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Validity of simplified Shockley-Read-Hall statistics for modeling carrier lifetimes in crystalline silicon

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Abstract - The Shockley-Read-Hall model, in its simplest and most common form, is often used to describe both injection- and temperature-dependent carrier lifetime measurements. Such lifetime modeling has provided the basis for novel, ultra-sensitive spectroscopic techniques for the study of recombination centres in crystalline silicon. However, this approximate model is only valid when the density of recombination centres is small enough to avoid trapping effects, which cause distortions in the excess mobile carrier concentrations. In this work, the simplified Shockley-Read-Hall model is compared with a more general solution of the continuity equations that takes account of carrier trapping. This comparison leads to an expression for the upper limit on the recombination centre density for which the simplified Shockley-Read-Hall model remains accurate. The limit depends not only on the dopant density, but also on the energy level and electron and hole capture cross-sections for a given type of recombination centre. The results allow experimental conditions that do not invalidate the use of the simplified Shockley-Read-Hall model to be determined.

1. INTRODUCTION

New techniques based on carrier lifetime measurements have been developed recently with the common goal of characterising impurities in crystalline silicon. One approach, which has been referred to as Injection Dependent Lifetime Spectroscopy (IDLS)[1], involves fitting Shockley-Read-Hall theory to injection-level dependent lifetime measurements. Within certain constraints, such a procedure allows the energy level and carrier capture cross sections of an impurity to be determined, often with superior sensitivity and accuracy to conventional techniques such as Deep-Level Transient Spectroscopy (DLTS). The IDLS technique has recently been applied to boron-oxygen complexes in Czochralski silicon[2,3] and also to iron-boron pairs in silicon[4-6], as well as other metallic species such as chromium, molybdenum and titanium[7,8]. Previously, it had been employed in analysis of recombination centres at silicon dioxide/silicon interfaces[9] and silicon nitride/silicon interfaces[9,10], which are of critical importance in solar cell applications. It has also been used in characterising recombination centres in electron-irradiated silicon[11,12]. In fact, simplified variations of the technique effectively formed the basis of well known, pioneering studies of iron-boron[13] and chromium-boron[14] pairs in silicon.

A second group of lifetime-based techniques, recently dubbed Temperature Dependent Lifetime Spectroscopy (TDLS), has also been developed[1]. By analysing the temperature dependence of the low-injection lifetime, the energy level of the dominant recombination centres can be inferred. So far it has found application in analysis of iron-related centres[15-17] and various other metallic centres[18], as well as electron-irradiated silicon[11,12]. It appears certain that lifetime-based techniques such as IDLS and TDLS will become more widespread as increasingly sensitive techniques are needed to track ever-diminishing quantities of impurities, and as the requirements of electronic devices become ever more stringent.

These two techniques rely heavily on the use of Shockley-Read-Hall (SRH)[19,20] statistics to model the behaviour of the recombination lifetime as a function of either injection-level or temperature. However, they generally make use of a simplified version of SRH theory that involves a number of assumptions[21,22] that must be satisfied when applying the model to experimental data. The most restrictive of these requires almost equal excess 'untrapped' electron and hole concentrations. As the recombination centre density N approaches a critical value N_{crit}, this simplified SRH model becomes increasingly inaccurate, due to the fact that the recombination centres in general also act as 'traps'. When this occurs, carriers spend some finite time trapped at the centre before either recombining or being ejected back into the band from which they came. Such trapping alters the overall carrier dynamics, often very significantly, and even if only one type of carrier is trapped. This restriction on the SRH model is often expressed as simply requiring that N be 'small'.

The purpose of this paper is to determine exactly how small N must be to ensure the simplified SRH model remains accurate, therefore

enabling lifetime-based spectroscopic techniques to be safely employed. This is achieved by comparing it with a more general model that explicitly accounts for the trapping properties of the defects and hence is valid for any value of N, provided that steady-state conditions prevail. This general model is used to find an expression for N_{crit} in terms of the dopant and excess carrier densities, and also the energy level and capture cross-sections of a given recombination centre. These latter parameters turn out to have a significant impact on the range of validity of the simplified SRH theory. Firstly, however, we begin with the continuity equations, which provide a general description of carrier dynamics within a semiconductor, and which are the basis for all the recombination models considered.

