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Surface photovoltage investigation of recombination at the a-Si/c-Si heterojunction

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ABSTRACT

We investigate the use of time-resolved surface photovoltage (SPV) transients as a means to determine band bending and recombination properties at amorphous/crystalline silicon (*a*-Si:H/*c*-Si) heterojunctions. Experimentally, it is shown that for *a*-Si:H film thicknesses above ~6 nm, SPV transients do not depend on the film thickness anymore. On this basis, a simple numerical model is proposed that consists of a single rechargeable gap state on the *c*-Si wafer surface, into which the properties of the *a*-Si:H/*c*-Si interface and the adjacent *a*-Si:H are lumped. It is shown that this model can reproduce all principal features of high excitation SPV transients, i.e. an initial fast decay shown to be due to Auger recombination, a plateau region for high injection conditions and a fast decay when the sample returns into low injection and the defect states are recharged. Under sufficiently high excitation, the SPV saturates at a value that is determined by the *a*-Si:H/*c*-Si interface band bending in the dark. From the slope of the transient decay, defect parameters (density, energetic position) can be extracted.

1. Introduction

Amorphous/crystalline silicon heterojunctions produced by plasma enhanced chemical vapour deposition (PECVD) of ultrathin (5–10 nm) hydrogenated amorphous silicon layers, *a*-Si:H, on crystalline silicon substrates, *c*-Si, are an interesting concept for high-efficiency solar cells on monocrystalline wafers, and to realize large area heterojunction cell concepts on for low-cost thin-film silicon. For those cell types, in order to achieve high efficiencies, it is necessary to suppress interface recombination at the *a*-Si:H/*c*-Si interface. We have shown previously [1], that this can be achieved by decreasing the density of interface defect states $D_{it}(E)$ of the *a*-Si:H/*c*-Si interface and/or by increasing the c-Si band bending $q\varphi_{s0}$. Low D_{it} can be obtained by reducing the *c*-Si surface defect density prior to *a*-Si:H deposition, and by choosing optimized *a*-Si:H deposition conditions [2], while the band bending is adjusted by the *a*-Si:H doping. The *a*-Si:H doping level has to be chosen as a trade-off between high band bending and high density of *a*-Si:H gap states at increased doping levels, which lead to enhanced recombination in the *a*-Si:H [3]. All those optimizations profit greatly from a tool to characterize the *a*-Si:H/*c*-Si interface recombination. To this end, we have been using surface photovoltage measurements (SPV), especially in the time-dependent and intensity-dependent modes (TD-SPV/ID-SPV) [4,5] and references therein], as a “fingerprinting” method to monitor the electronic properties of the *a*-Si:H/*c*-Si effective interface. With the present paper, using numerical simulations, we aim at a refined understanding of the mechanisms that determine the transient decrease of photovoltage over time after the short illumination light pulse. This will allow to extract *a*-Si:H/*c*-Si interface recombination properties that can be compared, for adequate sample structures, to those obtained by other means such as quasi-steady state and microwave photoconductance decay (QSSPC and µPCD).

2. Sample preparation

Phosphorous-doped n-type amorphous silicon (*a*-Si:H) layers were deposited by PECVD (base pressure 10^{-7} mbar) on high quality p-doped (resistivity 1–3 Ω cm) monocrystalline Si (*c*-Si) wafers with <111> surface orientation and bulk diffusion lengths of several 100 µm. For experimental details, see e.g. [3,4]. *a*-Si:H/*c*-Si solar cells produced using the same PECVD system have yielded maximum efficiencies of 19.8% [6]. The investigated set of samples consists of (n^+)*a*-Si:H/(p)*c*-Si (*a*-Si:H doping 10^3 ppm PH_3 in the gas phase) with increasing *a*-Si:H layer thickness (0.4 – 120 nm).

3. Experimental methods

3.1. Surface photovoltage

Surface photovoltage (SPV) is an electrical characterization technique that is well-established for the determination of the density of surface states especially at the silicon/silicon oxide interface [7]. The principle is described elsewhere [4,8] and will be briefly outlined here: The sample under test is sandwiched in a structure consisting of a transparent conductive front contact (TCO — typically zinc oxide), an

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Table 1
Parameters used in the numerical simulations with Silvaco ATLAS and AFORS-HET.

Silicon	
Volume lifetime	1 ms
Wafer thickness	300 µm
Doping	p-type, $1\times10^{15}/cm^2$
Rear surface	
ATLAS: constant surface recombination velocity	1000 cm/s
AFORS-HET: insulator, $E_g=5$ eV	
Defect on front side	
Type	Donor
Density	$3\times10^{10}/cm^2$
Hole capture cross section σ_p	1×10^{-16} cm^2
Electron capture cross section σ_n	1×10^{-14} cm^2
Energetic position	$E_V+0.45$ eV
SPV — laser parameters	
Wavelength	910 nm
Pulse length	ATLAS: 150 ns AFORS: 5–150 ns
Intensity	$\leq10^{22}$ Phot/(s cm^2)

insulating slab of mica, the sample and a back contact. Thus, a metal–insulator–semiconductor structure (MIS) is created. Upon intense illumination of the sample by a short laser pulse ($\lambda=910$ nm, pulse duration 150 ns, maximum intensity 10^{19} photons/(cm^2 s)) through the TCO, excess charge carriers are generated in the sample, leading to a flattening of the bands and a split-up of the quasi-Fermi levels of electrons and holes. The redistributed charge in the sample changes the surface potential, which is measured capacitively via the insulator as a photovoltage pulse V_{SPV}. Ideally, the system has reached steady state when the laser pulse is switched off. The maximum value of the SPV signal right after the laser pulse, $V_{SPV}(t=0)$, is given by the difference of the surface potentials in the dark and under illumination. If the illumination intensity was high enough to reach flat-band conditions in the sample, $V_{SPV}(t=0)$ (corrected by the Dember voltage, see below) gives directly the surface band bending in the dark, $q\varphi_{s0}$. This is the case under high injection conditions, when charge carrier densities n_{illum}, $p_{illum}\gg n_{dark}$, p_{dark}. After the light pulse has ended, the decay of the light-induced excess carriers due to recombination in the bulk and at the interfaces leads to a relaxation of the surface band bending into its dark equilibrium state. Thus, the time-dependent measurement of the surface photovoltage transient $V_{SPV}(t)$ yields information on the recombination processes and associated rate constants in the bulk and at the surfaces and interfaces of the sample.

