Theory of space-charge layer dynamics at oxide-semiconductor interfaces under optical modulation and detection by laser photocarrier radiometry

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The dynamic theory of the optically modulated space-charge layer (SCL) resulting from band bending at a Si–SiO_2 interface was developed in terms of the density of interface charges occupying band-gap energy states. Expressions were derived for these interface charge densities, interacting with the free-carrier density wave generated in the SCL and in the quasineutral region (bulk) by an intensity-modulated super-band-gap laser. The residual and modulated interface charge coverage affects the band-edge-to-impurity state recombination and the concomitant near-infrared photon emission comprising the photocarrier radiometry (PCR) signal. The PCR theory incorporating these effects was further developed. It was found to involve the dc, fundamental, and entire harmonic spectrum of the excitation frequency as a result of the optical modulation of the curvature of the energy bands and the SCL width at the interface. © *2005 American Institute of Physics*. [DOI: 10.1063/1.1850198]

I. INTRODUCTION

The technique of laser infrared photocarrier radiometry (PCR) was recently introduced as a sensitive method for electronic material transport property measurements under modulated laser light,[1,2] although it can also be used in a pulsed mode. The PCR signal consists of harmonically modulated near-infrared emissions within the spectral bandwidth of the InGaAs detector with a preamplifier and matched optical filters (0.8–1.7 μm). In Si, PCR is believed to be associated with room- or higher-temperature infrared photoluminescence, a phenomenon partly due to the indirect band-to-band transition, which in the past has invariably been associated with the presence of defects.[3] As a first step to the study of interface electronic effects affecting the PCR signal, a theory is developed for the optical modulation and relaxation of band bending toward photosaturation (flatband condition) at the Si–SiO_2 interface. The harmonic modulation of band bending through optical interactions with charged surface states in oxidized Si wafers is considered and the PCR signal from the width-modulated space-charge layer (SCL) and the quasineutral region beyond is derived. Expressions are thus developed for these interface charge densities, interacting with the free-carrier density wave generated in the SCL and in the quasineutral region (bulk) by an intensity-modulated super-band-gap photon source. The small radiative component of the recombination of free minority carriers in impurity states is assumed to be in the form of room-temperature photoluminescence measurable by PCR as near-infrared photon emission following the recombination event.

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II. THEORY OF OPTICALLY MODULATED *p*-SI–SIO_2 INTERFACE ENERGETICS IN THE PRESENCE OF CHARGED INTERFACE STATES

A. Interface energy-band configuration

To fix definitions and ideas, the following description of interface energetics focuses on a *p*-type semiconductor. *n*-type materials can be treated in an exactly analogous manner. In Fig. 1 we consider the SiO_2–Si interface energy diagram of *p*-type Si in the presence of the positively charged interface state density N_t (cm^{-2}) acting as traps of free minority carriers (electrons). At equilibrium in the dark,[4] the energy bands at the interface are bent with a total interface potential energy $q\psi_{s0}$, measured with respect to the intrinsic Fermi level. The interface depicted in Fig. 1 can either be in depletion or in inversion. At equilibrium the SCL width, W_0, serves as the reference value for the nonequilibrium configuration under optical incidence of intensity

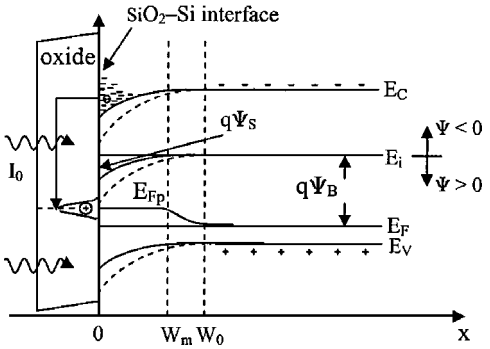

FIG. 1. Band-structure energetics at a *p*-type Si–SiO interface with a positively charged interface state (trap) density N_t assumed to be at energy E_t. The band bending is modulated by the external optical field. The various quantities have been defined in the text.

$I_0(\alpha, h\nu)$ $(\mathrm{W\,cm^{-2}})$, where α is the optical-absorption coefficient at the super-band-gap photon energy $h\nu$. The Fermi level is E_F in the bulk, but it splits up into E_{Fp} and $E_{Fn}(x)$ within the SCL, due to the presence of the interface state density N_t distributed over a narrow energy range centered at $E=E_t$. If many such interface state distributions are present, as in the case of several contaminants or mobile ions in the oxide, then the mean state density can be defined as a sum over the distribution of discrete state densities, or as an integral over a continuous distribution $N_{ti}(E_{ti})dE_{ti}$ across the band-gap range, $E_C \geqslant E_{ti} \geqslant E_V$, in the manner described by Kronik and Shapira.[5] Aberle *et al.*[6] have devised a computational method to deal with such distributions and their effects on Shockley–Read–Hall recombination at the SiO_2–Si interface. The single-state simplification in this work is not a serious limitation, as it leads to an effective density of states associated with an effective SCL width, which is all one can measure using nonspectrally resolved techniques. Details about the equilibrium configuration in an *n*-type semiconductor can be found in Ref. 4. The important results for *p*-type interfaces can be briefly summarized as follows, as they form the reference state for the theoretical development of the free-carrier-density-wave (CDW) dynamics under external optical modulation.

Charge neutrality across the two sides of the interface at $x=0$ requires that the accumulated free-electron charge density in the SCL must balance in detail the positive exterior charge density which causes the potential shift from the maximum ψ_{s0} to ψ_s,

$$Q_{si} = -Q_{sc} = \frac{\sqrt{2}\varepsilon_s k_B T}{qL_D} F\left(\frac{q\psi_s}{k_B T}\right), \tag{1}$$

where k_B, T, ε_s are Boltzmann's constant, the absolute temperature, and the dielectric constant of the semiconductor, respectively; L_D is the extrinsic Debye length for electrons,

$$L_D = \frac{1}{q}(k_B \varepsilon_s T / p_{p0})^{1/2} \tag{2}$$

and F is the normalized interface electric field defined as[7]

$$F(u) \equiv [(e^{-u} + u - 1) + (n_{p0}/p_{p0})(e^{u} - u - 1)]^{1/2}. \tag{3}$$

Here, p_{p0} and n_{p0} are the majority (holes) and minority (electrons) free-carrier densities, respectively, and $u = q\psi_s / k_B T$. In a *p*-type semiconductor under low-to-moderate injection conditions we have $(n_{p0}/p_{p0}) \ll 1$, which leads to a simplified relationship between the interface-state charge density and the potential,

$$Q_{si}(\psi_s) \cong \sqrt{2 p_{p0} \varepsilon_s k_B T}\left[\exp\left(-\frac{q\psi_s}{k_B T}\right) + \left(\frac{q\psi_s}{k_B T}\right) - 1\right]^{1/2}. \tag{4}$$

Within the $(n_{p0}/p_{p0}) \ll 1$ approximation, the SCL width can be found from the capacitance of the layer

$$W(u) = \varepsilon_s / C_d(\psi_s) = \varepsilon_s / (\partial |Q_{sc}| / \partial \psi_s) \cong \sqrt{2} L_D \left(\frac{\sqrt{e^{-u} + u - 1}}{1 - e^{-u}}\right). \tag{5}$$

