The Recombination Parameter γ : Modeling and Comments

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Abstract—The recombination parameter γ appears in mathematical expressions for the temperature coefficient of solar cells. This work presents a new analytical expression for this parameter. The expression is derived assuming that all nonradiative recombination occurs in the neutral region of the cell, where carrier diffusion is the dominant transport mechanism. The model shows a direct relation between γ and the temperature sensitivities of the carrier mobility and lifetime. Problems concerning the original definition of γ and its temperature and voltage dependence are discussed and, when possible, amended. A further investigation of the possibility of defect characterization through γ is presented. This yields two analytical expressions that link γ to defect characteristics. A numerical evaluation of the derived expressions is performed for a number of impurities. It is concluded that the recombination parameter γ alone may not be suitable for defect characterization.

Index Terms—Analytical expressions, open-circuit voltage, Shockley-Read-Hall (SRH) recombination, temperature coefficients (TCs), temperature sensitivity.

I. INTRODUCTION

T IS of general knowledge in the solar photovoltaic (PV) community that increasing temperature has a negative effect on the efficiency of solar cells [1], [2]. Solar cells are usually characterized under standard test conditions, which often differ from real operating conditions, and therefore, being able to describe the temperature sensitivity of solar cells is important to accurately predict the energy yield. For this, a single-valued temperature coefficient (TC) is usually employed [1], [3]. The TC of a solar cell parameter shows a general trend of how the respective parameter changes with the temperature. Among the solar cell quantities, the open-circuit voltage $V_{\rm oc}$ is the parameter whose temperature sensitivity has been studied the most [1], [3], [4]. The reason for this is that it has been shown in the scientific literature that the TC of $V_{\rm oc}$ accounts for approximately 80%–90% of the total temperature sensitivity of the cell [1].

Among previous research on the TC of $V_{\rm oc}$, the works in [1] and [4] are the most relevant for the present work. In [1], Green derived an analytical expression for the TC of $V_{\rm oc}$ and

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introduced the recombination parameter γ to account for the implicit temperature sensitivity of the mechanisms determining $V_{\rm oc}$ [5]. Later, in [4], Dupré et al. made use of the *external radiative efficiency* to include nonradiative recombination. This allowed to redefine the expression for the TC of $V_{\rm oc}$ previously derived by Green, yielding an explicit expression for γ . This was significant because it showed a direct connection between the TC of $V_{\rm oc}$ and material properties such as the ERE or the bandgap.

After its explicit derivation in [4], the γ parameter has been studied from an experimental perspective [6], [7], [8]. In the referred works, photoluminescence imaging (PLI) was used to construct spatially resolved images of the γ parameter in wafers and solar cells by applying Green's expression for the TC of $V_{\rm oc}$. Particularly, in [6] and [7], the γ parameter was used in the context of studying dislocation clusters in wafers. Low γ values, and even negative, were reported in areas of dislocation clusters with low $V_{\rm oc}$ temperature sensitivity.

Motivated by Green's [1] and Dupré et al.'s [4] papers, the present work intends to further explore the connection between γ and material parameters such as carrier lifetimes and mobility. The results of this exploration are shown in Section III, where a semiconductor physics approach is taken to relate minority carrier diffusion to γ . This results in an expression that shows an explicit dependence of γ with the temperature sensitivity of the carrier's lifetime and mobility.

The goal of the present work is to theoretically investigate the possibility of using γ to identify impurities in semiconductors dominated by Shockley–Read–Hall (SRH) recombination, such as crystalline silicon [9]. The hypothesis is that if the value of γ is unique and characteristic of an impurity, then it should suffice to measure the local $V_{\rm oc}$ and its TC to identify the aforementioned impurity. However, while studying this possibility, several problems regarding the definition of γ and its dependence on the temperature and $V_{\rm oc}$ itself are found. These problems are presented and discussed in Section IV. In Section V, possible solutions to these problems are suggested. Using these solutions, values of γ are calculated for several impurities, whose experimental data were obtained from the work in [10]. This work concludes that the recombination parameter γ , by itself, is not enough to uniquely identify impurities, but may be useful in laboratory settings in conjunction with other defect-characterization techniques. For the self-consistency of the present article, Section II gives an introduction to the γ parameter and its relation to the TCs. Readers familiar with this may skip this

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II. BACKGROUND

In the radiative limit and assuming nondegenerate conditions, the total current produced by a solar cell is given by Shockley's diode equation [11]

$$J = J_{\rm sc} - J_{\rm rad,0} \left[\exp\left(\frac{qV}{k_{\rm B}T}\right) - 1 \right] \tag{1}$$

where J_{sc} is the *short-circuit* current and $J_{rad,0}$ is the thermal recombination current [12]. The latter is given by

$$J_{\rm rad,0} = q \frac{2\pi}{c^2 h^3} \int_{E_{\rm g}}^{\infty} E^2 \exp\left(\frac{-E}{k_{\rm B}T}\right) dE. \tag{2}$$

In (1) and (2), h, q, c, and $k_{\rm B}$ are Planck's constant, the elementary charge, the speed of light, and Boltzmann's constant, respectively. As $J_{\rm sc}$ is several orders of magnitude larger than $J_{\rm rad,0}$, the approximation $J_{\rm sc}-J_{\rm rad,0}\approx J_{\rm sc}$ holds for solar cells described by (1). Using this approximation, the open-circuit voltage, $V_{\rm oc}$ can be obtained from (1) by setting J=0 [13]

$$V_{\rm oc} = \frac{k_{\rm B}T}{q} \log \left(\frac{J_{\rm sc}}{J_{\rm rad,0}}\right). \tag{3}$$

A. Temperature Coefficient

As mentioned earlier, the TC of a solar cell parameter describes how the parameter changes with the temperature. Letting X be an arbitrary solar cell parameter, the TC of X, denoted here $\beta_X(T)$, is defined as the derivative of X with respect to the cell temperature, i.e., [14]

$$\beta_X(T) = \frac{\mathrm{d}X}{\mathrm{d}T}.\tag{4}$$

In general, $\beta_X(T)$ is going to be a function of the temperature [15]. However, as the temperature dependence of most solar cell parameters is approximately linear for normal operating temperatures [1], the derivative in (4) is approximately constant and, therefore, referred to as the TC.

