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# Influence of the amorphous/crystalline silicon heterostructure properties on planar conductance measurements

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## ABSTRACT

We report a quasi-analytical calculation describing the heterojunction between hydrogenated amorphous silicon (a-Si:H) and crystalline silicon (c-Si) at equilibrium. It has been developed and used to determine the carrier sheet density in the strongly inverted layer at the a-Si:H/ c-Si interface. The model assumes an exponential band tail for the defect distribution in a-Si:H. The effects of the different parameters involved in the calculation are investigated in detail, such as the Fermi level position in a-Si:H, the density of states and the band offsets. The calculation was used to interpret temperature dependent planar conductance measurements carried out on (n) a-Si:H/ (p) c-Si and (p) a-Si:H/(n) c-Si structures, which allowed us to confirm a previous evaluation of the conduction band offset, $\Delta E_C = 0.18 \pm 0.05$ eV, and to evaluate the valence band offset: $\Delta E_V = 0.36 \pm 0.05$ eV at the a-Si:H/ c-Si heterojunction. The results are placed in the frame of recent publications.

## 1. Introduction

Hydrogenated amorphous silicon/crystalline silicon (a-Si:H/ c-Si) heterojunctions are of great interest in electronics since they combine the stable and good electronic properties of crystalline silicon with the low temperature processing of a-Si:H. Among the most critical properties of such a structure, the band discontinuities (conduction and valence band offsets, $\Delta E_C$ and $\Delta E_V$) strongly influence the band bending on each side of the heterojunction, as well as the charge carrier transport across the interface. Published values are unfortunately widely spread [1–4], and mostly based on optical measurements; doubts have been expressed about their validity to be used in order to explain electrical phenomena.

We recently measured planar conductance on a-Si:H/ c-Si samples in order to extract the band offsets. The method is based on the existence of a strongly inverted layer in the crystalline material at the interface if a highly doped (n) a-Si:H layer is deposited on a (p) c-Si substrate [5,6], or for the inverted structure [7]. This forms a conductive channel that strongly depends on the band bending and thus on the band offsets. Conductive probe atomic force microscopy measurements suggested that the valence band offset should be larger than 0.25 eV [8]; comparison with the heterojunction solar cell simulator AFORS-HET [9] allowed us to extract the conduction band offset with a good precision: $\Delta E_C = 0.15 \pm 0.05$ eV [6]. However, the temperature dependence of some parameters such as the bandgap energies was not fully considered and no detailed study on the effect of the structure parameters has been presented so far. For those reasons, a complete analysis of the heterojunction is necessary to validate our first results. Here we present this analysis and apply it to both (n) a-Si:H/ (p) c-Si and (p) a-Si:H/(n) c-Si heterojunctions.

## 2. Channel conductance calculations

We first give an overview on how we calculate the band-bending in c-Si to obtain the channel conductance of an (n) a-Si:H/ (p) c-Si heterojunction (see Fig. 1). The derivation is based on the charge neutrality equation in the whole structure, including the charge in the crystalline silicon $Q_{\text{c-Si}}$, the charge in the amorphous silicon $Q_{\text{a-Si:H}}$, and the charge in interface defects $Q_{\text{DB}}$.

The charge in c-Si is calculated from Frankl's work [10], and reads

$$Q_{\text{c}-\text{Si}} = 2qn_\text{i}L_\text{D}F(u_\text{S}, u_\text{B}) \tag{1}$$

where

$$F(u, u_\text{B}) = \text{sign}(u_\text{B} - u)\sqrt{2[\cosh(u) - \cosh(u_\text{B}) - (u - u_\text{B})\sinh(u_\text{B})]}. \tag{2}$$

In those expressions $q$ is the positive elementary charge, $n_i$ is the intrinsic carrier density in c-Si, $L_D$ given by $\frac{1}{L_\text{D}^2} = \frac{2q^2 n_i}{\varepsilon k_\text{B} T}$ is the intrinsic Debye length, $\varepsilon$ is the material's dielectric constant, $k_B$ is Boltzmann's constant and $T$ is the temperature. The reduced energy $u(x) = \frac{E_\text{F} - E_\text{i}(x)}{k_\text{B} T}$, with $E_i$ the intrinsic Fermi level energy, is used as the variable; $u_S$ and