2. RECOMBINATION MODELS

In a non-degenerate semiconductor under the influence of external illumination, the excess concentrations of free, untrapped electrons Δn and holes Δp are described by the following continuity equations[21]:

$$g_E - \frac{d\Delta n}{dt} = \frac{\Delta n}{\tau_n} = \frac{1}{\tau_{n0}}\left[\frac{(n_0 + n_1 + \Delta n)(\Delta n - \Delta p)}{N} + \frac{\Delta n n_1}{n_0 + n_1}\right] \quad (1)$$

$$g_E - \frac{d\Delta p}{dt} = \frac{\Delta p}{\tau_p} = \frac{1}{\tau_{p0}}\left[\frac{(p_0 + p_1 + \Delta p)(\Delta p - \Delta n)}{N} + \frac{\Delta p p_1}{p_0 + p_1}\right]. \quad (2)$$

Here, g_E is the rate of electron-hole pair generation by the illumination, n_0 and p_0 are the electron and hole concentrations in thermal equilibrium, τ_n and τ_p are the electron and hole lifetimes and N is the recombination centre density. The capture time-constants for electrons and holes, τ_{n0} and τ_{p0}, are related to the capture cross-sections σ_n and σ_p of the recombination centre, and also to the recombination centre density and the thermal velocities of electrons and holes v_{th}, via the following expressions:

$$\tau_{n0} = \frac{1}{N\sigma_n v_{th}} \qquad \tau_{p0} = \frac{1}{N\sigma_p v_{th}}. \quad (3)$$

The assumption of non-degeneracy is required to provide an unambiguous meaning to the capture cross-sections, since they represent 'average' cross-sections for carrier capture from *all* possible band-states[21]. The statistical factors n_1 and p_1 are the equilibrium concentrations of electrons and holes respectively when the Fermi level coincides with the energy of the recombination centre E_T:

$$p_1 = N_V \exp\left(\frac{E_C - E_G - E_T}{kT}\right), \qquad n_1 = N_C \exp\left(\frac{E_T - E_C}{kT}\right) \quad (4)$$

where E_C is the conduction band edge energy and E_G the energy gap. The densities of states at the conduction and valence band edges N_C and N_V are N_C=2.86×10^{19} and N_V=3.10×10^{19}cm^{-3} for silicon at room temperature[23].

The continuity equations (1) and (2) allow for all the possible interactions between the bands and the recombination centres, namely recombination via capture of an electron (or hole) and subsequent capture of a hole (or electron), or trapping via capture and release of an electron (or hole). The tendency of a specific recombination centre to act primarily as a trap or a recombination site, or as some combination of both, will depend on its energy and capture cross-sections, and also on the Fermi level.

As discussed by Blakemore[21], the time-dependent continuity equations (1) and (2) can only be solved analytically under very special conditions which are not of great practical interest. In the general case, complications arise due to the coupled nature of these expressions, which is a direct consequence of the fact that the centres may act as both recombination sites and as traps. Under steady-state conditions, however, the time-dependent terms are zero, the equations are less strongly coupled, and general solutions do exist. This was exploited by Shockley and Read[19], whose Equation 4.4 is precisely such a solution, the only underlying assumptions being those of non-degeneracy and steady-state conditions. Cast in this form, SRH theory is indeed quite general. However, in subsequent sections of their paper, Shockley and Read went on to develop only cases with restricted application. The first of these, in their sections 5 and 6, was for arbitrary modulation (values of Δn and Δp) but only small values of N. A later case, in Appendix A, was for arbitrary N but only small modulation. It is the first of these restricted manifestations of SRH theory, i.e. for small N, which is most widely used today. We shall refer to it as the 'simplified' SRH model, following the heading of Shockley and Read's own Section 5.

One route to the simplified SRH expression from the continuity equations involves

eliminating N by substitution from Equation (1) into Equation (2) under steady-state conditions. After some re-arranging, and upon use of the identities $n_0/(n_0+n_1)=p_1/(p_0+p_1)$ and $p_1n_1=p_0n_0$, the result is:

$$g_E = \frac{\Delta n}{\tau_n} = \frac{\Delta p}{\tau_p} = \frac{p_0\Delta n + n_0\Delta p + \Delta n\Delta p}{\tau_{p0}(n_0 + n_1 + \Delta n) + \tau_{n0}(p_0 + p_1 + \Delta p)}. \quad (5)$$