In Eq. (4), the potential ψ_s has been associated with the surface/interface barrier height and can be measured by the surface photovoltage technique.[8] Equation (5) can be evaluated under depletion conditions for $u < 1$, such that $\psi_B > \psi_s > 0$,

$$W(\psi_s) = (2\varepsilon_s \psi_s / q p_{p0})^{1/2}. \tag{6}$$

This is the same as the well-known depletion-layer expression under the one-sided abrupt junction approximation (Ref. 4, Chap. 2.3.1). For $\psi_s \gg \psi_B$ (inversion conditions, Fig. 1), the increasing exponential term in Eq. (3), when inserted in Eq. (5), eventually dominates the behavior, despite the smallness of (n_{p0}/p_{p0}), so that

$$W(\psi_s) = \frac{1}{q}\left(\frac{k_B \varepsilon_s T}{n_{p0}}\right)^{1/2} \exp\left(-\frac{q\psi_s}{2k_B T}\right). \tag{7}$$

This limit represents the inversion-layer portion of the SCL, i.e, when $E_{Fn}(x)$ crosses over the $q\psi(x)$ curve in Fig. 1 and the thickness of the layer decreases rapidly. Therefore, it is possible that optical modulation of the SCL width may pass through a series of configurations from inversion through depletion to flatbands, and possibly into accumulation, depending on the magnitude of the interface charge density (coverage). Within the depletion approximation, Eq. (6), the SCL width must take the thermal correction into account[9]

$$W(\psi_s) = \left(\frac{2\varepsilon_s}{q p_{p0}}[\psi_{s0} - \Delta\psi(I_0, h\nu) - (k_B T/q)]\right)^{1/2}, \tag{8}$$

where $\Delta\psi(I_0, h\nu)$ is the interface potential change in the presence of external optical photocarrier generation which perturbs the interface state charge density. Under room-temperature conditions in Si, $p_{p0} \approx N_A$, the total acceptor density $(\mathrm{cm^{-3}})$, since all hole impurity states would be essentially ionized. At flatbands, $\Delta\psi(I_0, h\nu) \sim \psi_{s0}$, and the SCL vanishes.

B. Interface-state occupation dynamics under modulated optical excitation

Let us assume the single interface energy trap state E_t, with N_t the number density of positive electron traps. The fraction N_{t0} of N_t is occupied through recombination into the traps of free thermal or photoexcited electrons within or beyond the SCL. Those occupied states become electrically neutralized and induce a change in the width of the SCL. The fraction $N_t - N_{t0}$ of states remains unoccupied, and therefore charged through thermal emission into the conduction band or through direct optical extraction of electrons by the incident photons. It must be mentioned that although super-band-gap photons are assumed throughout, the optical emission mechanism can also work with sub-band-gap energy photons, as long as $h\nu \geqslant E_C - E_t$. The rate equation of capture and release of minority (electron) carriers at the interface state under depletion/inversion conditions is

$$\frac{\partial N_{t0}}{\partial t} = [n_{p0} + \Delta n_p(0,t)]C_t(N_t - N_{t0}) - R_T N_{t0} - P_\alpha I_0(h\nu)N_{t0}, \tag{9}$$

where C_t is the probability for free-electron trapping at an interface state ($\mathrm{cm}^3\,\mathrm{s}^{-1}$). P_α ($\mathrm{cm}^2\,J^{-1}$) is the probability for incident photon absorption at an interface site (surface absorption), leading to ejection of a trapped minority carrier. P_α is usually small and delays the establishment of nonequilibrium steady state upon illumination of the surface.[8,10] R_T (s^{-1}) is the rate for thermal emission of electrons from the trap state into the conduction band,

$$R_T(T) = N_C C_t \exp[-(E_C - q\psi_s - E_t)/k_B T] \tag{10}$$

and $N_C = 2(2\pi m_e^* k_B T/h^2)^{3/2}$ is the effective minority-carrier state density in the conduction band of the semiconductor. $\Delta n_p(0,t)$ is the free photoexcited minority-carrier density at the edge of the conduction band. The foregoing picture of minority-carrier trapping at interface states depends on the ratio of electron and hole capture cross sections. At the Si–SiO_2 interface, Aberle *et al.*[6] have shown that this ratio is, indeed, on the order of 100; therefore, efficient capture of electrons by interface states is expected upon illumination of a *p*-type Si crystal, with not-so-efficient trapping of an *n*-type material. Insofar as the trapping efficiency affects the degree of band bending by means of optical biasing, these expectations were borne out experimentally,[11] achieving complete flatband conditions at *p*-type Si–SiO_2 interfaces and only partial removal of band bending at *n*-type Si–SiO_2 interfaces. At equilibrium in the dark, $\partial N_{t0}/\partial t = 0$ and $I_0 = 0$. Therefore, the charge density on the oxide side of the interface (mobile charges in the SiO_2 are neglected) is

$$Q_{si} = q[N_t - N_{t0}^{(e)}] = \frac{qR_T N_t}{C_t n_{p0}^{(e)} + R_T} \quad (\mathrm{C\,cm}^{-2}). \tag{11}$$

It is clear that the degree of band bending in the dark depends on the number density of thermally or otherwise ionized free minority carriers. In the extreme case, where $n_{p0}^{(e)} = 0$, then $Q_{si} = qN_t$, i.e. all interface states are unoccupied and positively charged, thus creating the largest possible band bending and the widest SCL width. From charge neutrality across the interface $x = 0$ it is established that $Q_{si} = -Q_{sc} = q n_{p0}^{(e)} W_0$, or

$$W_0 = \frac{R_T N_t}{n_{p0}^{(e)}[C_t n_{p0}^{(e)} + R_T]} = W_{\max}, \tag{12}$$

where $W_0 \equiv W(I_0 = 0)$ is the maximum value of the SCL width. For an interface at equilibrium, C_t is the product of the thermal velocity of an electron and the capture cross section of the interface state with energy E_t. Although the energy-band bending is modulated harmonically in time, the equilibrium configuration in the dark represents a physically meaningful and experimentally extremely useful reference state for optically driven band-curvature modulation, as part of the modulation cycle involves the complete shutoff of the radiation and temporary restoration of the dark equilibrium conditions, depending on the actual optical modulation wave form used. This configuration is, of course, attained only if trapped carriers in interface states during the illumination part of the modulation cycle can be reemitted fast enough into the conduction band during the dark part of the cycle. It is well known that saturation of surface photovoltage (SPV) signals versus illumination intensity in Si depends on modulation frequency due to incomplete carrier emission.[12,13]

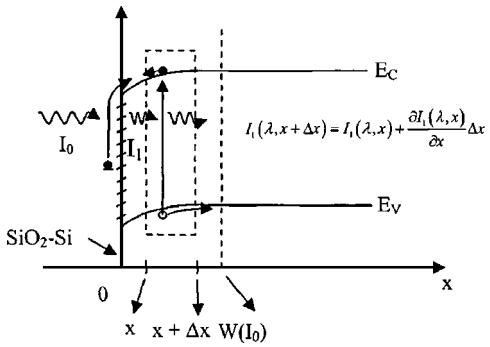

FIG. 2. Details of space-charge-layer optical excitation of a minority-carrier (electron) by an incident super-band-gap photon, showing an opposite sign carrier separation leading to Eq. (16).

