc.).

Of all these many parameters I shall here been concerned only with the lifetime $\tau$ against recombination. Because it is normally larger than the dielectric relaxation time $\tau_D$, one keeps up a non-equilibrium steady state between electrons and holes and can have lifetimes and diffusion lengths which are greater than zero. [The opposite situation $\tau \ll \tau_D$ characterises the so-called relaxation semiconductor in which the Fermi levels are locally coincident.]

In order to improve solar cells one has to increase $\tau$ further.

Lifetimes may be improved by gettering metallic impurities like Au, Fe, Cu which provide deep recombination centres, using a mixture of O$_2$ and HCl. Dislocations help to getter most impurities but unfortunately they provide recombination sites themselves, particularly in the presence of vacancies.

During processing the high temperatures induce the formation of thermal defects (vacancies, interstitials, etc.) some of which are quenched into the final material and cannot be annealed out altogether. Particularly when dislocation-free material is used, and dislocation gettering is the :fore not available, these mechanical defects tend to agglomerate and to give rise to aggregates of defects (some are known as "swirls") which also shorten lifetimes. This problem presents a "point defect dilemma" (9).
It should be remembered that a good understanding of lifetimes is desirable not only because one wants long lifetimes in solar cells. One additional reason is that lifetime monitoring is important in device processing. It is used for example in neutron transmutation doping in which the uniformly distributed isotope $^{30}\text{Si}$ is converted into phosphorus dopant which is therefore also uniformly distributed:

$$^{30}\text{Si} \rightarrow ^{31}\text{P}^{+} \text{Bray}.$$ 

Lifetime measurements designed to assess the quality of the starting ingot is also in use\(^{(10,11)}\). A second additional reason for understanding lifetimes is that for some device applications lifetime reduction is required, notably for fast-switching bipolar transistors. This reduction may be achieved (after fabrication) by electron beam irradiation, or (during fabrication) by introducing "killer centres" such as Au and Pt.

4. The residual defect in silicon

If one looks at measured silicon lifetimes as a function of doping, one finds the jumble of points shown in Figure 3.

However, one may consider only the best lifetimes for given doping on the argument that these crystals have attained some ideal lifetime, limited only by a particular, but unknown, defect. This defect could be mechanical (interstitial), chemical, or an association of several of these. In this view the dopants help to set the Fermi level, but do not participate in the recombination traffic which limits the lifetime. The recombination defects, on the other hand, although of low concentration, are included in the Fermi level equation. This is a kind of "separability assumption" for Fermi level and lifetimes and it will be adopted here. What are the characteristics of this "residual" lifetime limiting defect?

To answer this question we have added to the separability assumption, secondly the hypothesis that the defect has only one recombination level and that if it is occupied it is negatively charged; otherwise it is neutral. A third assumption is that the concentration of neutral defects is that which is "frozen in" at a temperature $T_f$ with an activation energy $E_a$, so that\(^{(13)}\)

$$N_d^X = \left(5 \times 10^{22}\right) \exp \left(-E_a/kT_f\right) \text{cm}^{-3}.$$  

(1)

The numerical factor is the atomic density of silicon.

The procedure now is to regard (1) as giving the maximum solubility of the neutral defect as $T_f$. This is independent of the location in the material and of Fermi level. The defect has a negative charge states linked to $N_d^X$ by

$$N_d^-/N_d^X = \exp \left[(F - E_a)/kT_f\right].$$

Hence an increase in n-doping, by raising the Fermi level, raises $N_d^-$ and so raises

$$N_d = N_d^X + N_d^-.$$ 

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Figure 3  Some experimental minority hole lifetimes in n-type silicon (a) from reference 12.
(b) from reference 13.
This leads to a lowering of $\tau_n(N_d)$ with doping. However, increase in p-doping lowers the Fermi level and hence $N_d$. This leads to longer lifetimes $\tau_n(N_A)$ with doping until these lifetimes are pulled down again by the band-band Auger effect as shown in Figure 4. Assumption 2 concerning the charge on the unknown defect enables therefore the model to reproduce the asymmetric behaviour observed experimentally as regards $\tau_n$ compared with $\tau_p$.