Further manipulation of this expression, along with the assumption of vanishing excess carrier densities, leads to Equations (A7) of Shockley and Read, which is the case for arbitrary N but restricted to small modulation. If, on the other hand, arbitrary excess carrier densities are allowed, but we insist that N is small enough to not noticeably perturb them, so that $\Delta n=\Delta p$, then we are led directly to Equation 5.3 from Shockley and Read, the simplified SRH model:

$$\tau_{SRH} = \tau_n = \tau_p = \frac{\tau_{p0}(n_0 + n_1 + \Delta n) + \tau_{n0}(p_0 + p_1 + \Delta n)}{n_0 + p_0 + \Delta n}. \quad (6)$$

Note that the simplifying assumption merely requires that $\Delta n=\Delta p$, but it is not clear exactly how small N must be to ensure this is so. This generates some uncertainty in applying the simplified SRH model to experimental data. As mentioned, however, this expression is widely employed in modeling carrier recombination for applications such as IDLS and TDLS. In order to quantify the limitations of the SRH model, it is useful to compare it with a more general solution to the continuity equations.

Blakemore has shown that general solutions of the continuity equations can be relatively easily found for the case of arbitrary excess carrier densities and values of N, making the assumptions in the simplified SRH model largely unnecessary. The only disadvantage of these general solutions over the simplified SRH model is that they are long.

When steady-state conditions prevail, the continuity equations (1) and (2) may be written as:

$$g_E = \frac{1}{\tau_{n0}}\left[\frac{(n_0 + n_1 + \Delta n)(\Delta n - \Delta p)}{N} + \frac{\Delta n n_1}{n_0 + n_1}\right] = \frac{1}{\tau_{p0}}\left[\frac{(p_0 + p_1 + \Delta p)(\Delta p - \Delta n)}{N} + \frac{\Delta p p_1}{p_0 + p_1}\right]. \quad (7)$$

This expression represents two equations containing three unknowns: Δn, Δp and g_E. Manipulating the two expressions on the right hand side of Equation (7) gives a quadratic equation involving only Δn and Δp. Upon applying the identities $n_0/(n_0+n_1)=p_1/(p_0+p_1)$ and $p_1n_1=p_0n_0$, the solution may be written as[21]:

$$\Delta n = \sqrt{\frac{1}{4}[A + \Delta p(k+1)]^2 - \Delta p N\left(\frac{p_0 - kp_1}{p_0 + p_1}\right)} - \frac{1}{2}[A + \Delta p(k-1)], \quad (8)$$

where we have defined $k=\tau_{n0}/\tau_{p0}$ and:

$$A = \frac{Np_0}{p_0 + p_1} + k(p_0 + p_1) + n_0 + n_1. \quad (9)$$

By choosing a range of values for Δp, we may calculate the corresponding values firstly for Δn, then g_E, and finally the carrier lifetimes via $\tau_n=\Delta n/g_E$ and $\tau_p=\Delta p/g_E$. The injection-level dependent lifetime curves obtained in this way may then be compared with the simplified SRH model. Of course it is also possible to express τ_n directly in terms of Δn and N, similarly for τ_p in terms of Δp and N. As expected, these expressions reduce to the familiar simplified SRH model when N is small. However, they are lengthy both to derive and express, as illustrated by Blakemore[21] in his Section 8.4, while the more compact approach shown here is more easily computed.

Note that if N is small then Equation (8) simplifies to $\Delta n=\Delta p$, as expected. Under these conditions the results will be identical to the simplified SRH model. However, in the general case $\Delta n\neq\Delta p$ and therefore $\tau_n\neq\tau_p$. This point has recently been highlighted by Karazhanov[24,25], who used Equations (5) in conjunction with the electroneutrality condition to calculate Δn and Δp and therefore τ_n and τ_p. In contrast, the approach used here involves direct solution of Equations (1) and (2), which implicitly contain the electroneutrality condition.

It may seem logical at this point to suggest replacing the use of the simplified SRH model in lifetime spectroscopy applications with this more general solution of the continuity equation. Indeed, this would remove entirely the need to be watchful for trapping effects. However, the general solution requires explicit knowledge of the value of N, while the simplified SRH model does not (although even in the simplified case N is required to determine the capture cross-sections, but not the capture time-constants). In many practical cases the value of N is not known, and so the simplified model may be the most useful, despite the restricted range over which it is valid.