For the calculation of the free-electron-density-wave generation rate in the SCL, Fig. 2 shows the relevant coordinate configuration. The incident modulated intensity (and its simplified form)

$$I(\lambda;\omega) = \frac{1}{2}I_0(\lambda)(1 + e^{i\omega t}) \rightarrow I_0(\lambda)e^{i\omega t} \tag{13}$$

creates electron-hole pairs (ehp) within a distance $\mu = [\alpha(\lambda)]^{-1}$, where α is the optical-absorption coefficient of the semiconductor at the incident wavelength λ. It is usually convenient to use the abbreviated form of the modulation factor above on the right; however, great care must be taken when nonlinear calculations mixing the dc level, the fundamental and higher harmonics are made, as is the case with photocarrier radiometry.[1] The modulated excitation generates a free-carrier density wave mostly within depth μ from the surface[14] that usually includes the very thin (~ 0.5 μm in Si) space-charge layer. This is a coherent excitation of minority carriers which is characterized by a frequency-dependent (ac) diffusion length

$$L_n(\omega) = \sqrt{D_n^* \tau_n/(1 + i\omega\tau_n)}, \tag{14}$$

where D_n^* is the ambipolar diffusion coefficient and τ_n is the bulk lifetime of the CDW. In practice, these parameters are composite (effective) quantities involving interface as well as bulk values.[15,16] In the Appendix it is shown that the interface lifetime value is affected by the details of the trapping dynamics. Those minority carriers (electrons) within an ac diffusion length from the edge of the SCL can be swept into it and slide down the energy-band slope of the SCL edge under depletion or inversion conditions for the majority carrier (holes). This increases the charge density within the SCL, which, in turn, affects the occupation of the interface state E_t. Under interface illumination with intensity $I_0(\lambda)e^{i\omega t}$ there is a nonzero probability that a fraction of the occupied interface states, N_{t0}, will absorb photons from the incident radiation and will eject trapped electrons into the

conduction-band edge, thus *increasing* the degree of band bending.[17] Assuming quantum efficiency one for this carrier extraction process and omitting the time-harmonic modulation factor, the interface-absorption-attenuated incident intensity transmitted through to the Si bulk is $I_1(\lambda)=I_0(\lambda)(1-\sigma_\alpha N_{t0})$, where σ_α is the absorption cross section (cm^2) for optical transitions depopulating the interface state E_t. For a uniformly illuminated cross-sectional area A, the net rate of CDW generation, $g_n(x,\omega)$, within the virtual slice $x, x+\Delta x$ is given by

$$\eta_Q A[I_1(x,\omega)-I_1(x+\Delta x,\omega)]=h\nu g_n(x,\omega), \tag{15}$$

where η_Q is the optical-to-electronic energy conversion quantum efficiency in the semiconductor. Expanding the second term in the brackets and retaining only the first order term in the expansion, and assuming the validity of the Beer–Lambert law, the free-electron-density-wave generation rate per unit volume, $G_n(x,\omega)=g_n(x,\omega)/A\Delta x$, is found to be

$$G_n(x,\omega)=\eta_Q[1-R(\lambda)]\frac{I_1(\lambda)\alpha(\lambda)}{2h\nu}e^{-\alpha x}(1+e^{i\omega t}) \quad (\mathrm{cm^{-3}\,s^{-1}})$$
$$\equiv G_n(0,\omega)e^{-\alpha x}, \tag{16}$$

where R is the reflectivity of the semiconductor-oxide interface, assuming that the oxide is essentially transparent to the incident laser radiation. In this picture, photocarrier radiometry monitors the near-infrared recombination emissions from free-electron-density oscillations photogenerated within an optical-absorption depth, α^{-1}, at the interface and within the SCL, and from those minority electrons migrating into the SCL from the quasineutral region from a statistical depth $W\leqslant x\leqslant|L_n(\omega)|$. In addition, CDW recombinations in the quasineutral region itself, within a statistical depth given by $\max[\alpha^{-1},|L_n(\omega)|]$, result in recombination emissions also captured by the IR detector. Finally, to complete the description of carrier dynamics at the interface, the rate equation for minority electrons in the conduction band within the SCL must be considered,

$$\frac{\partial\Delta n_p(0,t)}{\partial t}=-D_{nt}\Delta n_p(0,t)(N_t-N_{t0})+G_n(0,t)$$
$$+(P_\alpha I_0+R_T)N_{t0}-D_{ni}\Delta n_p(0,t)N_i. \tag{17}$$

Here, D_{nt} and D_{ni} are diffusion coefficients ($cm^2\,s^{-1}$) of conduction-band carriers into the interface charged states N_t and into other noncharged and defect states at the interface of density N_i (cm^{-2}), respectively. D_{nt} is related to C_t in Eq. (9). $G_n(0,t)$ is the generation rate per unit volume of Eq. (16) and acts as a harmonic source in the rate equation. It will be noted that free-carrier densities and generation or recombination/capture rates on the semiconductor side of the interface are considered to be volume quantities, whereas corresponding densities and rates on the oxide side are considered area quantities.[15] Unlike the rate equation (9) which is very specific to the occupation of the charged interface states at energy E_t that contribute to the electrical configuration of the SCL, Eq. (17) is more generally descriptive of the full recombination possibilities for the free minority carriers in the conduction band.

In adapting the foregoing interface carrier dynamics to optically modulated space-charge regions, the physical picture that emerges in a *p*-type semiconductor is as follows: ehp generation in the SCL and efficient separation of the two opposite sign carriers by an incident penetrating photon, unabsorbed by the interface states, lead to an extra free electron in the SCL under depletion. This added electron tips the electrical neutrality of the oxide-semiconductor interface and an electron must be trapped by an unoccupied charged state at the interface in order to reestablish charge balance. An increase in the fraction of occupied states occurs which decreases the net charge density to a minimum value $Q_{is}=q[N_t-N_{t0}(I_1)]$. The decreased potential ψ_s on the oxide side of the interface decreases the width of the SCL, Eq. (6). During the part of the modulation cycle when the light is off, the occupied states eject the electrons captured during the illumination part of the cycle in an effort to assume their equilibrium statistical density in the dark, at a rate which depends on the relaxation time of the trap (heretofore assumed fast compared to the period of the optical modulation, but accounted for by the interface capture and recombination lifetimes below). In the dark, the interface charge density reaches its maximum, $Q_{is}=q[N_t-N_{t0}^{(r)}]$, where $N_{t0}^{(r)}$ is the residual occupation density, conesponding to maximum SCL width. The value of $N_{t0}^{(r)}$ occurs for $I_1=0$ and is mainly determined by the thermal free-electron background density, $\Delta n_{p0}(T)$, in the conduction-band edge, and by hopping diffusion to the charged state from other types of occupied states which also contribute to the free-carrier density in the conduction band through thermal excitation (Appendix). These processes exist independently of the optical excitation and serve to determine the background potential bias at the interface which is responsible for the maximum (reference) band bending.