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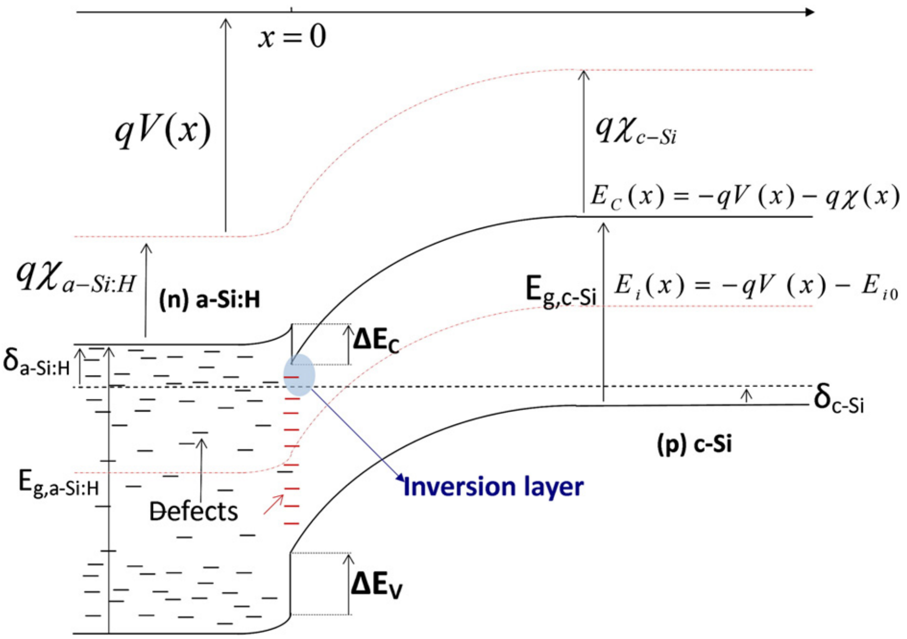

**Fig. 1.** Band diagram of an (n) a-Si:H/ (p) c-Si heterojunction at equilibrium. $\Delta E_C$ and $\Delta E_V$ are the conduction and valence band offsets; $\delta_{\text{a-Si:H}}$ and $\delta_{\text{c-Si}}$ locate the position of the closest band with respect to the constant Fermi level in each material. $E_i(x)$ is the intrinsic Fermi level. $\chi_{\text{a-Si:H}}$ and $\chi_{\text{c-Si}}$ are the electronic affinities.

$u_B$ are the values of $u$ at the interface ($x = 0$) and in the bulk ($x = +\infty$) respectively.

In order to obtain the charge in a-Si:H, Garin et al. followed the same approach as for the charge in c-Si [11]. However they did not consider the charge coming from defects in the bulk a-Si:H, which is actually the main contribution to the space charge density. In (n) a-Si:H, the Fermi level is expected to lie in the conduction band tail, which we represent by an exponential density of states (DOS) distribution: $N(E) = N_0 \exp\left(\frac{E-E_C}{k_B T_C}\right)$, $T_C$ being the characteristic temperature of the band tail. The occupation function of the conduction band tail states can be approximated by a step function since $T_C$, the parameter representing the thermal agitation of the network, is larger than $T$ in n-type a-Si:H. This is even truer in very thin films, which tend to be more defective than thick ones. Solving Poisson's equation and using Gauss' law lead to the expression of the charge in a-Si:H in the case where the flat band regime is reached far from the interface ($x = -\infty$):

$$Q^2_{\text{a-Si:H}} = 2\varepsilon q N(E_F) k_B T_C \left[ k_B T_C \left( \exp\left( \frac{(V(0)-V(-\infty))}{k_B T_C} \right) - 1 \right) - (V(0)-V(-\infty)) \right], \tag{3}$$

where $N(E_F)$ is the density of states at the Fermi energy and $V(0) - V(-\infty)$ is the potential drop in a-Si:H (all the energies are expressed in eV).