The lifetime curves for the correct concentration $N_d$ of defects, as calculated at $T_f$, are used at the lower measurement temperature $T$, assuming a generalised Shockley-Read mechanism. They follow roughly $(N_d)^{-1}$ with doping, until they are both pulled down by band-band Auger effects.

The notation for the recombination constant is shown in Figure 5. We use $B_1$, $B_2$, $B_3$ for band-band recombination and $T_1$, $T_2$, $T_3$, $T_4$ for recombination involving traps. A superscript S indicates a single-electron (non-Auger) transition, the other symbols refer to Auger effects. Following Fossum et al (13, 15) one can neglect $T_1$, $T_2$, $T_3$, $T_4$ and $B_3$ and adopt

$$E_a = 1.375 \text{ eV}, \quad T_f = 620 \text{ K}. \quad (2)$$

Position of defect level: 45 meV above mid-gap.

The resulting fit is shown in Figure 4.

We are left with two matters of controversy: (1) What is $T_f$ in eqn. (1)? (2) What is the nature of the defect specified in (2)?

As to the first question, recall the early quenching experiments on silicon which led to a relation of the type

$$\frac{1}{\tau} = C \exp \left( -\frac{E_a}{kT_q} \right)$$

where the activation energy was found to be 0.6 eV, $\tau$ was the minority carrier lifetime and $T_q$ was the temperature from which the sample was quenched.

Data enabling one to find $C$ was given later for these thermally generated recombination centres:

$$C \approx 2.13 \times 10^{13} \text{ s}^{-1}, \quad E_a = 0.9 \text{ eV}. \quad (17)$$

[18; note that the captions of Figures 8 and 10 should be interchanged]. More recently a thermally generated donor density

$$\nu = C' \exp \left( -\frac{E_a}{kT_q} \right)$$

was found with $C' \approx 8 \times 10^{23} \text{ cm}^{-3}$, $E_a = 2.5 \text{ eV}$ in "pure" $p$-type silicon.
Figure 4. Doping dependence of the best room temperature minority carrier lifetime in silicon according to experiments (points). Asterisks indicate that the band Auger process is included along with the normal Shockley–Read process (unasterisked). Circles (for holes) and square (for electrons) represent experimental points (14).

Figure 5. The notation for the recombination constants.
The appropriate level was located 0.37 eV above the valence band edge (19). These results suggest that (1) is a reasonable assumption and that the freezing-in temperature $T_f$ may be identified as the quenching temperature for infinitely rapid cooling at least for some heat treatment histories. This corresponds to the "perfect" quench. Departure from the perfect quench by slower cooling should lead to $T_f < T_q$. This relation between $T_f$ and $T_q$ needs further study.

The second question is made difficult by the variety of levels found by different methods in the forbidden gap of silicon. In particular we cite nine relevant pre-1980 papers on thermally generated and/or quenched-in centres in silicon (20-28). Thus a donor level at $E_V + 0.4$ eV was found in p-type silicon in (19,20) and in boron-doped silicon in (21), but not in (22) where the boron concentration was heavier. It was again found in (24) as a complicated defect. The thermally generated defects were found to be hard to anneal out in (25) and in later work.

In a series of later papers fast ("s") and slow ("r", "r'", "r'') thermal recombination centres were found and characterised. They have formation energies of 1.0 eV, 1.2 eV and 2.5 eV (26), the slower centres being less soluble. The high binding energy and the consequent difficulty of annealing out thermal centres was confirmed (27,28). The slow centres were attributed to vacancy-Cu complexes and later to vacancy-oxygen complexes (29). The fast centres were attributed to native defects [29, Figure 3].

As regards energy level structure, many inconsistencies remain. Some of the discrepancies between the various experiments have been attributed to electrically active defects connected with traces of iron in silicon which may have been present in varying amounts (30). They can be kept down to below $10^{14}$ cm$^{-3}$ by special treatment. Iron-related deep levels have, in fact, been studied separately (31) as has the level at 0.45 eV above the valence band edge (32).

Swirl defects (due to point defect agglomerates, presumably interstitial) of formation energy 1.3 eV - 1.4 eV were also noted in p-type floating zone grown heat-treated silicon (33), and their annealing characteristics differ from those of divacancies of a similar formation energy (1.3 eV).