B. Green's Model for the TC of V_{oc}

The TC of $V_{\rm oc}$, $\beta_{V_{\rm oc}}$, has been studied from an analytical perspective in multiple works. In [16], Green derived the first analytical expression for $\beta_{V_{\rm oc}}$. For this, the author noted that from (3), one can write

$$J_{\rm sc}(T) = AT^{\gamma} \exp\left(\frac{-E_{\rm g0}}{k_{\rm B}T}\right) \exp\left(\frac{qV_{\rm oc}}{k_{\rm B}T}\right)$$
 (5)

where A is a constant, $E_{\rm g0}$ is the bandgap linearly extrapolated to 0 K, and γ is a parameter that includes the temperature dependencies of the remaining parameters determining $J_{\rm rad,0}$. Taking the derivative with respect to the temperature at both sides yields

$$\frac{\mathrm{d}J_{\mathrm{sc}}}{\mathrm{d}T} = \left(A\gamma T^{\gamma-1} + AT^{\gamma} \frac{q}{k_{\mathrm{B}}T} \left[\frac{\mathrm{d}V_{\mathrm{oc}}}{\mathrm{d}T} - \left(\frac{V_{\mathrm{oc}} - E_{\mathrm{g0}}/q}{T} \right) \right] \right) \times \exp\left(\frac{q(V_{\mathrm{oc}} - E_{\mathrm{g0}}/q)}{k_{\mathrm{B}}T} \right).$$
(6)

At this point, Green argued that since J_{sc} is not strongly temperature dependent, the term ${}^{d}J_{sc}/{}_{d}T$ can be neglected in comparison to the remaining terms of the equality. Using then the definition of TC in (4), one can arrive at [16]

$$\beta_{V_{\text{oc}}} = \frac{\mathrm{d}V_{\text{oc}}}{\mathrm{d}T} = -\frac{E_{\text{go}}/q - V_{\text{oc}} + \gamma(k_{\text{B}}T/q)}{T} \tag{7}$$

from which Green concluded an approximately linear decrease in $V_{\rm oc}$ with an increasing temperature.

C. ERE and Dupré's Expression for γ

To account for nonradiative recombination, Green introduced, in [17], the concept of external radiative efficiency (ERE). The ERE is defined as the fraction of the total dark current recombination in the cell that results in radiative emission from the cell [17]. Dupré et al. inserted the ERE into (1) and (3), resulting in [4]

$$J = J_{\rm sc} - \frac{1}{\rm ERE} J_{\rm rad,0} \exp\left(\frac{qV}{k_{\rm B}T}\right) \tag{8}$$

$$V_{\rm oc} = \frac{k_{\rm B}T}{q} \log \left[\text{ERE}_{\rm oc} \frac{J_{\rm sc}}{J_{\rm rad,0}} \right]$$
 (9)

where ERE_{oc} is the ERE evaluated at an open circuit. From (9), $\beta_{V_{\text{oc}}}$ is obtained by taking the derivative of V_{oc} with respect to the temperature. This yields

$$\beta_{V_{\text{oc}}} = \frac{V_{\text{oc}}}{T} + \frac{k_{\text{B}}T}{q} \left(\frac{J_{\text{sc}}'}{J_{\text{sc}}} + \frac{\text{ERE}_{\text{oc}}'}{\text{ERE}_{\text{oc}}} - \frac{J_{\text{rad},0}'}{J_{\text{rad},0}} \right). \tag{10}$$

where the prime denotes the derivative with respect to the temperature. From (2), it can be shown that $J_{\rm rad,0}$ is well approximated by $J_{\rm rad,0} \sim k_{\rm B}TE_{\rm g}^2e^{-\frac{E_{\rm g}}{k_{\rm B}T}}$. The last term in (10) is then given by

$$\frac{J'_{\rm rad,0}}{J_{\rm rad,0}} = \frac{1}{T} + 2\frac{E'_{\rm g}}{E_{\rm g}} - \frac{E_{\rm g0}}{k_{\rm B}T^2}$$
 (11)

where the bandgap, $E_{\rm g}(T)$ has been linearized as $E_{\rm g}(T)=E_{\rm g0}+TE_{\rm g}'$. Substituting into (10) yields

$$\beta_{V_{\text{oc}}} = \frac{V_{\text{oc}}}{T} + \frac{k_{\text{B}}T}{q} \left(-\frac{1}{T} - 2\frac{E'_{\text{g}}}{E_{\text{g}}} + \frac{\text{ERE}'_{\text{oc}}}{\text{ERE}_{\text{oc}}} + \frac{J'_{\text{sc}}}{J_{\text{sc}}} + \frac{E_{g0}}{k_{\text{B}}T^{2}} \right)$$

$$= \frac{V_{\text{oc}}}{T} - \frac{E_{g0}}{qT} - \frac{k_{\text{B}}T}{q} \left(\frac{1}{T} + 2\frac{E'_{\text{g}}}{E_{\text{g}}} - \frac{\text{ERE}'_{\text{oc}}}{\text{ERE}_{\text{oc}}} - \frac{J'_{\text{sc}}}{J_{\text{sc}}} \right)$$

$$= \frac{1}{T} \left[V_{\text{oc}} - \frac{E_{g0}}{q} - \frac{k_{\text{B}}T}{q} \gamma \right]$$
(12)

with

$$\gamma = 1 + 2T \frac{E_{\rm g}'}{E_{\rm g}} - T \frac{\rm ERE_{\rm oc}'}{\rm ERE_{\rm oc}} - T \frac{J_{\rm sc}'}{J_{\rm sc}}.$$
 (13)

In [4], the notation $\frac{d \log X}{d \log T}$ was used instead of $T \frac{X'}{X}$. These are equivalent.

