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Light-intensity dependence of the steady-state photoconductivity used to estimate the density of states in the gap of intrinsic semiconductors

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Abstract

We present a method to obtain the density of states of photoconductive semiconductors based on the light-intensity dependence of the steady-state photoconductivity. A simple expression—relating the density of states at the electron quasi-Fermi level to measurable quantities—is deduced by performing suitable approximations from the analytical solution of the generalized equations that describe the photoconductivity of semiconductors. The validity of the approximations and the applicability of the final expression are verified from numerical simulations of the process. The usefulness of the method is demonstrated by performing measurements on a standard hydrogenated amorphous silicon sample.
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1. Introduction

The steady-state photoconductivity is one of the most widely studied properties of semiconductors. Light absorption increases the concentration of free carriers, whose lifetime is ultimately limited by recombination. Except for pure single crystalline semiconductors, a considerable density of localized states within the forbidden gap is known to exist. These defect states are usually the most efficient recombination centers which determine the transport properties and the photoconductivity. Therefore, many papers in the literature concern the photoconductivity and its dependence upon light flux or generation rate, with the aim to derive defect parameters of the material. For different semiconductor materials, like CdS, Sb_2S_3 or hydrogenated amorphous silicon (a-Si:H), a power-law dependence of the photoconductivity σ_{ph} on the light flux Φ has been observed: $\sigma_{ph} \propto \Phi^{\gamma}$. Several models have been proposed to explain this odd behavior of the photoconductivity, and to try to correlate the γ exponent to some part of the density of states (DOS) of the material. Rose [1] was the first to show that in an exponentially varying DOS, the exponent would be given by $\gamma = T_C/(T+T_C)$, where T is the temperature and T_C is the characteristic temperature that describes the exponentially decreasing conduction band tail. Following the work of Rose, many authors investigated the γ exponent in a-Si:H and commented on the link with the DOS [2–7]. While some authors suggested the possibility to estimate the DOS as a function of energy directly from photoconductivity measurements [4], other authors concluded that the γ coefficient is more sensitive to the total number of defects rather than to their distribution [7], thus throwing doubt on the possibility to develop a DOS spectroscopy from the dependence of the γ coefficient.

In this work we show that a DOS spectroscopy is indeed possible by using the dependence of the γ coefficient upon the temperature and the light flux, and we illustrate this concept on the basis of both numerical calculations and experimental results.

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2. Theoretical background

We will consider an arbitrary distribution of defect states throughout the gap of the semiconductor, characterized by the DOS function $N(E)$. When the solid is uniformly illuminated with photons of energy larger than the band gap, a constant generation rate per unit volume G of electron-hole pairs will result. Simmons and Taylor [8] have described the non-equilibrium steady-state statistics for such an arbitrary distribution of gap states. In the steady-state, the optical generation rate is balanced by recombination, according to the following rate equations:

$$\frac{\mathrm{d}n}{\mathrm{d}t} = 0 = G - \int_{E_V}^{E_C} c_n n[1 - f(E)]N(E)\mathrm{d}E + \int_{E_V}^{E_C} e_n(E)f(E)N(E)\mathrm{d}E - \beta np, \tag{1}$$

$$\frac{\mathrm{d}p}{\mathrm{d}t} = 0 = G - \int_{E_V}^{E_C} c_p f(E)N(E)\mathrm{d}E + \int_{E_V}^{E_C} e_p(E)[1 - f(E)]N(E)\mathrm{d}E - \beta np, \tag{2}$$

where n and p are the concentrations of electrons and holes in extended states, c_n and c_p are the capture coefficients, $e_n(E)$ and $e_p(E)$ are the emission coefficients for electrons and holes, respectively, t is the time, E_V is the energy at the top of the valence band, E_C is the energy at the bottom of the conduction band, $f(E)$ is the occupation function, and the term βnp is the rate of bimolecular recombination, which we will assume in the following to be much lower than the rate of recombination through localized states. As remarked in Ref. [8], if all the states belong to a single species of traps, so that the ratio c_n/c_p is energy-independent, a single occupation function describes the occupancy of all the traps,

$$f(E) = \frac{c_n n + e_p(E)}{c_n n + c_p p + e_n(E) + e_p(E)}. \tag{3}$$

Replacing Eq. (3) into Eq. (2) we get $G = \int_{E_V}^{E_C} \left[\frac{c_n n c_p p - e_n(E)e_p(E)}{c_n n + c_p p + e_n(E) + e_p(E)}\right] N(E)\mathrm{d}E$, which can be approximated to give [9]

$$G = \int_{E_{tp}}^{E_{tn}} \left[\frac{c_n n c_p p}{c_n n + c_p p}\right] N(E)\mathrm{d}E, \tag{4}$$

where E_{tn} and E_{tp} are the quasi-Fermi levels for trapped electrons and holes, respectively.