Two possible interpretations of the defect inferred here and characterised in (2) will now be proposed. The first suggestion is that it is a swirl. The A-type swirl, believed to consist of dislocation loops, loop clusters, etc., occurs in concentrations of typically $10^6$ - $10^7$ cm$^{-3}$, and is therefore not a serious candidate. B-type swirls are smaller and are found in concentrations up to $10^{11}$ cm$^{-3}$ or so (34). This is of the order ($10^{11} - 10^{13}$ cm$^{-3}$) of defect density implied by Figure 2 of (14). The formation activation energy of 1.3 - 1.4 eV (33) is also of the right order. If such swirls can supply an acceptor level near mid-gap (their energy level structure does not seem to be well known yet), the swirl B would be a serious candidate. This interpretation of the "residual" defect in silicon as used for semiconductor work, if correct, would be of importance for two reasons: In the first place swirl defects are known to have detrimental effects on silicon, and secondly the elimination of swirl defects is under active study. One can use slow or
Figure 6. Some deep levels in silicon due to divacancies $V_2$\textsuperscript{(36)} and due to metallic ions \textsuperscript{(37)}. 
fast crystal pulling rates, inert ambients during growth, or annealing after growth to reduce their occurrence.

A second candidate is the "s" (native, fast) recombination centre (29). The slow centres ("r, r', r'"") have levels which lie too close to the band edges, whereas the "s"-centre has a level near mid-gap. A recombination coefficient for minority carriers of $\sim 10^{-7}$ cm$^3$ s$^{-1}$ has been suggested (23) which is 100 times larger than our inferred values of $T_1 \sim T_2 \sim 10^{-9}$ cm$^3$ s$^{-1}$. This could, however, be understood in terms of different thermal histories. It is, of course, possible that the "s"-centre and the swirl B centre are the same defect. Even a very recent study (35) on the relation between recombination mechanisms and doping density leaves these matters unresolved. It is hoped that the above suggestions may, however, stimulate further work.

Deep level spectra are not well known, but some are shown in Figure 6 and it will be seen that they do not apply to the residual defect identified here.

5. Auger effects in trapping statistics

In the above discussion the Shockley-Read-Hall trapping mechanism has been invoked in order to arrive at a lifetime. However, the effect of additional Auger processes was not incorporated in the original version of 1952. This extension was made in 1963 (38) well before device engineers took an interest in heavy-doping phenomena. Because I believe this incorporation of Auger effects to yield an important new and useful concept, I have developed it and applied it from time to time (15, 39, 40). In the present context the motivation for such an extension of the Shockley-Read-Hall mechanism is particularly obvious: The reverse diode saturation current $J_0$ should be kept small in a solar cell to reduce loss by recombination. The minority (electron) carrier recombination rate per unit volume for the simplest picture of a p-type layer

$$\frac{n - n_p^0}{\tau_n} = \frac{n_p^0}{\tau_n} (\exp \delta v_n - 1) = \frac{n_i^2}{N_A n} (\exp \delta v_n - 1)$$

where $\delta v_n$ is the electron Fermi level excess over its equilibrium value divided by $kT$. It has also been assumed that the p-type material is non-degenerate with all acceptors ionised:

$$n_p^0 = n_i^2 = n_p^0 A n$$

The bulk recombination can therefore be held down by heavy doping and this brings in Auger effects as their rate tends to dominate over single carrier transitions at high carrier densities. [The improvement of the basic material by identifying and, if possible, removing deep level recombination, also indicated by the argument, was dealt with in section 4].

The need for heavy doping can also be seen from the open-circuit voltage of solar cells which in a simple theory should increase with doping but i
fact declines after going through a maximum. An early curve of this kind was given by Iles and Soclof(41).

Turning to the incorporation of the Auger effects shown in Figure 6 into the SRH trapping statistics scheme, the simplest way of doing the algebra may be as follows.