Dupré noted that (12) is the same as (7), and concluded that (13) explicitly described the γ parameter previously introduced by Green in [1]. From (13), it is seen that the recombination parameter γ corresponds explicitly to the temperature sensitivity of the mechanisms determining $V_{\rm oc}$ [4], [5].

D. Explicit Form of the ERE

From its definition given in [17], the ERE can be approximated by the ratio between the current produced by radiative recombination $J_{\rm rad}$ and the total dark current, here denoted $J_{\rm dark}$, i.e.,

$$ERE = \frac{J_{\text{rad}}}{J_{\text{death}}} \tag{14}$$

with J_{rad} being given by the last term on the right-hand side of (1). On the other hand, J_{dark} can be expressed as [13]

$$J_{\text{dark}} = J_{\text{diff}} + J_{\text{scr}} + J_{\text{rad}} \tag{15}$$

where $J_{\rm diff}$ is the current associated with minority carrier diffusion and $J_{\rm scr}$ is the current generated in the space charge region (SCR) of a p-n junction due to generation and recombination of carriers. $J_{\rm rad}$ may be significant in high-quality materials dominated by radiative recombination, such as GaAs. For the intended purposes of this work, nonradiative recombination will be assumed to be dominant, as this is the case for commercial silicon cells. Hence, $J_{\rm rad}$ will be negligible compared to $J_{\rm diff}$ and $J_{\rm scr}$ [13]. In semiconductors with an indirect bandgap, such as crystalline silicon, diffusion lengths are much longer than the width of the SCR. Most recombination, therefore, occurs in the neutral region of the p-n junction, i.e., outside the SCR, where diffusion is the dominant transport mechanism. Hence, $J_{\rm scr}$ can be neglected in comparison with $J_{\rm diff}$. Therefore, for nonideal materials with indirect bandgaps, $J_{\rm dark}$ may be approximated by

$$J_{\rm dark} \approx J_{\rm diff} = J_{\rm diff,0} \exp\left(\frac{qV}{k_{\rm B}T}\right)$$
 (16)

which allows re-expressing (8) and (9) in terms of $J_{\text{diff},0}$.

E. Diffusion Current

 $J_{\rm diff,0}$ results from the recombination of minority carriers in the neutral region [13]. Assuming that surface recombination is negligible, $J_{\rm diff,0}$ is well approximated by [13]

$$J_{\text{diff},0} = q n_i^2 \left(\frac{D_n}{N_n L_n} F_n + \frac{D_p}{N_d L_n} F_p \right) \tag{17}$$

where $N_{\rm a}$ and $N_{\rm d}$ are the densities of acceptors and donors, respectively. $L_j=\sqrt{D_j\tau_j}~(j=n,p)$ are the diffusion lengths, with τ_j being the carrier lifetimes and D_j the diffusion constants of the minority carriers. The latter is related to the mobility of carriers, μ_j , through Einstein's relation [13]

$$\mu_j = \frac{qD_j}{k_{\rm B}T}.\tag{18}$$

In (17), $F_j = \tanh(w/L_j)$ are factors that account for the cell thickness w. These simplify to $F_j = 1$ in the limit where the cell is thick compared to the diffusion lengths. This is the case if, e.g., $w \geq 3L_j$. Finally, n_i is the intrinsic carrier density and is given by

$$n_i^2 = N_{\rm v} N_{\rm c} \exp\left(-\frac{E_{\rm g}}{k_{\rm B} T}\right) \tag{19}$$

with N_x (x = c, v) being the effective conduction (CB) and valence (VB) band density of states and given by

$$N_x = 2\left(\frac{m_x^* k}{2\pi\hbar^2}\right)^{\frac{3}{2}} T^{\frac{3}{2}} \tag{20}$$

where m_x^* denotes the effective mass of the CB (VB) and \hbar is the reduced Planck constant.

III. ANALYTICAL EXPRESSION FOR γ

The explicit form of the ERE given by (14) allows for an explicit expression of the parameter γ . For this, assume a solar cell made of a p-doped wafer. Because the n layer is thin in comparison, most recombination processes will occur in the p region, and therefore, the expression for $J_{\rm diff,0}$ simplifies to

$$J_{\text{diff},0} = q n_i^2 \frac{D_n}{N_a L_n} F_n. \tag{21}$$

Taking now the derivative of $V_{\rm oc}$ with respect to the temperature yields

$$\frac{\mathrm{d}V_{\mathrm{oc}}}{\mathrm{d}T} = \frac{V_{\mathrm{oc}}}{T} + \frac{k_{\mathrm{B}}T}{q} \frac{\mathrm{d}}{\mathrm{d}T} \log \left(\frac{J_{\mathrm{sc}}}{J_{\mathrm{diff},0}}\right). \tag{22}$$