Introducing into Eq. (17) a harmonic time modulation of the free-electron density

$$\Delta n_p(x,\omega)=\Delta n_p(x)e^{i\omega t}, \tag{18}$$

which constitutes the free-electron-density wave, and a similar component to the interface state density determined by the modulated charge neutralizing occupation density (one electron neutralizes the positive charge of the state while it remains trapped during the part of the illumination cycle)

$$N_{t0}(\omega)=N_{t0}^{(r)}+N_1(\omega)e^{i\omega t} \tag{19}$$

and equating terms on both sides of the rate equation, yields the free photoexcited electron-density wave on the semiconductor side of the interface,

$$\Delta n_p(0,\omega)=\left(\frac{G_n(0,\omega)+(P_\alpha I_0+R_T)N_{t0}^{(r)}}{i\omega+D_{nt}[N_t-N_{t0}^{(r)}]+D_{ni}N_i}\right)e^{i\omega t}. \tag{20}$$

There are additional terms, both dc and $\propto e^{2i\omega t}$ appearing in the free-carrier density rate equation under harmonic modulation, but they are omitted here because the experimental configuration[11] involves lock-in detection at the fundamental frequency $f=\omega/2\pi$ only. Imposing the same type of harmonic modulation on the rate equation for interface-state occupation, Eq. (9), and equating terms $\propto e^{i\omega t}$ on both

sides result in an expression for the modulated component of the trap occupation density due to optical ehp generation,

$$N_1(\omega) = \left(\frac{C_t[N_t - N_{t0}^{(r)}]\Delta n_p(0) - P_\alpha I_0 N_{t0}^{(r)}}{i\omega + C_t n_{p0} + R_T} \right) e^{i\omega t}. \quad (21)$$

For simplicity, any losses of photons due to interface absorption at occupied states, as well as any resulting contributions to the free-carrier-density wave in the conduction band, have been neglected from both Eqs. (20) and (21), as they represent nonlinearities which become important only at very high incident modulated intensities (unlike the typical experimental situation) and/or occupation densities at the interface. Equating the dc terms on both sides of the rate equation (9) gives the residual density of occupied states due to the presence of thermal minority electrons in the conduction band without the external optical source under depletion/inversion conditions (equivalently, in the dark),

$$N_{t0}^{(r)} = \frac{C_t n_{p0} N_t}{C_t n_{p0} + R_T}. \quad (22)$$

This expression is consistent with Eq. (11) obtained under equilibrium conditions and attests to the fact that with regard to interface states with short emission/capture time constant, the dark part of the optical modulation cycle restores the interface to its equilibrium condition. The foregoing expressions for the modulated quantities help define an interface recombination lifetime for the photoexcited free-electron-density wave,

$$\tau_{ri} \equiv \frac{1}{D_{nt}[N_t - N_{t0}^{(r)}] + D_{ni} N_i}. \quad (23)$$

In terms of τ_{ri} the CDW can be written as

$$\Delta n_p(x,\omega) = \left(\frac{\tau_{ri}}{1 + i\omega\tau_{ri}} \right) [G_n(x,\omega) + P_\alpha I_0 N_{t0}^{(r)}] e^{i\omega t}. \quad (24)$$

Similarly, with regard to the interface state occupation-density modulation, the capture lifetime

$$\tau_c \equiv \frac{1}{C_t n_{p0} + R_T} \quad (25)$$

can be defined as the inverse of the background trapping rate into the state, so that the dc and modulated components of the occupation density can be expressed in terms of τ_C:

$$N_1(\omega) = \left(\frac{\tau_C}{1 + i\omega\tau_C} \right) (C_t[N_t - N_{t0}^{(r)}]\Delta n_p(0,\omega) - P_\alpha I_0 N_{t0}^{(r)}) e^{i\omega t} \quad (26)$$

and

$$N_{t0}^{(r)} = C_t \tau_C n_{p0} N_t. \quad (27)$$

C. Free photo-excited minority-carrier wave density in the quasineutral (bulk) and SCL regions

The interface carrier density expressions derived in Sec. II B are evaluated at $x=0$ regardless of where the quantity inside the SCL is considered, because the SCL acts as a thin spatial region ($\sim 0.5\ \mu$m) in which recombination is essentially absent due to efficient separation of the local ehp and the completely ionized impurity states at, or above, room temperature. As a consequence, the recombination lifetime in this region has been set equal to infinity, Fig. 3. Experimentally it is very hard to separate SCL recombination from other free-carrier sinks at the interface. However, it should be noted that if any recombination does occur inside the SCL, this would amount to an additional free-carrier sink which, in this work, is phenomenologically taken into account through the concept of surface (or interface) recombination velocity (SRV) adapted to the interface-state dynamics (Appendix). The opposite approach has also been taken in the literature: the surface recombination velocity and the SCL recombination lifetime have been combined into an effective "near-surface lifetime," τ_{SCL}.[16] Both of these descriptions are valid, as one usually does not know the detailed relationship between interface recombination velocity and near-surface lifetime for the (unknown) interface charge density energy distribution manifold in a given sample. Therefore, for simplicity, in calculating the number density of free photocarriers in the semiconductor bulk generated by the incident radiation $I_0(h\nu)$, it helps to think of the surface strip $0 \leqslant x \leqslant W(I_0)$ as serving only as a transport pathway of minority carriers which did not recombine radiatively in the quasineutral region (where they would have contributed to the PCR signal) to the interface, where they recombine mostly nonradiatively (contributing to the effective value of SRV which decreases the PCR signal). Of course, optical absorption and photocarrier excitation within the SCL generate a spatially dependent excess carrier density represented by the rate $G_n(x,\omega)$, Eq. (16); however, these carriers are assumed not to recombine within the SCL but rather join the transport flux to, and accumulation at the interface of, their peers which are generated in the bulk. Under these physical constraints the continuity boundary-value problem for minority electron-wave generation in the bulk is given by[14]

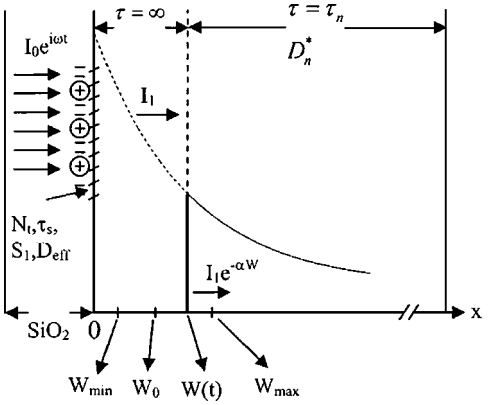

FIG. 3. Optical source depth profile and carrier-density-wave transport parameters in *p*-type semiconductor Si with a transparent surface oxide and interface state density N_t.

$$\frac{d^2\Delta n_b(x,\omega)}{dx^2} - \frac{\Delta n_b(x,\omega)}{L_n^2(\omega)} = -\frac{G_n(0,\omega)}{D_n^*} e^{-\alpha x + i\omega t};$$

$$W(t) < x \leqslant L, \tag{28}$$

where $G_n(0,\omega)$ is given by Eq. (16), with the simplification $I_1 = I_0$ subject to the boundary conditions

$$\left.\frac{d\Delta n_b(x,\omega)}{dx}\right|_{x=W(t)} = \frac{S_1}{D_{\text{eff}}}\Delta n_b[W(t),\omega] \tag{29a}$$

(conservation of photocarrier wave flux across the SCL interface); and

$$\Delta n_b(0,\omega) = \Delta n_b[W(t),\omega], \tag{29b}$$

$$\left.\frac{d\Delta n_b(x,\omega)}{dx}\right|_{x=L} = -\frac{S_2}{D_n^*}\Delta n_b(L,\omega). \tag{29c}$$

In the boundary condition (29a), the value of D_{eff} can either be the ambipolar value D_n^* for minority electron recombination in the quasineutral region, or the value for interface hopping diffusion, D_{eff} (Appendix), depending on the actual radiative recombination site. In most practical cases it will be taken as D_n^* as bulk recombination events far exceed interface hopping diffusion recombination. In Eqs. (28) and (29a), $W(t)$ denotes the oscillating width of the SCL with the frequency of the incident photocarrier generating radiation, because the photon flux changes the occupation density of the interface states via its effect on $N_1(\omega)$. This occupation density oscillation, in turn, modulates the SCL width W. A second possible mechanism for band bending, namely, the screening of the interface charge by free carriers[7,18] does not play as an important role in p-Si because surface trapping of minority carriers is a very efficient process due to the high capture cross section for electrons, $\sigma_n \sim 10^{-13}$–10^{-14} cm^2.[19,20] In Eqs. (28) and (29a)–(29c), S_1 and D_{eff} are the interface recombination velocity and effective diffusion coefficient, respectively, *at* $x=0$, despite the fact that the boundary condition is posed at $x=W(t)$. This is consistent with the assumption that there is no loss of carriers within the SCL, so all losses occur at the translated coordinate at the semiconductor-oxide interface. Conservation of the electron-density wave at $x=W(t)$ is assured by Eq. (29b) and the carrier-wave loss at the back surface $x=L$ is described by the recombination velocity and diffusion coefficient at that surface, Eq. (29c). The optical and transport parameter profiles across the semiconductor cross section are shown schematically in Fig. 3. Although the values of the interface parameters S_1 and D_{eff} are normally determined experimentally from the PCR signal as a function of modulation frequency,[1,2] it is possible to derive explicit expressions for them in terms of the interface state density configuration [see Appendix, Eqs. (A1) and (A8)].