A final point to note regarding these models is that they both neglect the possibility of tunneling transitions *between* recombination centres. If the wave-functions of these localised states overlap to an appreciable extent, then such tunneling transitions can affect properties such as lifetime and mobility. A well known example is amorphous silicon, which contains band-tail states of sufficiently high concentration to allow 'hopping' between them. Hattori *et al.*[26] recently developed a recombination model for amorphous silicon that contained three types of electronic state: the bands themselves, the band-tails, and deep states. Their model allowed transitions between the bands and both the band-tail and deep states, as well as between the band-tail states and the deep states. They also included tunneling transitions between band-tail states, and found that these were largely responsible for the form of measured drift mobility data. They did not however include tunneling transitions between deep states, since their density was kept below 10^{17}cm^{-3}, and hence their wave-functions are very unlikely to overlap. Similarly, in this work, we neglect tunneling transitions between the deep states, and any impact this might have on the lifetime, since in almost all practical cases the density of recombination centres will be well below 10^{17}cm^{-3}. Band-tails do not normally exist in crystalline silicon, unless it is extremely heavily doped, and so we do not include their effects here either.

3. COMPARISON OF THE TWO MODELS

Figure 1 provides a direct comparison between the general steady-state solution derived above and the SRH model for the specific case of interstitial iron in crystalline silicon. This particular recombination centre, which has an energy level[27] of E_V+0.38eV and capture cross-sections of $\sigma_n=5\times10^{-14}$ and $\sigma_p=7\times10^{-17}$cm^{-2}, was chosen because it provides a good example of the behaviour of a 'deep' centre. Three different values of the iron concentration are shown on the plot. For each of these, four lifetime curves are plotted: the simplified SRH lifetime, the electron and hole lifetimes from the general steady-state solution, and a mobility-weighted combination of these electron and hole lifetimes. The latter weighted curve will most accurately reflect lifetime measurements from photoconductance-based methods, which are unable to discriminate between carrier type since they merely record changes in conductivity. The weighted lifetime is calculated via $\tau_{wtd}=\Delta p_{wtd}/g_E$ where the mobility-weighted excess carrier density Δp_{wtd} is given by:

$$\Delta p_{wtd} = \frac{\Delta n\mu_n + \Delta p\mu_p}{\mu_n + \mu_p}. \qquad (10)$$

The four curves that represent the lowest concentration of iron are all in good agreement. In this case, the small concentration of centres causes negligible trapping, or, in other words, a minimal inequality between excess mobile electron and hole concentrations. The result is electron and hole lifetimes that are almost equal at all injection-levels, and hence one may safely apply the simplified SRH model in this case.

As the iron concentration increases, however, the electron and hole lifetimes start to become significantly different, especially at the lower injection-levels. This reflects an increasing breakdown of the simplified SRH model. The mobility-weighted lifetime curves reveal that the large hole lifetime causes the simplified SRH model to underestimate data obtained by photoconductance-based techniques. Note however that the curves are still in good agreement at higher injection levels.

The trends shown in Figure 1 are characteristic of deep recombination centres, which always generate lifetimes that increase (or remain constant) with increasing injection-level[1]. In contrast, shallow centres can result in either increasing or decreasing lifetimes, depending on the dopant density and the exact value of the energy level[21]. FeB pairs provide an example of shallow centres in silicon. Figure 2 gives a comparison of the SRH model and the general steady-state solution for FeB pairs, with an energy level[27] of E_C-0.23eV and capture cross-sections[6] of $\sigma_n=3\times10^{-14}$ and $\sigma_p=2\times10^{-15}$cm^{-2}. Once again, the results show that the SRH theory becomes increasingly inaccurate as the recombination centre density increases. For modern spectroscopy techniques that rely on the use of SRH theory, the important question then becomes – what is the critical recombination centre density above which the simplified SRH model will be inaccurate? This question is addressed in the following section.

4. THE CRITICAL RECOMBINATION CENTRE DENSITY

The upper limit on the recombination centre density N for which the simplified model is accurate will depend on the particular properties

of the recombination centre (i.e. the energy level and capture cross-sections), and also on the dopant density. In general, it will also depend on the concentration of excess carriers, since, if sufficiently numerous, these may overwhelm any trapping effects. A convenient way to express this limit is by defining a parameter N_{crit}, such that the simplified SRH model is only valid if $N \ll N_{crit}$.

