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Density of states in the gap of microcrystalline silicon determined from thermally-stimulated currents

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Abstract

This paper presents the determination of the density of states (DOS) in the energy gap from the Fermi level towards the conduction band edge in microcrystalline silicon (μc-Si:H) from experimental and numerically simulated thermally-stimulated currents (TSC). The simulation is based on the numerical solution of the rate equations and takes recombination, thermal emission and trapping into account. A combined experiment–simulation approach allowed to provide the evidence of the strong and weak retrapping regimes. In this approach different simulations have been performed in order to reproduce the experimental TSC and then to get the DOS from which the band tail parameter is deduced.

Keywords: Microcrystalline silicon; Thermally-stimulated currents; Defect; Electrical and electronic properties

1. Introduction

Recently, the promising prospect of high efficiency solar cells on the basis of microcrystalline silicon (μc-Si:H) has attracted considerable attention [1–4]. However, a clear physical understanding of the underlying photoelectronic properties remains necessary. Localized states and defects facilitate recombination, resulting in poor collection of excess carriers, which thus leads to poor photovoltaic properties. Since the localized states also affect the transport properties of excess carriers, the knowledge of the density of states (DOS) in the forbidden gap band is very important. The thermally-stimulated current (TSC) technique has been applied to determine the DOS profile and trap parameters in amorphous semiconductors [5–8]. The method consists of cooling the sample to a low temperature T_0 at which the sample is illuminated in order to fill the traps. The light is switched off and the sample is kept in dark at T_0 during a relaxation time t_{rel}. The temperature is increased, usually as a linear function of time, and the trapped carriers are released concomitantly as the quasi-Fermi level moves downward in the energy gap. These released carriers contribute to an excess conductivity measured as an excess current in the presence of an electric field. This excess conductivity, found by subtraction of the dark conductivity is the TSC conductivity σ_{TSC}.

In much of the TSC literature [9–14], quasi-equilibrium conditions are assumed, in which the rate of change of excess free carriers is small. TSC then arises from an instantaneous 'balance' between the net thermal emission rate (re-emission minus retrapping) and recombination. An important distinction can further be made [9], between the 'weak' retrapping case, where released charge carriers simply recombine, and 'strong' retrapping, where released carriers may be retrapped many times before recombining. In the 'weak' retrapping case, the quasi-Fermi energy descends into the energy gap at a rate defined by the attempt-to-escape frequency, ν_0, of the traps.

Fritzsche and Ibaraki [14] developed an analysis of TSC based on continuous DOS and a multiple trapping model. Fritzsche and Ibaraki also considered the effect of variations in carrier lifetime which occur as the TSC temperature scan progresses, and which affect the emission–recombination 'balance'. To describe empirically the effects of strong retrapping, Fritzsche and Ibaraki introduced an 'effective attempt-to-escape frequency' ν_{eff}. In practice, in such a case, *retrapping* into states around E_m, the energy at which the instantaneous emission rate is at a peak, plays a significant role during TSC and leads to a slowing in the descent of E_m toward the Fermi level. Consequently ν_{eff} is smaller than the actual attempt-to-escape frequency ν_0. We note that in the

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literature ν_0 is taken around 10^{11} s^{-1} and 10^{13} s^{-1} [15]. By separate photoconductivity measurements taken over the same temperature range, to reveal the mobility lifetime product, their approach has been successfully applied in order to obtain the DOS in hydrogenated amorphous silicon and related alloys (a-Si:H and a-SiN_x:H) which is in good agreement with that determined from other experimental techniques as space-charge-limited currents.

In this paper, TSC has been carried out on μc-Si:H samples with high and low crystalline volume fraction. Taking into account retrapping, recombination and emission, a simulation [16,17] has been applied in order to reproduce experimental TSC curves and to get the profile of the DOS labelled here TSC–DOS. The analyses of experimental and simulation results allowed to determine the retrapping regime (weak or strong) related to each sample.

2. Experimental details and analysis

The thin film μc-Si:H samples were deposited by hot wire chemical vapor deposition (HWCVD) with high (HC) and low (LC) crystalline volume fraction of about 34% and 79% respectively, determined from Raman spectroscopy measurements. Heat treatment is carried out at a temperature of around 150 °C for 30 min. During TSC measurements the time-dependent current was recorded by an electrometer. The sample was illuminated at T_0 for 3 min by a light emitting diode (LED) with wavelength $\lambda=640$ nm and photon flux of about 10^{16} cm^{-2} s^{-1}. The excitation was turned off and the sample was allowed to relax for a time t_{rel}. Then it was heated at constant heating rate b in the dark.