The solution to the boundary-value problem (28) and (29a)–(29c) is[14]

$$\begin{aligned}\Delta n_b(x,\omega) = &\left[\frac{\eta_Q(1-R)I_0\alpha}{2h\nu D_n^*(\alpha^2-k^2)}\right]e^{-\alpha W(\omega)}(1+e^{i\omega t})\\ &\times\left[\frac{g}{G_2-G_1e^{-2kL}}(G_2e^{-k[x-W(\omega)]}\right.\\ &\left.+e^{-k[2L-x-W(\omega)]})-e^{-\alpha[x-W(\omega)]}\right],\end{aligned} \tag{30}$$

where

$$g \equiv \frac{S_1+\alpha D_{\text{eff}}}{S_1+k(\omega)D_{\text{eff}}};\quad G_1 \equiv \frac{k(\omega)D_{\text{eff}}-S_1}{k(\omega)D_{\text{eff}}+S_1};$$

$$G_2 \equiv \frac{k(\omega)+S_2}{k(\omega)D_n^*-S_2} \tag{31}$$

are minority CDW interfacial coupling and accumulation/depletion coefficients. $k(\omega)$ is the minority electron CDW wave number (magnitude of the complex wave vector in one dimension) defined as

$$k(\omega) \equiv \left(\frac{1+i\omega\tau_n}{D_n^*\tau_n}\right)^{1/2}. \tag{32}$$

In view of the fact that the SCL width is almost always very small compared to the typical thickness of bulk semiconductor materials, $L \gg W_0$, collecting terms from the space-charge region, Eq. (24), and from the bulk of the semiconductor, Eq. (30), a complete description of the CDW everywhere on the semiconductor side of the p-type material can be obtained,

$$\begin{aligned}\Delta n_p(x,\omega) = &\left[\frac{\eta_Q(1-R)I_0\alpha}{2h\nu}\right](1+e^{i\omega t})\\ &\times\begin{cases}\left(\dfrac{\tau_{ri}}{1+i\omega\tau_{ri}}\right)e^{-\alpha x}+\dfrac{e^{-\alpha W(\omega)}}{D_n^*(\alpha^2-k^2)}\left[\dfrac{g(G_2+e^{-2kL})}{G_2-G_1e^{-2kL}}-1\right]; & 0 \leqslant x < W(\omega)\\ \dfrac{e^{-\alpha W(\omega)}}{D_n^*(\alpha^2-k^2)}\left\{\dfrac{g}{G_2-G_1e^{-2kL}}[G_2e^{-k[x-W(\omega)]}+e^{-k(2L-x)}]e^{-\alpha[x-W(\omega)]}\right\}; & W(\omega) < x \leqslant L\end{cases}\end{aligned} \tag{33}$$

It should be noticed that the term $P_\alpha I_0 N_{t0}^{(r)}$ in Eq. (24) was neglected in comparison with $G_n(x,\omega)$, because the number density of ejected carriers by direct absorption at the interface is too small compared to the bulk photogenerated carrier density required to shift the curvature of the energy bands in order to have any measurable effect on the PCR signal (or,

alternatively, on the surface photovoltage[8]).

In Eq. (33) there is an apparent CDW discontinuity at $x=W$ due to the inability of the SCL to exchange particle fluxes with the quasineutral (bulk) region in the absence of intralayer and interlayer diffusion. Recall that only drift of photocarriers across the layer is considered based on the well-known dominant transport mechanisms across this very thin layer and in order to keep the mathematical formulation tractable. The term proportional to $[\tau_{ri}/(1+i\omega\tau_{ri})]e^{-\alpha x}$ is the result of CDW confinement within the SCL under depletion and/or inversion conditions of the *p*-type semiconductor created by the presence of interface charged states and it depends on the trapping time constant τ_{ri}. The discontinuity can also be viewed as the consequence of assuming an abrupt ending of the departure of the potential energy, $q\psi(x)$, from the intrinsic Fermi level, E_i, at $x=W$. Through this term, the SCL can freely communicate with the interface states. Through the remaining terms it facilitates and accelerates the transit to the interface of bulk-generated carriers swept under the influence of the built-in electric field that exists inside the SCL. The obvious analog of this situation is the charge-density discontinuity of an abrupt *p-n* junction at the edge of the SCL (e.g., Ref. 4, Chap. 2.3), which is in general agreement with experimental results.

D. SCL width modulation as a function of laser-beam intensity

The effect of band-bending modulation under an external optical field on the interface charge density at the oxide side can be described in terms of static and modulated components,

$$Q_{si}(\omega) = Q_{si}^{(r)} + Q_1(\omega)e^{i\omega t} = q[N_t - N_{t0}^{(r)}] - qN_1(\omega)e^{i\omega t}. \tag{34}$$

Using Eqs. (26) and (27) for the respective interface state densities yields

$$Q_{si}^{(r)} = qN_t\left(\frac{R_T}{C_t n_{p0} + R_T}\right) \tag{35}$$

and

$$Q_1(\omega) = -qN_t\left(\frac{C_t\tau_C^{\,2}}{1+i\omega\tau_C}\right)[R_T\Delta n_p(0,\omega) - P_\alpha I_0 N_{t0}^{(r)}]e^{i\omega t}. \tag{36}$$

The negative sign above indicates that Q_1 increases when the occupation of interface states decreases, since a charge is neutralized for each minority electron captured at an interface state. During one modulation period the SCL width W oscillates between its maximum (dark) value, $W_{\max}=W_0$, and a minimum which depends on the incident intensity: $W_{\min}=W(I_0)$. Ideally, the absolute minimum occurs at the flatband intensity, $I_{\rm FB}$, in which case $W(I_{\rm FB})=0$. The total charge density in the SCL is obtained by integrating Q_{sc} over the SCL width,

$$Q_{sc} = -q[n_{p0}W(I_0) + e^{i\omega t}\int_0^{W(I_0)}\Delta n_p(x,\omega)dx]. \tag{37}$$

From the charge distribution in the SCL, Eq. (33), it is straightforward to show that

$$-Q_{sc}/q = n_{p0}W(I_0) + CI_0\{T_{ri}(\omega)[1-e^{-\alpha W(I_0)}] + \alpha F(\omega)W(I_0)e^{-\alpha W(I_0)}\}e^{i\omega t}, \tag{38}$$

where frequency and intensity dependencies of the various parameters are highlighted, as they correspond to experimentally controlled variables in PCR measurements. The following definitions were introduced to simplify notation

$$C \equiv \frac{(1-R)\eta_Q}{2h\nu}; \quad T_{ri}(\omega) \equiv \frac{\tau_{ri}}{1+i\omega\tau_{ri}};$$

$$F(\omega) \equiv \frac{1}{D_n^{\,*}(\alpha^2-k^2)}\left[\frac{g(G_2+e^{-2kL})}{G_2-G_1e^{-2kL}} - 1\right]. \tag{39}$$