A direct approach to calculating N_{crit} is to consider the excess carrier ratio $\Delta n/\Delta p$ as determined by the general steady-state model above. For conditions under which the simple SRH model is accurate, trapping must be negligible, and this ratio will be close to unity. An expression for $\Delta n/\Delta p$ can be arrived at from Equation (7):

$$\frac{\Delta n}{\Delta p} = \frac{n_0 + n_1 + \Delta n + k(p_0 + p_1 + \Delta p) + kp_1 N/(p_0 + p_1)}{n_0 + n_1 + \Delta n + k(p_0 + p_1 + \Delta p) + p_0 N/(p_0 + p_1)}. \quad (11)$$

Firstly, it is clear from this expression that the right hand side will always equal unity when

$$p_0 = kp_1 = \frac{\tau_{n0}}{\tau_{p0}} p_1. \quad (12)$$

If this condition holds, trapping will *always* be negligible, irrespective of the recombination centre density N. In practice however, this condition is only satisfied by rare coincidence. In physical terms, it represents the unique combination of energy level and capture cross-sections that cause a perfect balance between majority and minority carrier trapping[21].

In the more general case, the right-hand side of Equation (11) will also be close to unity when the two terms involving N either do not contribute much to the numerator or denominator, or contribute very similarly. A convenient way to express this in a single inequality is to state that the *magnitude of their difference* must be much less than the other terms. After some rearranging, we then arrive at the following expression for N_{crit}:

$$N_{crit} = \frac{(p_0 + p_1)[n_0 + n_1 + \Delta n + k(p_0 + p_1 + \Delta p)]}{|p_0 - kp_1|}. \quad (13)$$

If we require the simplified SRH model to be accurate to within 10%, then N must be at least an order of magnitude smaller than N_{crit}. Under high-injection conditions, a greater concentration of recombination centres can be tolerated, since N_{crit} increases due to the Δn and Δp terms. However, it is often the value of N_{crit} under low-injection conditions which is of interest. For a p-type sample with $p_0 = N_A$ such that $n_0 = n_i^2/p_0$ is negligible, the relevant expression for N_{crit} in low-injection is:

$$N_{crit} = \frac{(N_A + p_1)(n_1 + kN_A + kp_1)}{|N_A - kp_1|}. \quad (14)$$

This expression can be simplified further if the recombination centres are deep, meaning that both p_1 and $n_1 \ll N_A$. In such cases, provided k is not excessively large, then:

$$N_{crit} = N_A \frac{\tau_{no}}{\tau_{p0}}. \quad (15)$$

This final expression in fact represents the lowest possible, and hence most restrictive, value for N_{crit} for *any* recombination centre energy, deep or shallow. In this sense, deep levels are the most likely to cause the simplified model to become invalid for a given value of N. This does not necessarily mean, however, that they will always be the most difficult to study using the simplified SRH model. In general, fewer deep recombination centres are required to produce a given lifetime, counterbalancing the fact that N_{crit} is smaller for such centres.

Another important feature of this final expression is that N_{crit} depends only on the *ratio* of τ_{n0} and τ_{p0}, and not on their magnitudes. This reflects the fact that the centres must not cause significant trapping of carriers, as has been discussed above. The extent to which this trapping occurs is characterised by the ratio τ_{n0}/τ_{p0}, since this is essentially a measure of the proportion of time that the carriers remain untrapped. It is not surprising then that this parameter has a heavy bearing on the boundaries of accuracy of the simple SRH model.

It is worth noting at this point that Shockley and Read also considered under which conditions their simplified theory would be valid (as discussed in their Appendix A). They concluded that the simplification would hold provided N is small compared with any one of n_0, p_0, n_1 or p_1. However, the conditions under which they arrived at this conclusion were only valid for infinitesimal modulation. In contrast, the expression for N_{crit} given in this work also accounts for arbitrary modulation, hence the appearance of Δn. Furthermore, the expression derived here also accounts for the potential impact of highly asymmetric cross-sections, as

manifested in the value of k, which was not considered in Shockley and Read's approximate approach.

Figure 3 depicts the dependence of the low-injection limit of N_{crit}, normalised with respect to N_A, as a function of the recombination centre energy, which appears indirectly in Equation (14) through n_1 and p_1. Five curves are shown, corresponding to different values of the capture cross-section ratio k. The spikes on the curves correspond to the conditions of Equation (12) – a very special and narrow range of energies for which the effect of trapping will be negligible. Of more general interest however, the curves show that there is a broad range of energy levels near the middle of the band-gap that has the most detrimental impact on N_{crit}. These are referred to as deep centres, and the magnitude of their impact on N_{crit} is determined directly by the value of k.