Although bulk and interface defects may be correlated [12], especially in ultra-thin films, we treat them independently for more generality. Interface defects are assumed to be correlated dangling bonds of surface state density $N_{DB}$ (per unit area per unit energy) so that the charge of interface defects is obtained from:

$$Q_{DB} = q \int_{E_V}^{E_C} N_{DB}(E) \left[ f_0^+(E) - f_0^-(E) \right] dE, \tag{4}$$

where $f_0^+(E)$and $f_0^-(E)$are the equilibrium occupation functions of positively and negatively charged dangling bonds [13,14] calculated at the interface, and are functions of $u_s$. The integration is performed numerically in the case of a Gaussian defect distribution, whereas Eq. (4) become $Q_{DB} = qD_{it}(f_0^+(E_T) - f_0^-(E_T))$ for a single trap located at an energy $E_T$, with $D_{it}$ the surface density (per unit area) of defects.

$Q_{\text{c-Si}}$ and $Q_{DB}$ are functions of $u_s$. From the band diagram shown in Fig. 1, we can also relate the potential drop in a-Si:H to $u_S$:

$$(V(0)-V(-\infty)) = -\Delta E_C - E_{g,c-Si} + \delta_{a-Si:H} + \delta_{c-Si} + k_B T(u_S - u_B), \tag{5}$$

where $\delta_{\text{a-Si:H}}$ and $\delta_{\text{c-Si}}$ are the positions of the Fermi level in both materials ensuring the local charge neutrality in both bulk materials, far from the interfaces.

Inserting Eq. (5) in Eq. (3), the charge in a-Si:H also becomes a function of $u_s$. The statement of charge neutrality:

$$Q_{\text{c-Si}} + Q_{\text{a-Si:H}} + Q_{DB} = 0, \tag{6}$$

can then easily be solved numerically to find the value of $u_s$, from which we obtain the band bending in c-Si. More details about the presented derivation can be found elsewhere [15].

To derive the temperature dependence of $u_s$ we considered the temperature dependence of the gap of crystalline silicon:$E_{g,c-Si}(T) = E_{g,c-Si}(0) - \alpha \frac{T^2}{T+\beta}$ with $\alpha = (4.9 \pm 0.2) \times 10^{-4}$ eV/K, $\beta = 655 \pm 40$ K and $E_{g,\text{c-Si}}(0) = 1.1692$ eV [16], as well as that of the gap of amorphous silicon:$E_{g,\text{a-Si:H}}(T) = E_{g,\text{a-Si:H}}(0) - 2.25.10^{-4} T$ [17], and of the effective density of states in the valence and conduction bands in c-Si:$N_V(T) = \left(\frac{T}{300}\right)^{1.5} \times 1.8 \times 10^{19} \text{cm}^{-3}$ and $N_C(T) = \left(\frac{T}{300}\right)^{1.5} \times 2.8 \times 10^{19} \text{cm}^{-3}$. The band offsets $\Delta E_C = \chi_{c-Si} - \chi_{a-Si:H}$ and $\Delta E_V = E_{g,\text{a-Si:H}} - E_{g,\text{c-Si}} - (\chi_{\text{c-Si}} - \chi_{\text{a-Si:H}})$ are de facto temperature dependent through the variations of the gaps with temperature. We analyzed several possibilities for the temperature dependence of the band offsets. Experimental results can be best reproduced if the valence band offset stays constant in the experimental range of temperature (150 K–500 K), while the conduction band offset changes according to the variations of the gaps [15]. This is consistent with findings in the literature: Aljishi et al. have shown that the conduction band tail dips strongly with temperature, while the valence band tail shows a much smaller slope [18]. As the mobility edges, which are the relevant quantities in the context of the present electrical measurements, depend on the tail slopes, the same trend is to be expected for the band offsets. Our measurements were reproducible as long as the temperature stayed under the deposition temperature (≈450 K), suggesting that the films were not altered during the measurements.