Furthermore, the modulated space-charge layer width can be written as

$$W(I_0) = W_0 - W_m(I_0)e^{i\omega t}. \tag{40}$$

Q_{sc} in Eq. (38) is complex and given by $+Q_{si}=q\{[N_t - N_{t0}^{(r)}] - N_1(\omega)e^{i\omega t}\}$ in Eq. (34). However, the right-hand side (rhs) of Eq. (38) contains a full harmonic spectrum of the angular modulation frequency ω when multiplexed with the SCL modulation function Eq. (40). Upon introducing a Principle of Detailed Charge Neutrality for each harmonic order, the components of each order $O(e^{in\omega t})$; $n=0,1,2,\ldots$, on both sides of the equal sign in Eq. (38) must be, one-to-one, equal across the oxide-semiconductor interface. For synchronous lock-in PCR detection, however, we only need the dc and $O(e^{i\omega t})$ components of Eq. (38) to match with the respective terms of Q_{si}/q. To perform this calculation upon insertion of Eq. (40) into Eq. (38), the following expansions to order $e^{i\omega t}$ are required:

$$e^{-\alpha W} = e^{-\alpha\Delta W}(1+\alpha W_m e^{i\omega t}), \tag{41a}$$

$$We^{-\alpha W} = e^{-\alpha\Delta W}[\Delta W - W_m(1-\alpha\Delta W)e^{i\omega t}];$$

$$\Delta W \equiv W_0 - W_m. \tag{41b}$$

To obtain physically meaningful results requires using the full modulation function $\frac{1}{2}(1+e^{i\omega t})$ instead of the modulus $e^{i\omega t}$ with all modulated quantities, and keeping in mind the origin of the various dc and ac terms so that they can be grouped together with similar terms (e.g., the unity above must accompany the ac component) when the complex equation

$$n_{p0}W(I_0) + CI_0\{T_{ri}(\omega)[1-e^{-\alpha W(I_0)}] + \alpha F(\omega)W(I_0)e^{-\alpha W(I_0)}\} = [N_t - N_{t0}^{(r)}] - N_1(\omega)e^{i\omega t}$$

is separated out into its harmonics. The outcome of computational demultiplexing is

dc term,

$$N_t - N_{t0}^{(r)} = n_{p0} W_0; \tag{42}$$

$O(e^{i\omega t})$ term,

$$N_1(\omega, I_0) = C\alpha W_m I_0 [T_{ri}(\omega) + (1 - \alpha \Delta W) F(\omega)] e^{-\alpha \Delta W}. \tag{43}$$

Equation (42) can be used to calculate the background (dc) charge coverage of the interface state and thus define the SCL reference width in the dark

$$W_0 = \frac{N_t - N_{t0}^{(r)}}{n_{p0}} = \frac{R_T N_t}{n_{p0}(C_t n_{p0} + R_T)}. \tag{44}$$

The rightmost expression is derived from Eq. (22) and can be compared to the equilibrium SCL in the dark, Eq. (12). In principle, from Eq. (44), knowledge of the SCL maximum width W_0 and of the thermally induced minority electron density, n_{p0}, can be used to infer the equilibrium interface charge density $N_t - N_{t0}^{(r)}$. This has been accomplished experimentally.[11] Further knowledge of the interface capture and thermal emission rates C_t and R_T suffices to estimate the trap density N_t and thus completely determine the interface equilibrium charge configuration. In practice, these interface quantities are unknown and the calculated (maximum) value of W_0 may be used to extract the active doping concentration in the SCL from the experimental data. With SPV measurements under depletion conditions, it is relatively straightforward to use Eq. (6) with the Kelvin probe-determined surface potential ψ_s to solve for p_{p0}.[21] As there is no electrical interface with PCR, only W_0 measurements under inversion conditions can be used to determine the SCL active dopant density, N_{sc}, from the equation [Ref. 4, Sec. 7.2.1, Eq. (28)]

$$W_0 = \left[\frac{4\varepsilon_s k_B T \ln(N_{sc}/n_i)}{q^2 N_{sc}} \right]^{1/2}, \tag{45}$$

as was done by Roman *et al.* using SPV.[22] Here n_i is the intrinsic carrier concentration in Si. In PCR, the known value of W_0 must be used in the determination of W_m from Eq. (43). Given that the left-hand side of Eq. (43) is an amplitude (real number), the equality can only be understood also in terms of the amplitude of the rhs. For $I_0 = 0$ Eq. (43) yields $N_1(\omega, 0) = 0$. This is consistent with the expectation that there should be no photocarrier generation in the dark. $N_1(\omega, 0) = 0$ also if $W_m = 0$ in the same equation, again consistently with the requirement that the condition $W_m = 0$ must be equivalent to the dark configuration of the energy bands at the surface, so that $W = W_0$. For $I_0 = I_{FB}$, the flatband intensity, we require that $\Delta W = 0$, i.e., $W_m = W_0$. Equation (43) provides a nonlinear method to extract the I_0 dependence of the SCL width W_m, provided that the oscillating interface charge coverage is known. In practice, the reverse is more likely to happen; the $W_m(I_0)$ dependence may be extracted from the PCR data, and then used with Eq. (43) to estimate the magnitude of the oscillating charge coverage, $N_1(\omega, I_0)$. Similarly, using a variable dc optical bias intensity, I_{DC}, to change W_0 under the conditions where W_m is negligible, the $W_0(I_{DC})$ dependence may be extracted from the PCR data using Eq. (42) to calculate the steady interface charge coverage.[11] Equation (43) can also be used to determine the magnitude of incident laser intensity required to drive the interface to the flatband condition,

$$I_{FB} = I_{0,\max} = \frac{n_{p0}}{(1 - R)\eta_Q \alpha |T_{ri}(\omega) - F(\omega)|}. \tag{46}$$

At flatbands the modulated interface charge density is

$$Q_{si}(I_{FB}) = q n_{p0} W_0 \left[1 - \frac{1}{2}(1 + e^{i\omega t}) \right] = \begin{cases} q n_{p0} W_0; & e^{i\omega t} = -1 \\ 0; & e^{i\omega t} = +1. \end{cases} \tag{47}$$

At the instant of maximum fluence of the sinusoidal optical intensity modulation this relation shows that the charge is fully neutralized instantaneously (in reality, at times short compared to the capture time constant) and accompanied by shrinkage of the SCL width to zero. At the dark (zero fluence) instant of the period, the interface state occupation due to illumination ceases and the residual charge density $q n_{p0} W_0$ (C cm^{-2}) emerges unbalanced. Again, it is emphasized that these predictions can only be achieved if the trapping time constant of the interface state is short compared to the inverse of the light modulation period: $\omega \tau_{ri} \ll 1$. Otherwise, there will be a delayed response amounting to a PCR phase shift, leading to complications akin to those known in the field of surface photovoltage spectroscopy as "photomemory effect."[23]

In view of the fact that optical intensity bias is the primary experimental control of the SCL width, the relationships of Eqs. (42) and (43) between the dark (reference) SCL width and the incident intensity with the interface-state charge coverages (occupation densities) $N_t - N_{t0}^{(r)}(I_0)$ and $N_1(\omega, I_0)$, respectively, are of great importance. however, it is clear from the foregoing that they cannot be easily determined from first principles. Experimental data of the PCR signal versus the incident optical intensity must be obtained and fitted into the appropriate expressions with W_0 and W_m as parameters. Experimentally, these quantities can be obtained conveniently from PCR frequency scans and/or intensity scans with a super-band-gap optical source.