Figure 4 shows that the breadth of the flat region due to deep centres is determined by the dopant density. For lightly-doped samples, the range of recombination energies which generates the most severe trapping is reduced. Furthermore, shallow centres of a given energy level impose a less stringent limit on N_{crit} in more lightly-doped material. Figures 3 and 4 reveal that whether a centre behaves as a deep centre or not depends not only on its energy, but also on the dopant density and the value of k. Therefore, care must be taken to avoid applying Equation (15) to centres which, despite having energy levels far from the band edges, may not behave as deep states. It should be noted that in both Figures 3 and 4, the value of N_{crit} exceeds 10^{17}cm^{-3} at some points. It is possible that tunneling transitions between the deep states would significantly alter the carrier dynamics if the actual value of recombination centres, N, also exceeded this value. In such cases a more complex model such as that developed by Hattori *et al.* would be required.

If a recombination centre is known to be deep, then N_{crit} is given by Equation (15) for low-injection conditions. As discussed above, interstitial iron is a deep centre in silicon, and its low value of k results in a limit of $N_{crit}=1.4\times10^{12}$cm^{-3} for the dopant density in Figure 1 ($N_A=10^{15}$cm^{-3}). The plots in Figure 1 show that when $N \ll N_{crit}$, (i.e. the $N=10^{11}$cm^{-3} case), the SRH model is accurate across all injection-levels. For higher recombination centre densities, mid- to high-injection lifetime measurements may still be accurately modeled with the SRH theory, provided the excess carrier concentration is high enough to ensure that $N \ll N_{crit}$, where N_{crit} is given by Equation (13).

For shallow centres, the value of N_{crit} depends on the factors n_1 and p_1 also. An example of such a shallow centre is given by FeB pairs, which give a value of $N_{crit}=3.6\times10^{15}$cm^{-3} for the conditions in Figure 2 ($N_A=10^{15}$cm^{-3}). Once again, the curves reveal that the value of N_{crit} provides an effective demarcation between the regions over which SRH theory is valid for all injection-levels and those over which it is not. It should be noted that, while referred to as shallow, FeB pairs are still some considerable distance from the conduction band edge. As a result, the terms containing n_1 and p_1 in Equation (13) moderate the value of N_{crit}, but not to a massive extent. However, for very shallow centres, N_{crit} is likely to be much larger, due to the overwhelming magnitude of either p_1 or n_1.

A. Modeling more than one type of centre simultaneously

In many practical situations, more than one type of recombination centre may be present in significant quantities. As mentioned, one such example is provided by interstitial iron and FeB pairs. Both centres may occur with similar concentrations, and both may impact significantly on the overall, or *effective*, recombination lifetime.

A question naturally arises as to how to correctly deal with such cases. A common approach is to treat the different types of recombination centres as 'independent', and then proceed to sum the inverse lifetimes due to each type of centre to obtain the effective lifetime.

In using this approach, it is assumed that any additional terms arising from interactions between the various types of centres are negligible[21]. If being used in conjunction with the simplified SRH model, it is only valid when *all* types of recombination centre are present in small enough quantities to avoid trapping, that is they must all satisfy the requirement $N \ll N_{crit}$. Even if only one such centre traps carriers to any significant extent, the resulting change in the free carrier populations can cause very large changes to the recombination dynamics of *all* the centres. An extreme case is described by the Hornbeck-Haynes model[28], which was developed for the situation in which one type of centre acts only as a recombination centre, and another only as a trap. This model shows that the trapping centres do indeed have a dramatic impact on the behaviour of

the recombination centres, and has been used to explain unusual photoconductance measurements in single-crystal silicon and germanium[28-30] and multicrystalline silicon[31].

B. An Experimental Example

Figure 5 shows photoconductance-based lifetime measurements, taken from Ref. 6, of a silicon sample with a total Fe concentration of 2.5×10^{13}cm^{-3}. The iron was introduced by ion-implantation, and the sample annealed to distribute the iron uniformly throughout the bulk, taking care to avoid precipitation[6]. The lifetime measurement was performed using the quasi-steady-state photoconductance (QSSPC) technique[32]. Unfortunately, it was not possible to measure the iron-related lifetime at lower carrier densities than shown, because of the existence of trapping centres associated with the surface passivating film which overwhelm the photoconductance[6]. In this sample, only 20% of the iron was present in interstitial form, the rest was paired with boron dopant ions.