 $J_{\rm sc}$ is dependent on the cell temperature through the bandgap, which is here assumed to vary linearly with the temperature, i.e.,

$$E_{\rm g}(T) \approx E_{\rm gc} + T \frac{\partial E_{\rm g}}{\partial T} \bigg|_{T=T_{\rm o}} + \mathcal{O}(T^2)$$
 (23)

where $E_{\rm gc}=E_{\rm g}(T_c)+E_{\rm g}'(T_c)T_c$ and $T_c=300$ K. For, e.g., crystalline silicon, $E_{\rm gc}=1.206$ eV and $E_{\rm g}'=-2.73\times 10^{-4}$ eV K⁻¹ [1]. Accounting for the temperature dependence of the bandgap, given by (23), and inserting (21) into (22), allows expressing $\beta_{V_{\rm sc}}$ as

$$\beta_{V_{\text{oc}}} = \frac{V_{\text{oc}} - \frac{E_{\text{gc}}}{q} - \frac{k_{\text{B}}T}{q}\gamma}{T}$$
 (24)

with γ now given by

$$\gamma = \frac{7}{2} - x_n \mathrm{csch}(2x_n) - T\frac{J_{\mathrm{sc}}'}{J_{\mathrm{sc}}} + [1 - 2x_n \mathrm{csch}(2x_n)] T\frac{\mu_n'}{2\mu_n}$$

$$-\left[1 + 2x_n \operatorname{csch}(2x_n)\right] T \frac{\tau_n'}{2\tau_n} \tag{25}$$

where $x_n = w/L_n$ and csch is the hyperbolic cosecant function. The csch function has a fast decay rate to zero when its argument increases. Therefore, if the cell is thick compared to the diffusion lengths, (25) simplifies to

$$\gamma = \frac{7}{2} - T \frac{J_{\text{sc}}'}{J_{\text{sc}}} + T \frac{\mu_n'}{2\mu_n} - T \frac{\tau_n'}{2\tau_n}.$$
 (26)

This expression for the γ parameter is equivalent to (13) [4]. The difference here is that the ERE has been explicitly quantified, allowing for a connection between γ and material properties. Finally, note that for an n-doped semiconductor, the expression for γ would take the same form, but the subscript n would change to p.

IV. DISCUSSION

The next step toward finding a link between material impurities and the recombination parameter γ is to assume that the nonradiative recombination in the cell is dominated by SRH recombination [18], [19]. The last term in (26) should then be evaluated at $\tau_n = \tau_{\rm SRH}$. One can then proceed to evaluate the derivative. By doing so, a series of issues, that can be traced back to the definition of γ , appear. In this section, these issues are pointed out and, when possible, amended.

A. Temperature Dependence of γ

It is worth noting that even though (26) describes the same γ parameter as (13), these are not the same γ as the one appearing in (5) and (7). The reason for this lies in the definition of γ that Green gave in [1]. If γ is supposed to include the temperature dependencies of the parameters determining J_0 (or $V_{\rm oc}$ [4]), then, unless these are constants, γ must be a function of the temperature and should, therefore, be included in the derivative in (6). In fact, note that (13) and (26) show both explicit and implicit dependencies with the temperature. The latter is implied in the derivatives. To address this issue, let $\gamma = \gamma(T)$. Taking the logarithm on both sides of (5) gives

$$\log J_{\rm sc} = \log A + \gamma \log T - \frac{E_{\rm g0}}{kT} + \frac{qV_{\rm oc}}{kT}.$$
 (27)

Taking now the derivative with respect to the temperature and neglecting $J'_{\rm sc}$ results in

$$0 = (\log T) \frac{d\gamma}{dT} + \frac{1}{T}\gamma + \frac{E_{g0}}{kT^2} - \frac{qV_{oc}}{kT^2} + \frac{q}{kT} \frac{dV_{oc}}{dT}$$
(28)

which is equivalent to

$$\beta_{V_{\rm oc}} = -\frac{1}{T} \left(\frac{E_{\rm g0}}{q} - V_{\rm oc} + \frac{kT}{q} \left[\gamma + (T \log T) \frac{\mathrm{d}\gamma}{\mathrm{d}T} \right] \right). \tag{29}$$

Note that for constant γ , the last term in (29) is zero and (7) is recovered. Two conclusions can be drawn from the discussion presented in this section. First, Green's γ in (7) only equals Dupre's γ in (13) in the particular case $\gamma =$ constant. Second, and most important, as γ is, in general, temperature dependent, it should not be considered a single-valued parameter.

B. Voltage Dependence of γ

Next, note that already in (9), the term $\text{ERE}_{\text{oc}} = \text{ERE}(V_{\text{oc}})$ is introduced, implying that (9) is an implicit equation in V_{oc} of the form $V_{\text{oc}} = f(V_{\text{oc}})$. Because of this, when deriving an expression for $\beta_{V_{\text{oc}}}$, the derivative with respect to the temperature should be taken implicitly. This yields a general expression of the form

$$\beta_{V_{\text{oc}}} = \frac{\mathrm{d}V_{\text{oc}}}{\mathrm{d}T} = \frac{\mathrm{d}}{\mathrm{d}T} f(V_{\text{oc}}) = \sum_{i=1}^{n} \frac{\partial f}{\partial x_i} \frac{\mathrm{d}x_i}{\mathrm{d}T} + \frac{\partial f}{\partial V_{\text{oc}}} \frac{\mathrm{d}V_{\text{oc}}}{\mathrm{d}T}$$
$$= \sum_{i=1}^{n} \frac{\partial f}{\partial x_i} \frac{\mathrm{d}x_i}{\mathrm{d}T} + \frac{\partial f}{\partial V_{\text{oc}}} \beta_{V_{\text{oc}}}$$
(30)

where x_i are the remaining physical quantities in (3). The general form in (30) can be identified in (12). As $ERE_{oc} = ERE(V_{oc})$, the term in (13) involving the derivative of ERE_{oc} with respect to

the temperatures depends on both $V_{\rm oc}$ and $\beta_{V_{\rm oc}}$. Therefore, (12) is an implicit equation in $\beta_{V_{\rm oc}}$, and γ is a function of both $V_{\rm oc}$ and $\beta_{V_{\rm oc}}$.