III. PHOTO-CARRIER RADIOMETRIC SIGNAL DEPENDENCE ON SCL

The PCR signal in a semiconductor, with infrared absorption (equivalently, emission) coefficient $\alpha_{IR}(\lambda_{IR})$, averaged over the spectral bandwidth of the photodetector, is given by[1]

$$S_p(\omega, \lambda_{IR}) = \frac{\eta_R W_{eR}(\lambda_{IR})}{A} \left[\frac{1 - R_1(\lambda_{IR})}{1 - R_1(\lambda_{IR}) R_2(\lambda_{IR}) e^{-2\alpha_0(\lambda_{IR})L}} \right] e^{i\omega t} \times \int_0^L e^{-\alpha_0 z} [\alpha_{fc}(z, \omega; \lambda_{IR}) - \alpha_0 J(z, \omega; \lambda_{IR})] dz, \tag{48}$$

where R_1, R_2 are the reflectivities of the front and back surface at the infrared emission wavelength, respectively; η_R is the radiative quantum efficiency for the emission of an infrared photon through carrier recombination; $W_{eR}(\lambda_{IR})/A$ is the

probability density for a radiative emission within an area A; and

$$\alpha_{\mathrm{IR}}(z,\omega;\lambda_{\mathrm{IR}}) = \alpha_0(\lambda_{\mathrm{IR}}) + \alpha_{fc}(z,\omega;\lambda_{\mathrm{IR}})e^{i\omega t}, \tag{49a}$$

$$J(z,\omega;\lambda_{\mathrm{IR}}) \equiv \int_0^z \alpha_{fc}(x,\omega;\lambda_{\mathrm{IR}})dx. \tag{49b}$$

Here, α_0 is the background sub-band-gap infrared absorption coefficient of the semiconductor in the dark, and $\alpha_{fc}(z,\omega;\lambda_{\mathrm{IR}})$ is the excess infrared absorption coefficient due to the free photoexcited CDW by means of an incident modulated optical beam emitting super-band-gap photons. Equation (48) is a simplification of the infrared absorption field valid in the limits of low reflectance R_2 and reasonably constant spectral dependence of $\alpha_0(\lambda_{\mathrm{IR}})$ within the detector bandwidth. For Si the residual $\alpha_0(\lambda_{\mathrm{IR}})$ in the near sub-band-gap region is very low;[24] $\alpha_0(\lambda_{\mathrm{IR}}) \ll \alpha_{fc}(z,\omega;\lambda_{\mathrm{IR}})$. According to Kirchhoff's law stemming from the Principle of Detailed Balance,[25] the infrared absorption and emission coefficients are equal at all wavelengths. Now, the modulated part of the absorption coefficient can be linked to the free photocarrier density wave as[26]

$$\alpha_{fc}(z,\omega;\lambda_{\mathrm{IR}};\alpha) = K\lambda_{\mathrm{IR}}{}^2\Delta n_p(z,\omega;\alpha);$$

$$K \approx 10^{18}\ \mathrm{cm}^2/\mu\mathrm{m}^2, \tag{50}$$

for both n- and p-type semiconductors, where Δn_p is the minority-carrier density, and α is the optical-absorption coefficient at the excitation wavelength. Therefore, for $\alpha_0 L \ll 1$ in Eq. (48), the PCR signal can be obtained, to first approximation, from the depth integral of the free-photocarrier density generated throughout the thickness of the semiconductor

$$S_P(I_0,\omega;\alpha) \cong C_0(R_1,R_2;\alpha_{\mathrm{IR}})\int_0^L \Delta n_p(x,\omega;\alpha)dx, \tag{51}$$

where C_0 is a depth- and frequency-independent constant. Carrying out the integration using Eqs. (33) and (40) and retaining only terms on the $O(e^{i\omega t})$ for lock-in detection of the fundamental Fourier component of the PCR signal using expansions (41a) and (41b), yields the expression

$$\begin{aligned} S_P(I_0,\omega;\alpha) \cong C_0(R_1,R_2;\alpha_{\mathrm{IR}})&\left[\frac{\eta_Q[1-R_1(\lambda_\alpha)]I_0\alpha}{2h\nu}\right] \\ &\times\left(\frac{T_{ri}(\omega)}{\alpha}[1-(1+\alpha W_m)e^{-\alpha\Delta W}]\right. \\ &+\frac{1}{D_n{}^*(\alpha^2-k^2)}\left\{\frac{g}{k(G_2-G_1e^{-2kL})}\right. \\ &\times[\{(1+\alpha W_m)-[1+(\alpha-k)W_m]e^{-kL}\} \\ &\times(G_2+e^{-kL})+[\Delta W - W_m(1-\alpha\Delta W)] \\ &\times(G_2+e^{-2kL})]-\frac{1}{2\alpha}[(1+\alpha W_m)-e^{-\alpha L}] \\ &\left.\left.-[\Delta W - W_m(1-\alpha\Delta W)]\right\}e^{-\alpha\Delta W}\right)e^{i\omega t}. \end{aligned} \tag{52}$$

Here, λ_α denotes the wavelength of the excitation radiation. Experimentally,[11] this equation can be applied with super-band-gap radiation of absorption coefficient $\alpha(h\nu) > 10^3\ \mathrm{cm}^{-1}$, such that the semiconductor material is entirely opaque to the incident radiation, $e^{-\alpha L}\approx 0$. The quantities g, G_1, G_2, and k have been defined in Eqs. (31) and (32). $T_{ri}(\omega)$ was defined in Eq. (39). The effective SCL width $\Delta W = W_0 - W_m$ and W_m are functions of I_0, as described in Eq. (43). In the limit of $I_0 = 0$, there exists no photocarrier density wave, therefore $S_P = 0$. If there exist no charged surface states, then $\Delta W = 0$ and $W_0 = W_m(I_0) = 0$ for all $I_0 > 0$, as gathered from Eqs. (42) and (43), respectively. In this limit Eq. (52) reduces to the conventional PCR signal expression[1] with linear dependence on I_0,

$$\begin{aligned} S_P(I_0,\omega;\alpha) \cong C_0(R_1,R_2;\alpha_{\mathrm{IR}})&\left[\frac{\eta_Q[1-R_1(\lambda_\alpha)]I_0\alpha}{2h\nu D_n{}^*(\alpha^2-k^2)}\right] \\ &\times\left\{\frac{g}{k(G_2-G_1e^{-2kL})}[(G_2+e^{-kL})(1-e^{-kL})]\right. \\ &\left.-\frac{1}{\alpha}(1-e^{-\alpha L})\right\}e^{i\omega t}. \end{aligned} \tag{53}$$