Also shown are the simplified SRH lifetimes for the relevant concentrations of Fe_i and FeB pairs, calculated using the capture cross-sections and energy levels given above, as well as the combined lifetime achieved by adding the inverses of these two components. The general, mobility-weighted steady-state solutions are also shown. The general solution and the simplified model are in good agreement for all injection-levels for the FeB pairs, but a discrepancy emerges at lower carrier concentration for Fe_i. As a result, a similar disagreement appears for the combined recombination lifetimes.

The values of N_{crit} for this dopant density (9×10^{13}cm^{-3}) are 1.6×10^{11} and 3.6×10^{15}cm^{-3} for interstitial iron and FeB pairs respectively. Therefore we expect the simplified theory to be valid for all injection-levels for the FeB pair component, since $N_{FeB}\ll N_{crit\text{-}FeB}$. This is clearly not true for the interstitial iron component however. As a result, the simple SRH model is not valid for this sample across all injection-levels. However, at higher injection-levels the simplified model remains valid due to the swamping of the trapping effects by excess carriers. For trapping effects to impact on the measurement by no more than 10%, we require that $N_{crit\text{-}Fei}$ be an order of magnitude larger than $N_{Fei}=5\times10^{12}$cm^{-3}. From Equation (13), this is satisfied when $\Delta n=\Delta p=4.5\times10^{13}$cm^{-3}. Figure 5 shows that this is indeed the region in which the general model and the simplified SRH model converge within 10% for the Fe_i curves. Since interstitial iron accounts for about only half of the total recombination lifetime at this carrier density, the effective value for Δp is around 2×10^{13}cm^{-3}.

4. CONCLUSIONS

The simplified Shockley-Read-Hall model is a powerful and widely-used tool in lifetime-based techniques for characterising impurities and defects in semiconductors. However, to be confident that its use is valid, it is necessary to verify that the recombination centre density N is small enough to avoid excessive trapping effects. An expression for the critical value of N, above which the simplified SRH model becomes invalid, has been presented. It reveals that the most severe restrictions on the region of validity of the simplified SRH model occur for deep centres with highly asymmetric capture cross-sections. These restrictions should be considered routinely when using spectroscopic techniques based on either injection-level or temperature dependent lifetime modeling.

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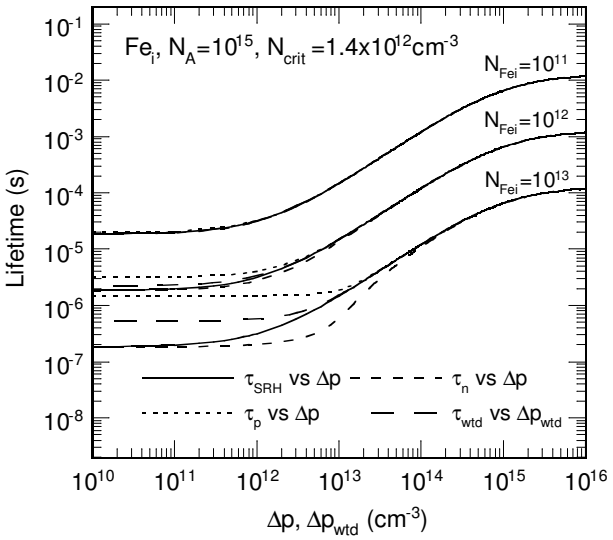

FIG. 1. Comparison between the injection-level dependence of the simplified SRH lifetime and the electron and hole lifetimes as calculated from the general steady-state solution, using the recombination parameters of interstitial iron. Curves are shown for three values of the iron concentration. The electron and hole lifetimes are plotted against the excess hole concentration Δp. Also shown for each iron concentration is a fourth curve, τ_{wtd}, which represents the mobility-weighted combination of τ_n and τ_p plotted against a similarly weighted excess carrier concentration Δp_{wtd}.

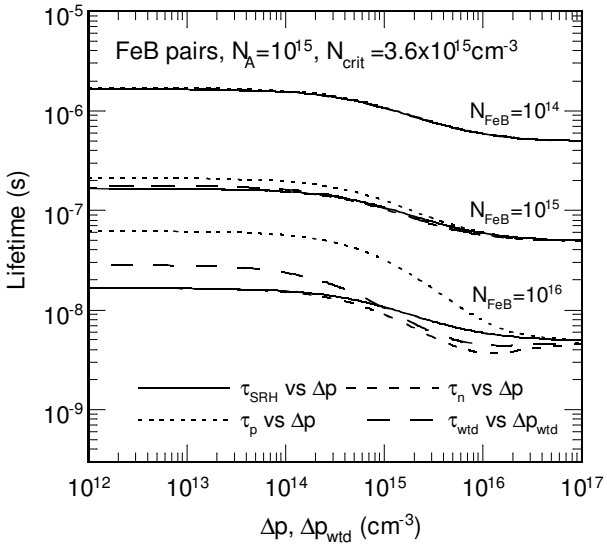

FIG. 2. Comparison between the injection-level dependence of the simplified SRH lifetime and the electron and hole lifetimes as calculated from the general steady-state solution, using the recombination parameters of FeB pairs.