On the other hand, the condition of charge conservation between dark equilibrium and steady-state under illumination gives the following condition

$$n_0 - p_0 + \int_{E_V}^{E_C} f_0(E)N(E)\mathrm{d}E = n - p + \int_{E_V}^{E_C} f(E)N(E)\mathrm{d}E, \tag{5}$$

where the subscript "zero" stands for dark equilibrium values. In defective semiconductors, where the concentration of excess free carriers is negligible compared to the concentration of trapped carriers, the terms $(n_0 - p_0)$ and $(n - p)$ can be neglected compared to the integrals in Eq. (5). This is true even for device-quality a-Si:H [5]. Moreover, in a low-temperature approximation we have that $f(E) \approx 0$ for $E > E_{tn}$; $f(E) \approx c_n n/(c_n n + c_p p)$ for $E_{tp} < E < E_{tn}$; and $f(E) \approx 1$ for $E > E_{tp}$. Following the work of Taylor and Simmons [9] and combining Eqs. (4) and (5) with the preceding approximate expressions for $f(E)$, after some easy calculations we can write

$$G = \frac{n}{\tau_n} \approx c_n n \int_{E_{F0}}^{E_{tn}} N(E)\mathrm{d}E, \tag{6}$$

and, as well, $G = \frac{p}{\tau_p} \approx c_p p \int_{E_{tp}}^{E_{F0}} N(E)\mathrm{d}E$, where $\tau_n(\tau_p)$ is the free electron (hole) lifetime and E_{F0} is the dark equilibrium Fermi level. Without lost of generality we will consider in the following a semiconductor where electrons are the majority carriers, so that $n O p$ and $c_n n O c_p p$, and we will derive a simple expression relating the DOS at E_{tn} to measurable quantities. If holes were the dominant type of carriers, a similar relation could be derived for the DOS at E_{tp}. Under this assumption of n-type character, the photoconductivity can be approximated by $\sigma_{ph} \cong q\mu_n(n - n_0)$, where μ_n is the mobility of the electrons in the extended states. Also, the quasi-Fermi level for trapped electrons is almost equal to that for free electrons, E_{Fn},

$$E_{tn} \approx E_{Fn} = E_{F0} + k_B T \ln\left(\frac{n}{n_0}\right), \tag{7}$$

where k_B is the Boltzmann's constant and T is the absolute temperature.

Thus, Eq. (6) expresses the generation rate as a function of n. By taking the logarithmic derivative, we get

$$\frac{\mathrm{d}(\ln G)}{\mathrm{d}(\ln n)} = 1 + \frac{c_n n}{G}\frac{\mathrm{d}}{\mathrm{d}E_{Fn}}\left[\int_{E_{F0}}^{E_{Fn}} N(E)\mathrm{d}E\right]\frac{\mathrm{d}E_{Fn}}{\mathrm{d}(\ln n)} = 1 + \frac{c_n n}{G} N(E_{Fn}) k_B T. \tag{8}$$

Defining the parameter γ_n as

$$\gamma_n^{-1} = \frac{\mathrm{d}(\ln G)}{\mathrm{d}(\ln n)}, \tag{9}$$

from the combination of Eqs. (8) and (9) we obtain the very simple expression $N(E_{Fn}) = \frac{G}{k_B T c_n n}\left[\frac{1}{\gamma_n} - 1\right]$. Since under the usual illumination conditions $n \gg n_0$, we have $\sigma_{ph} \cong q\mu_n n$, and hence

$$N(E_{Fn}) = \frac{q\mu_n G}{k_B T c_n \sigma_{ph}}\left[\frac{1}{\gamma_n} - 1\right]. \tag{10}$$

Eq. (10) expresses the DOS at the quasi-Fermi energy as a function of material parameters (c_n and μ_n) and experimental magnitudes that can be easily measured (temper-

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