Let $N_0$ and $N_1$ be the concentration of centres or defects without a trapped electron and with a trapped electron, and let $N_d = N_0 + N_1$ be the total defect concentration. Let $n$, $p$ be electron and hole concentrations so that for non-degenerate material we have

\[
\begin{align*}
\text{Electron capture rate} &= nN_0 \\
\text{Electron emission rate} &= N_1 \\
\text{Hole capture rate} &= pN_1 \\
\text{Hole emission rate} &= N_0
\end{align*}
\]

The coefficients of proportionality, which we shall identify later, are also shown. All one needs is the steady state condition for the centres, by equating the nett electron and hole capture rates per unit volume:

\[
G(nN_0 - n_1N_1) = H(pN_1 - p_1N_0)
\]

This gives steady-state occupation fractions

\[
\frac{N_1}{N_d} = \frac{Gn + Hp_1}{G(n+n_1)+H(p+p_1)},
\]

so that

\[
\frac{N_0}{N_d} = 1 - \frac{1}{N_d}
\]

Substitution for $N_0$ and $N_1$ from (4) into the left-hand side of (3) gives the steady-state trap recombination rate per unit volume:

\[
U_{\text{st}, \text{st}} = \frac{np - n_1p_1}{(N_dH)^{-1}(n+n_1)+(N_dG)^{-1}(p+p_1)}
\]

This has the general shape of the usual S.R.H. result, except that $n_1$, $p_1$, $G$, $H$ need interpretation.

The factors $n_1$ and $p_1$ are not interesting; they follow from (3) if detailed balance is assumed.
\[ n_1 = \frac{nN_0}{N_1} \text{eq} = N e^{\frac{E_{\text{tr}}}{kT}} \]  

(6)

where \( n_1 \) and \( n_c \) are the energies of trap level and conduction band edge, each divided by \( kT \). Similarly

\[ P_1 = \frac{nN_1}{N_0} \text{eq} = e^{\frac{\eta - \eta_d}{kT}} \]  

(7)

where \( \eta_v \) refers to the valence band edge. It follows that

\[ n_1P_1 = (np) \text{eq} = n_1^2. \]

However, \( G \) and \( H \) are more interesting: we must include all the six trapping processes of Figure 5, making the electron capture rate per unit volume

\[ G_nN_0 = T_S nN_0 + T_1n^2N_0 + T_2npN_0, \]

i.e. \( G = T_1 + T_2n + T_2p. \)  

(8)

Similarly

\[ H = T_2^S + T_2n + T_3p \]  

(9)

The picture is completed by adding the band-band recombination rate per unit volume

\[ Fnp, \quad F = B^S + B_1n + B_2p \]  

(10)

Hence the total steady-state recombination rate per unit volume is

\[ U = [F + \frac{1}{(N_dH)^{-1}(n+n_0)(N_oG)^{-1}(p+p_1)}](np-n_1^2) \]  

(11)

We now proceed to some special cases of interest.

Consider now the minority carrier lifetimes. In p-type material one has \( p = p_0 \) (the equilibrium concentrations receive now a suffix zero) so that

\[ \frac{1}{n_n} = \frac{U}{n-n_0} \Rightarrow \frac{(n-n_0)p}{n-n_0} = [F + \frac{N_oG}{p+p_1}] = pF + \frac{p}{p+p_1} N_oG. \]  

(12)
\[
\frac{1}{\tau_p} = \frac{U}{p-p_0} \propto \frac{(p-p_0)^n}{p-p_0} \left[ F + \frac{N_d}{n+n_1} \right] = nF + \frac{n}{n+n_1} N_d H. \tag{13}
\]

If \( n_1 \ll n \), \( p_1 \ll p \), one has, underlining terms liable to dominate,

\[
\frac{1}{\tau_n} \propto \left( B_1^S + B_1 n + B_2 p \right)_n + \left( T_1^S + T_1 n + T_2 p \right) N_d \tag{14}
\]

\[
\frac{1}{\tau_p} \propto \left( B_1^S + B_1 n + B_2 p \right)_n + \left( T_2^S + T_2 n + T_3 p \right) N_d \tag{15}
\]

These formulae were in reasonable agreement with earlier (1962) experiments on Germanium when these results were first tested shortly after they were proposed (42). However, it took a surprising eighteen years before an explicit test was made (43). Some of the results are shown in Figure 7 and Table 1. There is reasonable agreement between theory, equation (15) in this case, and experiment. [The classical S.R.H. results are found if one puts

\[
B_1^S = B_1 = B_2 = T_1 = T_2 = T_3 = T_4 = 0. \tag{16}
\]