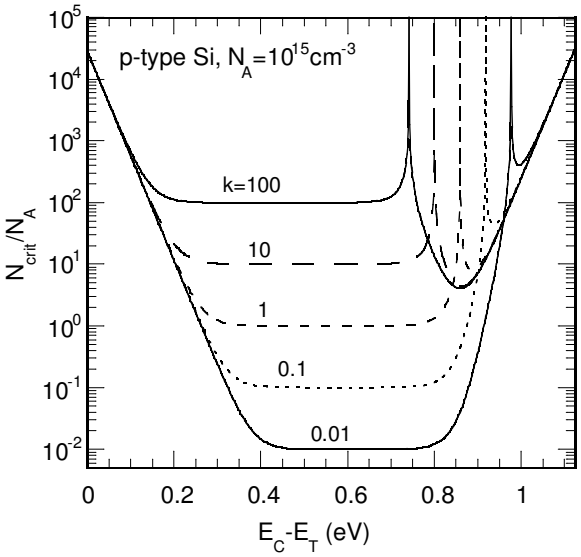

FIG. 3. Values of the low-injection limit of N_{crit}, normalised with respect to N_A=10^{15}cm^{-3}, as a function of the recombination centre energy level E_C-E_T. Curves are shown for different values of the capture cross-section ratio k.

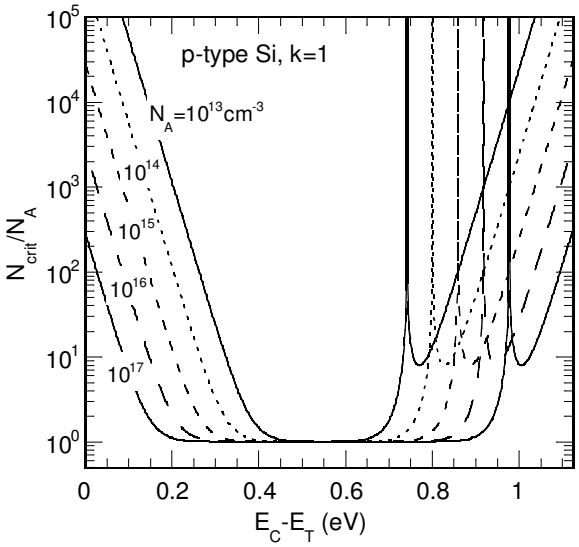

FIG. 4. Values of the low-injection limit of N_{crit}, normalised with respect to N_A, as a function of the recombination centre energy level E_C-E_T. Curves are shown for different values of N_A. The capture cross-section ratio k is unity.

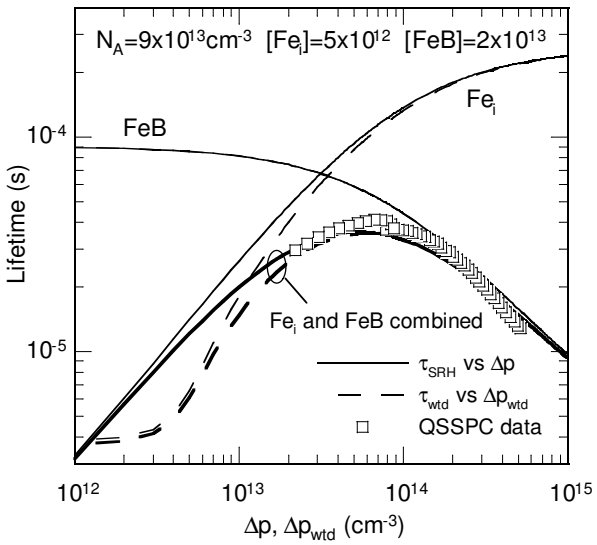

FIG. 5. Comparison between experimental data (from Ref. 6) and modeled lifetime curves for a silicon sample containing interstitial Fe and FeB pairs as the dominant recombination sources.