In the case of the expression derived for γ in this work, since the ERE is voltage dependent, so is $J_{\rm diff,0}$. This can be easily shown with the example of a semiconductor dominated by SRH recombination. For a p-doped semiconductor, the carrier lifetime τ_n is given by

$$\tau_{\rm SRH} = \tau_{\rm n0} \left[1 + \frac{p_{\rm t}}{N_{\rm a} + \Delta n} \right] + \tau_{\rm p0} \left[\frac{n_{\rm t} + \Delta n}{N_{\rm a} + \Delta n} \right] \tag{31}$$

where τ_{j0} (j = n, p) are the capture time parameters of electrons and holes, and with $n_{\rm t}$ and $p_{\rm t}$ being the electron and hole densities when their quasi-Fermi level matches the trap energy level $E_{\rm t}$. These are given by

$$p_{\rm t} = N_{\rm v} \exp\left[\frac{-E_{\rm t}}{kT}\right] \tag{32}$$

$$n_{\rm t} = N_{\rm c} \exp\left[\frac{E_{\rm t} - E_{\rm g}}{kT}\right]. \tag{33}$$

Equation (31) also contains the excess carrier density, Δn . For a p-doped semiconductor, Δn follows from

$$np - n_i^2 \approx N_a \Delta n + \Delta n^2 = n_i^2 \left[\exp\left(\frac{V}{V_t}\right) - 1 \right].$$
 (34)

Note from (34), that Δn is a function of the voltage $\Delta n(V)$. This explicitly demonstrates the dependence of $J_{\rm diff,0}$ with the voltage.

One important point to note when deriving an expression for $\beta_{V_{oc}}$ is that Δn cannot be chosen independently but must follow from (34) evaluated at an open circuit, i.e., at $V = V_{\rm oc}$. Therefore, one should technically write $J_{\text{diff},0;\text{oc}}$ instead of $J_{\rm diff,0}$ at an open circuit. This is the same problem as with $ERE_{oc} = ERE(V_{oc})$, but it is now explicit: The dependence of the ERE with the voltage comes from the dependence of $J_{\rm diff,0}$ with injection-dependent lifetimes. In (25), γ will be dependent on $\Delta n(V_{\rm oc}) = \Delta n_{\rm oc}$ and its derivative with respect to the temperature. Explicitly, the dependence of τ_n with $V_{\rm oc}$ can be seen by evaluating the derivative in the last term in (26). When taking the derivative of the lifetime with respect to the temperature, a term dependent on $\beta_{V_{\rm oc}}$ will also appear. To see this let $\tau_n = \tau_n(x_1(T), x_2(T), \dots, x_n(T), \Delta n_{\text{oc}}(T); T)$, where the x_i correspond to capture cross-sections, thermal velocities, etc. The last term in (26) becomes

$$\frac{\tau_n'}{\tau_n} = \sum_{i=1}^n \frac{\partial \log \tau_n}{\partial x_i} \frac{\mathrm{d}x_i}{\mathrm{d}T} + \frac{\partial \log \tau_n}{\partial T} + \frac{\partial \log \tau_n}{\partial \Delta n_{\rm oc}} \frac{\mathrm{d}\Delta n_{\rm oc}}{\mathrm{d}T}$$
(35)

with

$$\frac{\mathrm{d}\Delta n_{\mathrm{oc}}}{\mathrm{d}T} = \frac{\partial \Delta n_{\mathrm{oc}}}{\partial V_{\mathrm{oc}}} \frac{\mathrm{d}V_{\mathrm{oc}}}{\mathrm{d}T} + \frac{\partial \Delta n_{\mathrm{oc}}}{\partial T} = \frac{\partial \Delta n_{\mathrm{oc}}}{\partial V_{\mathrm{oc}}} \beta_{V_{\mathrm{oc}}} + \frac{\partial \Delta n_{\mathrm{oc}}}{\partial T}$$
(36)

from where it is clear that γ is, in general, dependent on both $V_{\rm oc}$ and $\beta_{V_{\rm oc}}$.

V. Isolating the Voltage Dependence of γ

As γ is dependent on both the cell temperature and $V_{\rm oc}$, it is clearly not, in general, a single-valued parameter for a particular impurity. Although one could, e.g., tabulate values of γ at T=300 K, the voltage dependence of γ complicates relating γ to specific impurities as two cells contaminated with the same impurity will have different values of γ if they have different values of $V_{\rm oc}$. A possible solution to amend this problem is to isolate the dependence of γ with $V_{\rm oc}$ and $\beta_{V_{\rm oc}}$, i.e., writing γ as $\gamma=f(V_{\rm oc},\beta_{V_{\rm oc}};T)+\Gamma(\mathbf{x}(T),\mathbf{x}'(T);T)$, where $\mathbf{x}(T):=\{x_1(T),\ldots,x_n(T)\}$. As all $V_{\rm oc}$ -dependence has been isolated in f, Γ is only dependent of the physical mechanisms (and their temperature derivatives) intrinsic to the impurity.