Finally, in the presence of a nonzero density of charged interface states, qQ_{si}, when the PCR intensity is such that $I_0 = I_{\mathrm{FB}}$, Eq. (46), the amplitude of the modulated SCL width is maximum, $W_m = W_0$, and the signal, Eq. (52), reduces to the following expression:

$$\begin{aligned} S_P(I_0,\omega;\alpha) \cong C_0(R_1,R_2;\alpha_{\mathrm{IR}})&\left[\frac{\eta_Q[1-R_1(\lambda_\alpha)]I_0\alpha}{2h\nu}\right] \\ &\times\left(-T_{ri}(\omega)W_0+\frac{1}{D_n{}^*(\alpha^2-k^2)}\right. \\ &\times\left\{\frac{g}{k(G_2-G_1e^{-2kL})}[\{(1+\alpha W_0)\right. \\ &-[1+(\alpha-k)W_0]e^{-kL}\}(G_2+e^{-kL}) \\ &\left.-W_0(G_2+e^{-2kL})]-\frac{1}{2\alpha}[(1+\alpha W_0)-e^{-\alpha L}]\right. \\ &\left.\left.+W_0\right\}\right)e^{i\omega t}. \end{aligned} \tag{54}$$

What differentiates this case from the previous one where there was no interface state density present is that, when the flatband condition is satisfied, there is a temporary neutralization of the interface states; however, the dependence on $N_t - N_{t0}{}^{(r)}$ renders the PCR signal a function of the residual trap density via Eq. (42). Physically, even when the flatband condition is satisfied during the dark part of the modulation cycle, the surface states remain a locus of carrier trapping/emission.

IV. CONCLUSIONS

A dynamic theory of the optically modulated space-charge layer at a Si–SiO_2 interface was developed in terms of the density of intraband-gap interface charges, both residual (background) and harmonically modulated, as a result of a free photoexcited minority carrier density wave (CDW). The theory was incorporated into a quantitative analysis of the PCR signal which was found to involve the dc, fundamental, and all higher harmonics of the excitation frequency as a result of the modulation of the curvature of the energy bands. The dependence of the interface charge density (dc and fundamental components) on the intensity of the excitation source (laser) and on the transport properties of the CDW was derived and led to the formulation of the PCR signal dependence on the SCL width under optical modulation. In conclusion, the presented combined ac/dc laser source PCR theory offers a method for quantitative monitoring of the optical flattening of the energy bands at the interface of a semiconductor under depletion or inversion conditions.

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APPENDIX: DETERMINATION OF S_1, D_S, AND D_{EFF} AT A SEMICONDUCTOR-OXIDE INTERFACE WITH A CHARGED INTERFACE-STATE DENSITY

The definition [Eq. (23)] of the recombination lifetime in terms of semiconductor-oxide interface diffusion rates D_{nt} and D_{ni} describes the hopping occupation of positively charged (D_{nt}) and noncharged or defect (D_{ni}) states. A connection can be made to the Shockley–Reed definition of surface recombination velocity,[27] when properly adapted to the present configuration. Let

$$S_1 = \sigma_{nt} v_{\rm th} [N_t - N_{t0}{}^{(r)}] + \sigma_{ni} v_{\rm th} N_i \equiv S_{1t} + S_{1i}, \tag{A1}$$

where σ_{nt} and σ_{ni} are the capture cross sections (cm^{-2}) for electrons at charged states N_t and noncharged or defect states N_i, respectively. $v_{\rm th}$ is the thermal velocity on the interface plane. Therefore, the interface recombination lifetime can be defined as

$$\frac{1}{\tau_{ri}} = \left(\frac{D_{nt}}{\sigma_{nt} v_{\rm th}}\right) S_{1t} + \left(\frac{D_{ni}}{\sigma_{ni} v_{\rm th}}\right) S_{1i} \equiv \frac{S_{1t}}{d_t} + \frac{S_{1i}}{d_i}, \tag{A2}$$

where d_t and d_i are electron hopping diffusion coefficients (cm). They can be interpreted as probabilities for a hopping surface carrier to reach a trap distance d_t or d_i away from its current location, respectively. Now defining interface carrier lifetimes τ_t and τ_i before trapping, as $\tau_t = d_t / S_{1t}$ and $\tau_i = d_i / S_{1i}$, we obtain

$$\tau_t = \frac{d_t}{\sigma_{nt} v_{\rm th} [N_t - N_{t0}{}^{(r)}]}; \quad \tau_i = \frac{d_i}{\sigma_{ni} v_{\rm th} N_i}. \tag{A3}$$

Equations (A2) and (A3) lead to the physically expected rate equation $\tau_{ri}{}^{-1} = \tau_t{}^{-1} + \tau_i{}^{-1}$. Equations (A1), (A2), and (23) can also be combined to yield

$$\frac{1}{\tau_{ri}} = \frac{1}{v_{\rm th}} \sum_j \left(\frac{D_{nj}}{\sigma_{nj}}\right) S_{1j}, \tag{A4}$$

where (j) denotes all the available surface (interface) trapping sites that will affect the value of the surface (interface) lifetime. Assuming a single rate-limiting carrier trapping state, E_t, consistently with the assumptions of the theory, the following relationship can be written between the interface lifetime $\tau_{ri} = \tau_s$ and the single component of the interface recombination velocity, S_1:

$$\frac{1}{\tau_s} = \frac{1}{v_{\rm th}} \left(\frac{D_{nt}(1-f)}{\sigma_{nt}}\right) S_1. \tag{A5}$$

Here $f = f(E_t)$ stands for the occupation probability of a charge state at the Si–SiO_2 interface. For p-Si, typical values of the diffusion constants in Eq. (A5) are $v_{\rm th} = (3k_B T / m_e{}^*)^{1/2} = 2.257 \times 10^7$ cm/s (Ref. 4; Sec. 5.4.3); $\sigma_{nt} = 5 \times 10^{-14}$ cm^2.[6] The value of $D_{nt}(1-f)$ depends on the details of the space-charge state energy distribution and cannot be calculated from first principles. An adequate approximation for modeling purposes can be obtained in the range of low S_1 values, in which case $\tau_s \approx (L/2S_1)$ where L is the thickness of the semiconductor. This approximation is valid to within 4% for $S_1 < D_n / 4L$.[28] When combined with Eq. (A5), it yields an empirical figure of merit for the hopping charge diffusion coefficient at the interface: $D_{nt}(1-f) \sim (2 v_{\rm th} \sigma_{nt} / L) = (2.257 \times 10^{-6} / L)$ cm^2/s. If more than one interface trapping processes are competing for carriers, combining Eqs. (23) and (A4) gives an expression for the effective (mean) hopping diffusion coefficient,

$$D_s = D_{nt} \left[\frac{N_t - N_{t0}{}^{(r)}}{N_t - N_{t0}{}^{(r)} + N_i}\right] + D_{ni} \left[\frac{N_i}{N_t - N_{t0}{}^{(r)} + N_i}\right]. \tag{A6}$$

Considering the effective recombination rate which is equal to the sum of the interface and bulk recombination rates[29] one may write,

$$\frac{1}{\tau_{\rm eff}} = \frac{1}{\tau_B} + \frac{1}{\tau_s}. \tag{A7}$$

Here, $\tau_{\rm eff}$ is the effective recombination lifetime, τ_s is given by Eq. (A5), and τ_B is the bulk recombination lifetime. Using the definitions of the respective diffusion lengths we find from Eqs. (A5)–(A7) that the effective carrier diffusivity can be expressed as,

$$D_{\rm eff} = D_n{}^* + \left[\frac{L_{\rm eff}{}^2 (1-f) S_1}{v_{\rm th} \sigma_{nt}}\right] D_{nt}. \tag{A8}$$

For small values of S_1 and D_{nt} values in the range of 10^{-5} cm^2/s, the second term on the right can be neglected in most cases, so that $D_{\rm eff} \approx D_n{}^*$.

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