For the *a*-Si:H/*c*-Si samples investigated here, the chosen excitation wavelength of 910 nm corresponds to sub-bandgap light for the *a*-Si:H film ($E_{phot}=1.36$ eV$<E_{g,a\text{-Si:H}}\approx1.7$ eV). Thus, electron-hole pairs are generated in the *c*-Si substrate, and recharging of *a*-Si:H/*c*-Si interface or *a*-Si:H defect states should mainly occur through injection of electrons and holes from the *c*-Si into the thin *a*-Si:H film.

3.2. Numerical simulation

The numerical simulations have been carried out using the computer program AFORS-HET [9] which allows to simulate the output of measurement techniques for an arbitrary sequence of semiconducting layers and interfaces with an arbitrary number of defects. Since version 2.1, AFORS-HET is also capable of simulating transient effects, which is the basis for the present investigation. For some cases, a comparison with transient simulations using the commercial ATLAS device simulator from Silvaco® International was carried out to check the reliability of AFORS-HET's transient mode against a reference. However, it was found that the transient calculations using ATLAS did only converge to stable solutions for very small band bending at the *c*-Si surface.

The structure used in all simulations consisted of a 300 µm thick p-doped *c*-Si wafer with either a constant rear side recombination velocity of 1000 cm/s (a typical value for an oxide-covered *c*-Si surface) for the calculations using ATLAS, or with a 1 nm thin wide-gap semiconductor as insulating, SiO_2-like layer on the back ($E_g=5$ eV, i.e. below $E_{g,SiO2}$, for increased numerical stability) for the AFORS-HET simulations. Regarding the simulation results, both types of back surfaces lead to very similar results. This is to be expected, as the front surface recombination velocity for the simulated structure, calculated using the Shockley–Read–Hall formalism, is between ~3×10^4 and ~350 cm/s at $\Delta n_s<10^{12}$ and $>10^{17}$ cm^{-3}, respectively, for the defect parameters chosen here. Thus, either the front surface recombination dominates (at low injection levels) or both interfaces contribute about equally (at high injection level, for the case of constant S = 1000 cm/s).

Based on the results of SPV measurements on the *a*-Si:H thickness series (see below), the gap defect states (*c*-Si dangling bonds and *a*-Si:H gap states) on the front of the wafer were lumped into a single donor-like defect in the band gap at $E_V+0.45$ eV, i.e. slightly below *c*-Si midgap. The recombination via this defect is described by the general time-dependent Shockley–Read–Hall formalism (e.g. [10] and references therein). In addition, a fixed charge on the sample surface is used to control the surface band bending. The presence of fixed charges on the *a*-Si:H surface also had to be assumed by Olibet et al. [11] to simulate correctly the dependence of effective lifetime vs. excess carrier density in QSSPC. The simulation parameters are summarized in Table 1.

4. Results and discussion

4.1. SPV on (n$^+$)a-Si:H/(p)c-Si structures with varying a-Si:H thickness

Fig. 1 shows the TR-SPV measurements for the series of (n$^+$)*a*-Si:H/(p)*c*-Si samples with varying *a*-Si:H thickness, together with the data obtained from an unprocessed wafer covered with native oxide. The light pulse ends at $t=0$ and is not resolved on the µs time scale.

For the *a*-Si:H/*c*-Si samples, all transients show a fast initial decay at $t<10$ µs. For the sample covered with 0.4 nm *a*-Si:H – a nominal layer thickness, the *a*-Si:H forms no closed film but islands on the *c*-Si at such low coverages [12] – the transient voltage then decreases quickly up to $t\approx40$ µs and subsequently tails off with a relatively small slope, as compared to the other samples. The sample covered with 4.3 nm *a*-Si:H already shows a plateau region for times $t<60$ µs after the light pulse, followed by a steep decrease to $V_{SPV}<10$ mV at $t>100$ µs. For all other samples with *a*-Si:H layer thicknesses of 6–

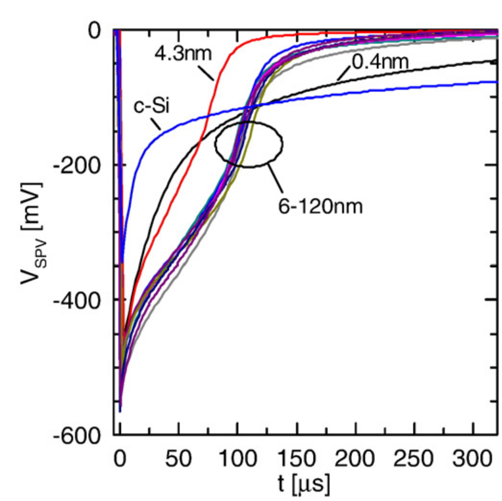

Fig. 1. Surface photovoltage transients measured on (n$^+$)*a*-Si:H/(p)*c*-Si structures for *a*-Si:H film thicknesses from 0.4 to 150 nm. A transient measured on the *c*-Si substrate covered by its native oxide is also included.