Looking at (25) and (26), obtaining $\Gamma(\mathbf{x}(T),\mathbf{x}'(T);T)$ may only be possible in the limit where the cell is sufficiently thick, compared to the diffusion lengths, as otherwise the terms involving $\mathrm{csch}(w/L_n)$, which are dependent on Δn_{oc} , will make it impossible to isolate the dependencies on V_{oc} and $\beta_{V_{\mathrm{oc}}}$. In (26), only the term involving the derivative of the lifetime with respect to the temperature is dependent on Δn_{oc} . Then, if one can write $\tau'_n/\tau_n = h(V_{\mathrm{oc}},\beta_{V_{\mathrm{oc}}};T) + g(\mathbf{x}(T),\mathbf{x}'(T);T)$, a voltage-independent Γ can be obtained. An example of this is $h(V_{\mathrm{oc}},\beta_{V_{\mathrm{oc}}};T) = \beta_{V_{\mathrm{oc}}}/V_{\mathrm{oc}} = \beta_{V_{\mathrm{oc}}}^T$, which yields expressions for $\beta_{V_{\mathrm{oc}}}$ and γ similar to (24) and (26). With a bit of manipulation, one can write

$$\beta_{V_{\text{oc}}} \left(1 - \frac{1}{2v_{\text{oc}}} \right) = \frac{V_{\text{oc}} - \frac{E_{\text{gc}}}{q} - \frac{k_{\text{B}}T}{q}\Gamma}{T}$$
(37)

where $v_{\rm oc} = qV_{\rm oc}/k_{\rm B}T$ and

$$\Gamma = \frac{7}{2} - T \frac{J'_{sc}}{J_{sc}} + T \frac{\mu'_n}{2\mu_n} - \frac{1}{2} T g(\mathbf{x}(T), \mathbf{x}'(T); T).$$
 (38)

If the cell in a study is dominated by SRH recombination, $g(\mathbf{x}(T), \mathbf{x}'(T); T)$ will contain the physical mechanisms intrinsic to the impurity and one may say that the Γ presented in (38) is characteristic to the impurity. However, this very particular case, in general, will not hold. This is because isolating the V_{oc} -dependence already constitutes a transcendental equation and only a few of these equations have closed-form solutions. Among the few possible analytical solutions, it is worth mentioning $\tau_n = \tau_n(\mathbf{x}(T), \mathbf{x}'(T); T)$, i.e., carrier lifetimes that are not voltage dependent. This possible solution will be further explored in the following section.

A. Low Injection

The goal of this section is to show that under low-level injection (LLI) conditions, it is possible to obtain analytical expressions for γ that are not voltage-dependent. For this, assume first a sufficiently thick solar cell, so that γ is given by (26). Assume also that the cell is dominated by SRH recombination. The lifetime τ_n then follows $\tau_n = \tau_{\text{SRH}}$, where τ_{SRH} is given by (31) with

$$\tau_{j0} = \frac{1}{N_t v_i \sigma_i} \tag{39}$$

where N_t is the density of traps, v_j is the thermal velocity of the charged carrier, and σ_j is the capture cross-section of the minority carriers. Both v_j and σ_j are temperature dependent. The former follows from $\frac{1}{2}m_x^*v_j^2=\frac{3}{2}k_{\rm B}T$. The temperature dependencies of σ_j are characteristic of the capture mechanism and can be found in the literature (see, e.g., [20]). From (31), (32), and (33), one can see that the value of $\tau_{\rm SRH}$ depends essentially on the trap energy level E_t , the excess carrier density Δn , and the capture cross-sections. The latter can be accounted for through the symmetry factor k defined by $k(T)=\tau_{\rm p0}/\tau_{\rm n0}\approx\sigma_n/\sigma_p$ [20]. The value of k, which, in general, is a function of the temperature, is characteristic of the impurity in question.

Under LLI conditions, i.e., $\Delta n \ll N_{\rm a}$, (31) simplifies to

$$\tau_{\text{SRH}}^{\text{LLI}} = \tau_{\text{n0}} \left[1 + \frac{p_{\text{t}}}{N_{\text{a}}} + k(T) \frac{n_{\text{t}}}{N_{\text{a}}} \right].$$
(40)

Given an impurity, i.e., at fixed k(T), the position of the trap within the bandgap will determine whether further simplification is allowed. Assume now, a defect positioned in the *transition region* of the bandgap, i.e., in between what would be considered $deep (E_t \to E_g/2)$ and $shallow (E_t \to E_{c,v})$ [20]. Dividing the bandgap in two halves, (31) simplifies to

$$\tau_{\text{SRH}}^{\text{LLI}} = \begin{cases} \left(1 + \frac{p_t}{N_{\text{a}}}\right) \tau_{n0} & \text{lower band gap half (L)} \\ \\ \left(1 + k \frac{n_t}{N_{\text{a}}}\right) \tau_{n0} & \text{upper band gap half (U)} \end{cases}$$
 (41)

Equation (41) is of interest because it automatically accounts for all the possible cases where further simplification can occur (see [20, Tab. 3.1]): For a deep defect, $p_t, n_t \ll N_{\rm a}$ and therefore, (31) simplifies to $\tau_{\rm SRH} = \tau_{n0}$. On the other hand, for a shallow defect close to, e.g., the VB edge, $p_t \gg N_{\rm a}$ and (31) simplifies to $\tau_{\rm SRH} = \tau_{n0}(p_t/N_{\rm a})$. An analog discussion holds for a defect close to the CB edge.

To shorten the notation, let $\hat{n}_t = n_t/N_a$ and $\hat{p}_t = p_t/N_a$. Inserting (41) into (26) yields

$$\gamma_{\rm L} = \frac{15}{4} - \frac{1}{2} \frac{\hat{p}_t}{1 + \hat{p}_t} \left(\frac{3}{2} + \frac{E_t}{k_{\rm B}T} \right) - T \frac{J'_{\rm sc}}{J_{\rm sc}} + T \frac{\mu'_n}{2\mu_n} + T \frac{\sigma'_n}{2\sigma_n}$$
(42)

$$\gamma_{\rm U} = \frac{15}{4} - \frac{1}{2} \frac{k \hat{n}_t}{1 + k \hat{n}_t} \left(\frac{3}{2} + T \frac{k'}{k} + \frac{E_{\rm gc} - E_t}{k_{\rm B} T} \right) - T \frac{J_{\rm sc}'}{J_{\rm sc}} + T \frac{\mu'_n}{2\mu_n} + T \frac{\sigma'_n}{2\sigma_n}$$
(43)

where U and L denote the upper and lower bandgap halves, respectively. Note that γ_L and γ_U are not voltage dependent and are fully determined by the characteristics of the defect.