<table>
<thead>
<tr>
<th>Table 1</th>
</tr>
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<tbody>
<tr>
<td>Some inferred values from a fit of equation (15) to the data of Figure 7 at 300K. Based on reference 43</td>
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<table>
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<tr>
<th></th>
<th>( (T_2^S N_d)^{-1} )</th>
<th>( T_3 N_d )</th>
<th>( T_3 / T_2^S )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Au diffusion at 850°C</td>
<td>15 ( \times 10^{-8} ) s</td>
<td>5.3( \times 10^{-12} ) cm s</td>
<td>7.95 ( \times 10^{-19} ) cm³</td>
</tr>
<tr>
<td>Au diffusion at 920°C</td>
<td>1.3 ( \times 10^{-8} ) s</td>
<td>8.2( \times 10^{-12} ) cm s</td>
<td>10.7 ( \times 10^{-19} ) cm³</td>
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We thus have a method, capable of being applied to experiments, which is the natural extension of S.R.H. statistics. As Auger effects have often to be taken into account, this method should rival S.R.H. statistics in popularity. The only complication is the need to know the additional recombination coefficients. But as was seen in (16) some of these may be put equal to zero in specific cases.

There is a question of a more academic nature which the above results bring up: The steady-state occupation probability (4) of the recombination
Figure 7. Hole lifetime in n-type Si as a function of electron concentration for different temperatures. The samples were diffused with Au: (a) at 850°C, (b) at 920°C. The curves are fits of equation (15) to the data with $B_1 = B_2 = T_4 = 0$ (43).
centres should go over into the normal Fermi-Dirac function in equilibrium:

\[
\frac{N_l}{N_d} = \frac{1}{\exp(\eta_d - \gamma_o) + 1} \tag{17}
\]

where \( \gamma \) is the equilibrium Fermi level divided by \( kT \) and the degeneracy factor has been absorbed in \( \eta_d \). At first sight it is not easy to see how this can come about. However, one can rewrite (4) as

\[
\frac{N_l}{N_d} = \frac{1}{h \exp(\eta_d - \gamma_o) + 1} \tag{18}
\]

which solves the problem provided one can show that \( h + 1 \) in thermal equilibrium. This is so. In fact one finds

\[
h = \exp[\gamma_o - \frac{1}{2}(\gamma_e + \gamma_h)] \frac{\cosh[a + \frac{1}{2}(\gamma_h - \gamma_o)]}{\cosh[a + \frac{1}{2}(\gamma_e - \gamma_o)]} \tag{19}
\]

where

\[
\exp a = G_{nl}/H_{p0}. \tag{20}
\]

In thermal equilibrium \( h + 1 \), as expected. The results (18) - (20) seem to be new. They were first found in reference 44.

A question not investigated much (but see (40)), though it could be of importance for lifetimes, is the following: How is the recombination lifetime changed if \( N_d \) levels at an energy \( E_d \) are spread out with constant density to extend from \( E_d - \varepsilon \) to \( E_d + \varepsilon \)? This doubt arises occasionally in modelling situations. To answer this question one can use the generalised S.R.H. process, assuming that defect-defect transitions are negligible. This matter is under investigation. Preliminary results suggest that, depending on the position of \( E_d \) and on the excess carrier concentration, the recombination rate can move in either direction. For a defect at midgap a decrease is more likely, while an increase is favoured if the defect is in the upper part of the gap provided the excess carrier concentration is not too large. More details will be reported in due course.
6. Additional comment after the work was completed.

A defect similar to the one inferred here (in section 4) appears to have been found in swirl- and dislocation-free float zone grown silicon by deep level transient spectroscopy and derivative surface photovoltage (45). This dominant recombination level was located at $E_v + 0.56\text{eV}$ with a capture cross section for holes equal to twice the capture cross section for electrons:

$$\sigma^S_2 = 2\sigma^S_1 = 10^{-14}\text{ cm}^2$$  \hspace{1cm} (21)

in fair agreement with the specification (2), above, of the defect identified here. If one puts

$$T^S_2 = f \nu \sigma^S_2 \ (\nu \sim 10^7 \text{ cm/s} \ - \text{thermal velocity})$$

and inserts our value for $T^S_2$ and relation (21) the factor $f$ (giving a recombination efficiency) turns out to be

$$f = 0.05.$$ 

The same result is found if $T^S_1$ and $\sigma^S_1$ are used. These authors suggest that the defect may be a self-interstitial or a cluster of these - this is a third possibility in addition to the two noted in section 4.
REFERENCES