The TSC–DOS at energy E_m below the conduction band edge is expressed by [18]

$$\mathrm{DOS}(E_m) = \frac{\sigma_{\mathrm{TSC}}(T)}{e(\mu\tau)_n W(T)}. \tag{1}$$

Here e denotes the elementary charge. W and E_c-E_m are b- and T_0-dependent parameterised functions determined in [18]. The

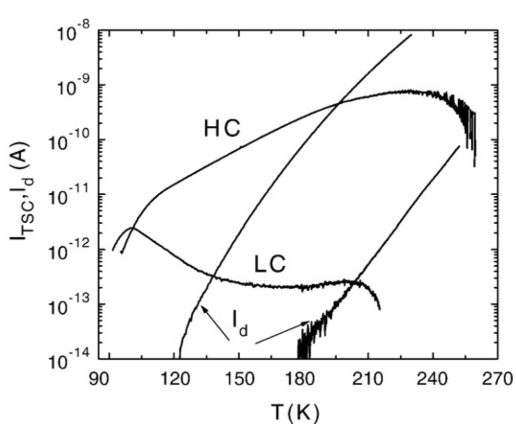

Fig. 1. Experimental thermally-stimulated and dark current carried out on samples LC and HC. The experimental parameters are: for sample LC, $T_0=90$ K, $b=0.032$ K/s, while for sample HC, $T_0=96$ K, $b=0.052$ K/s.

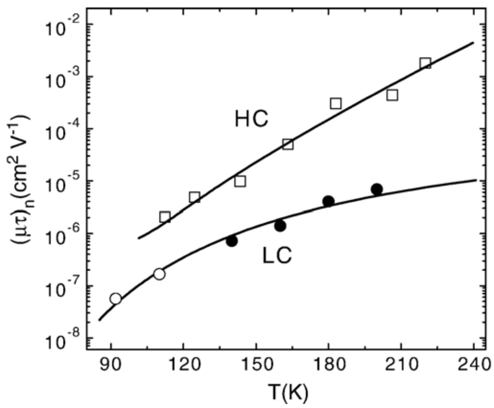

Fig. 2. Temperature dependence of the mobility lifetime product $(\mu\tau)_n$ for electrons for both samples LC and HC. Open symbols show extrapolated data of $(\mu\tau)_n$, while full symbols show experimental data.

electron mobility lifetime product $(\mu\tau)_n$ in Eq. (1) is determined from steady state photoconductivity measurements by $(\mu\tau)$

$$(\mu\tau)_n = \frac{\sigma_p}{eG}, \tag{2}$$

where G is the photogeneration and σ_p is the photoconductivity. The latter is related to the photogeneration rate by

$$\sigma_p = G^{\lambda}. \tag{3}$$

Here γ is known as the light intensity exponent of the photoconductivity. The photon flux was adjusted with neutral density filters such that

$$\sigma_p(T) = \sigma_{\mathrm{TSC}}(T). \tag{4}$$

Eq. (4) is used in order to extrapolate the experimental current data to the low current. The extrapolation is not needed if the measurable photocurrent range covers the TSC current.

A quasi-Fermi level is given by

$$E_c - E_q = kT\ln\left(\frac{\sigma_0}{\sigma_{\mathrm{TSC}} + \sigma_d}\right), \tag{5}$$

where σ_0 is the conductivity prefactor and σ_d is the dark conductivity.

3. Results

The experimental parameters used for the sample LC are: $b=0.032$ K/s and $T_0=90$ K, while for the sample HC, $b=0.052$ K/s, and $T_0=96$ K.

Fig. 1 shows the variation of the thermally-stimulated (I_{TSC}) and dark (I_d) current of μc-Si:H for the samples LC and HC. For sample LC, the TSC current increases initially with increasing temperature showing a maximum at $T_m=100.2$ K. The current then decreases until 145 K. A shoulder appears over a wide range of temperature between 145 K and 203 K. Finally a sharp drop of I_{TSC} is shown from 203 K to 216 K. The dark current of the sample HC is 3 orders of magnitude larger than that of the sample LC. For the sample HC, an initial rise appears upon a