VI. NUMERICAL RESULTS

This section presents a numerical evaluation of the expressions for γ derived in this work. The simulations are performed for silicon (Si) cells, with $E_{\rm g}=1.125$ eV at T=300 K. The bandgap is assumed to be linearly dependent on the cells' temperature. The temperature dependence of the carrier mobilities

Defect	E _t (eV)	$\sigma_n(T) \text{ (cm}^2)$			$\sigma_p(T) \ ({\rm cm}^2)$			
		$\sigma_0 (\mathrm{cm}^2)$	α	E_a (eV)	$\sigma_0 (\mathrm{cm}^2)$	α	E_a (eV)	I I
Tii	0.86	2.57×10^{-14}	-	0.0039	1.35×10^{-15}	-	-	1.82
Ti _i	0.26	3.90×10^{-12}	1.00	-	1.09×10^{-16}	-	0.0027	2.51
CrB	0.20	2.00×10^{-12}	1.20	-	4.30×10^{-12}	1.20	-	1.81
Fe _i	0.34	3.47×10^{-11}	1.48	-	4.54×10^{-16}	-	0.05	2.37
FeB	0.87	5.10×10^{-09}	2.50	-	3.32×10^{-11}	-	0.262	1.86
$ $ Zn_s	0.29	9.90×10^{-16}	-	-	2.00×10^{-14}	-	-	3.08
Zn _s	0.62	3.70×10^{-10}	-	0.136	1.80×10^{-05}	3.93	-	5.76
Mo _i	0.33	4.20×10^{-08}	2.95	-	6.05×10^{-14}	1.07	-	1.63
W	0.32	1.20×10^{-15}	-	0.017	1.20×10^{-16}	-	0.018	3.43
Au _s	0.31	2.90×10^{-11}	2	-	3.50×10^{-15}	-	-	2.09
Au _s	0.56	8.50×10^{-17}	-	-	1.50×10^{-11}	1.30	-	3.11

 $TABLE\ I$ Temperature Dependence of the Capture Cross-Sections of Different Impurities [10]

The temperature dependencies of the capture mechanisms for the displayed impurities have one of the following forms: (1) $\sigma_j(T) = \sigma_0 = \text{constant}$, (2) $\sigma_j = \sigma_0 \left({^{T_0}/T} \right)^{\alpha} \text{or } \sigma_j = \sigma_0 \exp\left[{^{-E_a}/k_{\rm B}T} \right]$ [10], [20]. The furthest right column displays the corresponding values calculated with (26), i.e., for short diffusion lengths, at LLI conditions and T = 298 k.

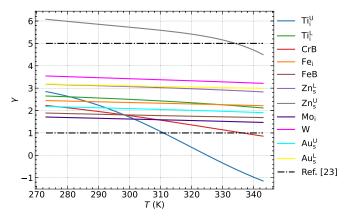


Fig. 1. Values of γ as a function of the temperature for the impurities displayed in Table I calculated at LLI conditions with (26). The superscripts U and L, used in the Ti₁, Zn_s, and Au_s defects, signify their position, upper and lower half, within the Si bandgap (see Table I). Values of γ previously mentioned in [23] are displayed with dotted lines.

is calculated through Klaassen's model [21], [22]. The studied defects and the temperature dependence of their capture cross-sections are obtained from [10]; a review paper that compiles experimental data of defect recombination processes in silicon from multiple articles of the scientific literature. A summary of these is displayed in Table I. Here, the subscripts i and s indicate *interstitial* and *substitutional* impurities, respectively. The density of traps is assumed to be a constant with respect to the temperature and has been set to $N_t = 3 \times 10^{12} \ \rm cm^{-3}$. Finally, the doping density has been set to $N_a = 5 \times 10^{16} \ \rm cm^{-3}$.

Fig. 1 shows γ as a function of the temperature for the impurities displayed in Table I. In Fig. 1, the curves were obtained using (26) evaluated at $\tau_n = \tau_{\rm SRH}^{\rm LLI}$, with $\tau_{\rm SRH}^{\rm LLI}$ given by (40). Using (24) yields the same values. In the furthest right column of Table I, the numerically calculated γ values of the studied defects at T=298 K are displayed. These were also obtained with (26). From the plot and table, it is worth noting that the γ values span the interval [1,6] at T=298 K. This is in agreement with the values of γ previously mentioned in the

literature, which are displayed in Fig. 1 with dotted lines [4], [16], [23]. From Fig. 1, it is worth noting that γ decreases with increasing temperature, although some of the studied defects show a nearly constant behavior. The latter can be seen in the curves of FeB and Mo_i in Fig. 1.

A. Long Diffusion Lengths

The numerical results presented earlier were obtained by means of (26). This expression for γ was obtained from its general form in (25) by assuming a thick cell compared to the diffusion lengths. Although this assumption may be true for highly contaminated cells, in commercial and industrial Si cells, diffusion lengths should be much higher than the cell thickness to ensure high quality. This can be deduced from (17): Higher diffusion lengths result in a smaller recombination term and, therefore, higher efficiency.

The reasoning behind assuming short diffusion lengths compared to the cell thickness was to isolate the voltage dependence of γ , so that it would be possible to obtain analytical expressions, such as (42) and (43) in the case of LLI. However, the numerical experiments show that evaluating (26) at $\tau_n = \tau_{\rm SRH}^{\rm LLI}$ is the safest way to compute γ values as approximating (40) by (41) may not always hold. The general form of γ , which does not make any assumptions on the diffusion lengths, can also be evaluated at LLI. Indeed, at LLI, the diffusion lengths in the argument of the csch functions are not voltage dependent. While it may not be possible to derive analogs to (42) and (43) using this method, evaluating (25) under LLI conditions yields a γ value that depends exclusively on the defect's properties and the width of the cell.