DISCUSSION

SCHUMACHER: Well, Peter, I guess I don't understand the whole story here, but after all, in the Shockley-Read-Hall treatment of lifetime, the shifting of the Fermi level is taken into account, and there is an occupancy factor that tells you how many electrons, how many majority carriers there are in the centers for recombination. Then, as a result of that, the lifetime in less heavily doped material is higher than the lifetime in more heavily doped material. Of course, if you change the total number of recombination centers, then you can change the lifetime. You are saying that the number of recombination centers is changing because of the position of the Fermi level, not just the occupancy number. In order for what you saying to be true, it would be necessary for the total number of recombination centers to change.

LANDSBERG: Right. And so it does. I think I might not have made it clear. It is entirely my fault. Perhaps what I didn't explain quite well enough is that these dopants don't act as recombination; a kind of separability assumption that the defect acts as a recombination center. The dopant is merely there to set the Fermi level. Now, what happens is, as you said, the lifetime increases because the total number of defects has decreased.

SCHUMACHER: Then the X is the total number of defects.

LANDSBERG: No. The X is the total number of neutrals. So the neutral defect density is given by the solubility of the defect in the silicon.

SCHUMACHER: Then $N_d^X$ is not the total number of defects?

LANDSBERG: There is an old paper by Hall and Shockley many years ago that discussed solubility. There were other people after this. They were talking largely about the solubility of the neutral species. That is always uniform; it is not affected by the p-n junction, and so on, because it doesn't react in an electric field because it is neutral.

TAN: Peter, I have two simple comments, made in good faith, and I hope you will accept them in good faith too. The first one is that in one early slide you said that in order to specify the material, silicon, you have something called a mechanical property. Those of us who work in the material characterization field refer to that as a physical defect. This is simply a misnomer, not important. The important part is that to my knowledge, up to today, we do not know how to specify that property in the same sense as you would with your electrical property.

LANDSBERG: I think it is a very interesting point you are making, because it is just where I am rather ignorant.

TAN: That is why I mentioned I made these comments in good faith.

LINDHOLM: I will be very brief, but some of the people here might want to know where some of these things were published. Can you tell us what is the status of that manuscript?
LANDSBERG: We didn't pay any reprint charges because we couldn't afford to.

LINDHOLM: That is a good comment for the sponsors to listen to.

LANDSBERG: Therefore, it is delayed. It is in the Journal of Applied Physics. The proofs have been seen but as far as I know it has not appeared yet.

LINDHOLM: As a point of clarification in sort of following up Joe Loferski's question: I think that your $T_f$ on the slide stands for temperature of formation. You have an activation energy of 1.3 eV, and roughly figuring that out, that must mean around 600K. Do you remember that?

LANDSBERG: Yes. It was around 620K, something of that order.

SCHWUTTKE: Just a comment in supporting the characterization people on the previous comment. Looking back to my early years as a student, there was one hot subject, and you will remember this as well as I do. People were totally concerned for what we called color centers, and they studied this from a to b to c. And every month, almost, they discovered a new symbol. Then later on, once I graduated, they discovered one particle of matter, another particle of matter and I don't know how many particles of matter they have discovered by now. And then we were very proud that we defined crystal perfection by zero dislocation density and so we got accustomed to zero dislocation density and crystal perfection -- to characterize crystal perfection by the number of dislocations. And then, I believe, a lot of nuclear physicists got into silicon, and from there on we have had this tremendous confusion about crystal perfection. Today crystal perfection does not mean that you have zero dislocation. You are really addressing the state, the point defect state, in the materials. Basically, you can only talk about crystal perfection if you know the condition of every atom and what else is floating around. You are faced with some very difficult problems if you want to calculate something, because we just cannot provide you with the necessary detailed information that you need to make the proper calculation. So it is basically our shortcoming, not yours, and I would like apologize for that.