Matlab minority carriers documentation
What does the app do?

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(Dated: May 11, 2020)

The analysis of time-resolved photoluminescence lifetime data as a function of temperature is needed in order to understand the dominant recombination mechanisms of a material. This will give evidence of device performance, and can suggest whether material growth quality can improve. Here, a MATLAB application is created which allows for further analysis of lifetime results and it's subroutines are discussed. The format of the documentation will be closer to article-style, to allow for reference in future manuscript drafting. A walkthrough of the MATLAB application will be provided in a powerpoint format to understand the proper buttons that need to be pushed for data analysis.

Usage: The documentation will allow for quick and easy reference for understanding the MATLAB app, and will provide for discussion of recombination mechanisms and formulas used to model the lifetime.

I. INTRODUCTION: MOTIVATION

The mechanisms that are attributed to the minority carrier lifetime contain multiple components. Understanding the constituents that make up the lifetime character of a sample provides evidence of device performance. For background limited performance (BLIP), the photon generation rate per unit area needs to be greater than the thermal generation rate per unit area,[1] or

$$\eta_a \Phi_B > \frac{n_{th} t}{\tau}, \tag{1}$$

where η_a is the absorption efficiency, Φ_B the background flux, n_{th}, t, and τ are the density of thermal carriers, thickness of the material and lifetime of the carriers, respectively. For best performance, the lifetime needs to be at a maximum. The minority carrier lifetime will be considered here because the material system of interest are direct band gap materials.

II. DATA ANALYSIS

The minority carrier lifetime can be characterized by it's recombination mechanisms,

$$\frac{1}{\tau_{tot}} = \frac{1}{\tau_{SRH}} + \frac{1}{\gamma \tau_{rad}} + \frac{1}{\tau_{Auger}}, \tag{2}$$

where τ_{SRH} is the Shockley-Read-Hall (SRH) lifetime, γ the photon recycling factor, τ_{rad} the radiative lifetime and τ_{Auger} is the Auger lifetime. The lifetime components are added as recombination rates in order to calculate the total lifetime, which is why the reciprocals are added in Eq. 2.

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A. Shockley-Read-Hall Recombination

The recombination of photoexcited carriers with defects in a material is the SRH recombination mechanism. This is observed because there are defect levels, E_t that occur within the forbidden band gap of a material. The lifetime due to SRH recombination is[2, 3]

$$\tau_{SRH} = \frac{\tau_{p0}(n_0 + n_1) + \tau_{n0}(p_0 + p_1)}{n_0 + p_0}. \tag{3}$$

In the case of an n-type sample, and approximating with Boltzmann statistics and parabolic bands[4] we can define the quantities in Eq. 3 by

$$n_0 - p_0 = D \tag{4}$$
$$n_0 p_0 = n_i^2 = N_c N_v \exp\left(-E_g/kT\right) \tag{5}$$
$$\Rightarrow n_0 = \frac{1}{2}\left(\sqrt{D^2 + 4n_i^2} + D\right) \tag{6}$$
$$n_1 = N_c \exp\left(E_t - E_c\right)/kT \tag{7}$$
$$N_c = \frac{1}{4}\left(\frac{2m_e^* kT}{\pi\hbar^2}\right)^{3/2} \tag{8}$$
$$\tau_{p0} = \frac{1}{\sigma_p v_{th} N_t} \tag{9}$$
$$v_{th} = \sqrt{\frac{8kT}{\pi m^*}} \tag{10}$$

where D is the doping concentration, n_0 is the concentration of electrons in thermal equilibrium, n_1 is the density of electrons for the case of the fermi level falling at the trap level E_t, N_c is the effective electron density of states, τ_{p0} is the lifetime for holes injected in a p-type sample, and v_{th} is the thermal velocity. The quantities τ_{n0}, p_0, p_1, etc. can be found by similar equations and through the relation $p_0 = n_i^2/n_0$. When analyzing the total lifetime, the doping D, trap level E_t, and the product σN_t are fit parameters to the data. In the case of degenerate materials, such as highly doped materials, metals or

materials with a negative band gap, Fermi-Dirac statistics will need to be considered. This then causes the approximation of the right hand side of Eq. 5 to become invalid.

B. Radiative Recombination

Photoexcited carriers in the conduction band recombine with vacancies in the valence band and release the excess energy in the form of a photon, we can model the radiative lifetime through the thermal generation rate introduced by Van Roosbroeck and Shockley,[5]

$$G_R = \frac{8\pi}{h^3c^2}\int_0^\infty \frac{\epsilon(E)\alpha(E)E^2dE}{\exp\left(E/kT\right)-1}, \tag{11}$$

where ϵ is the relative dielectric constant which is typically aproximated by the static dielectric constant taken at energies below the fundamental absorption edge, ϵ_∞, α is the absorption coefficient, and E is the photon energy. The integral can be integrated numerically with indirect experiments[6] of the absorption coefficient, such as transmission. Another method is through simulation[7, 8] by using a 14 band **k.p.** theory software.[9] Here, we will compute the integral by giving an approximate analytic form of the absorption coefficient, where the same method was used on analyzing the radiative lifetime on Ge[10] and HgCdTe[11–13] material systems. The analytic form of the absorption coefficient is

$$\alpha_{direct} = \frac{2^{3/2}}{3\epsilon_\infty^{1/2}}\frac{m_0e^2}{\hbar^2}\left[\frac{m_e^*m_h^*}{m_0(m_e^*+m_h^*)}\right]^{3/2}\left(1+\frac{m_0}{m_e^*}+\frac{m_0}{m_h^*}\right) \times\left(\frac{E-E_g}{m_0c^2}\right)^{1/2}, \tag{12}$$

where m_0 is the free electron rest mass, m_e^* is the conduction electron effective mass, m_h^* is the valence heavy hole effective mass, and E_g is the material band gap. Inserting this in Eq. 11, we have

$$G_R = n_i^2 5.8\times10^{-13}\epsilon_\infty^{1/2}\left(\frac{m_0}{m_e^*+m_h^*}\right)^{1/2}\left(1+\frac{m_0}{m_e^*}+\frac{m_0}{m_h^*}\right) \times\left(\frac{300}{T}\right)^{3/2}\left(E_g^2+3kTE_g+3.75(kT)^2\right). \tag{13}$$

The effective masses used for the group III-V material systems will be the effective masses of the major consitutents. For example, for an $InAs_{0.91}Sb_{0.09}$ alloy, the effective mass[14] and static dielectric constant of bulk InAs[15] will be used.

The radiative generation rate developed in Eq.13 is valid for the internal radiative generation and in a doped sample the internal radiative lifetime becomes

$$\tau_{rad} = \frac{n_i^2}{G_R(n_0+p_0)}, \tag{14}$$

but when analyzing the minority carrier lifetime from external measurements such as Time-resolved photoluminescence (TRPL) the simulations tend to underestimate the radiative lifetime. What needs to be considered is the photon recycling factor; this is where the emitted photon is reabsorbed in the active region of a material

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