To see the effect of accounting for the cell thickness, Fig. 2 shows γ , given by (25) at LLI and T=298 K, as a function of the normalized parameter $x_n=w/L_n$. From this figure, it is worth noting that assuming short diffusion lengths may have a big impact on the value of γ . Take, e.g., $\mathrm{Zn_s}~(E_{\mathrm{t}}=0.62~\mathrm{eV})$. For this defect, the magnitude of γ increases with increasing diffusion length. In the limit where $w\gg L_n$, $\mathrm{Zn_s}~(E_{\mathrm{t}}=0.62~\mathrm{eV})$

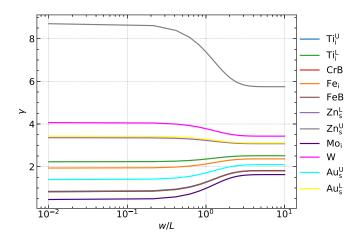


Fig. 2. Values of γ as a function of the normalized cell thickness, $x_n = w/L_n$, for the impurities displayed in Table I calculated at LLI conditions and T = 298 K with (25).

has a γ value of 5.76 at T=298 K (see Table I). When the diffusion length is higher, say $x_n\approx 0.01$, the γ value of Zn_s ($E_t=0.62\,{\rm eV}$) increases to 8.73. Another 3 of the 11 studied defects also show an increasing dependence of γ with the diffusion length while the remaining 7 show the opposite behavior. Fig. 2 suggests a symmetry axis around $\gamma\approx 3$ where the dependence of γ with the cell thickness is inverted, i.e., where the derivative of γ with respect to x_n changes sign.

B. Applicability of γ

The numerical results presented earlier show that the γ values for two different impurities may be quite similar. Examples of this are the γ values for $\rm Zn_s$ with $E_{\rm t}=0.29$ eV and $\rm Au_s$ with $E_{\rm t}=0.59$ eV. Although these are different defects, at different trap levels and with different capture cross-section mechanisms, their γ values differ by less than 1%. Furthermore, from Fig. 2, note that it is virtually impossible to distinguish between the curves of Ti ($E_{\rm t}=0.86$ eV), CrB, and FeB. Moreover, from Fig. 1 and focusing on Ti ($E_{\rm t}=0.86$ eV), it is worth noting that this impurity could be identified as six different defects, depending on the temperature at which the measurements were taken. This example shows that the hypothesis of a γ being unique to a defect is, in general, not true.

It is clear that a single value of γ , by itself, is not enough to uniquely identify impurities. Still, this does not mean that γ cannot be used to reduce the number of possible candidates. Take, e.g., the γ maps obtained in [6] and [7]. There, the highest reported value of γ was $\gamma=4$. Then, based on the γ values displayed in Table I, it is unlikely that the studied cells/wafers were contaminated with $\mathrm{Zn_s}$ ($E_{\mathrm{t}}=0.62~\mathrm{eV}$), given that the γ value of a silicon cell contaminated with this defect is closer to 6 at 298 K in the short diffusion length limit.

An important note to this discussion is areas within wafers containing multiple impurities or impurity mixes. These are not unusual in real wafers and cells. A γ value cannot account for these, at least in the way, it has been studied so far in the literature

and the present work. In this context, γ may be used to see how impurities distribute within the wafer. Say that one wanted to know how Zn_s impurities distribute within a silicon wafer. Then one could, e.g., contaminate a wafer with Zn_s and obtain a γ map through PLI. Areas with high γ values (around 6 if the cell is highly contaminated, following Table I and Fig. 2) should be indicative of how the recombination centers distribute. The same argument applies to wafers contaminated with several impurities. For example, suppose that one knew, through other characterization techniques, that a silicon wafer is contaminated with Mo_i and W. Areas with low and high γ values, respectively, in a γ map would be indicative of how these two impurities distribute within the wafer. This shows the potential of γ in combination with other characterization techniques for defect identification.

Finally, it is worth mentioning that obtaining γ maps at multiple temperatures may be useful to characterize defects as the temperature dependence of γ may give extra information regarding the impurity in question.

VII. CONCLUSION

In this work, analytical expressions for the recombination parameter γ have been derived. This was possible by using the formal definition of the ERE and assuming that, for commercial cells, radiative recombination can be neglected, and nonradiative recombination occurs mainly within the neutral zone of the junction. This allowed relating γ to minority carrier diffusion and resulted in an expression that shows its dependence on the temperature sensitivities of the mobility and lifetime.

In the further theoretical exploration of the usability of γ for defect characterization, a series of problems involving its definition and temperature and voltage dependence were identified. Under LLI conditions, analytical expressions for γ were derived. These expressions for γ were fully determined by defect characteristics, which opened the possibility of impurity identification. From numerical examples, however, it was concluded that γ alone is not sufficient to uniquely identify impurities, as two different impurities may have quite similar γ values. Still, it was discussed that γ may be useful in conjunction with other characterization techniques to study defects in silicon wafers. Particularly, it was suggested the applicability of γ maps in studying how impurities distribute within wafers.

As a final note, with respect to further developments, the present work has suggested applications of γ under LLI conditions. The voltage and temperature dependence of γ were regarded as problems in the context of defect identification. However, if this was not the goal, obtaining information on these dependencies of γ for a given impurity may be beneficial for further characterization of the wafer in the study. This could be done by, e.g, obtaining γ maps at multiple temperatures and light conditions. It is important to note that under these circumstances, Auger recombination may become relevant and should, therefore, be included in the modeling of γ . These possibilities should be further studied both theoretically and experimentally.

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