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FIELD EFFECT STUDIES ON a-Si:H FILMS

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Abstract.— The density of localized gap states $N(E)$ is calculated using a new scheme, which computes the charge density $\rho(V)$ without explicit solution of Poisson's equation directly from the experimental field effect data avoiding fitting procedures and loops. — In a second step $N(E)$ is computed from $\rho(V)$ considering finite temperature statistics. This method is applied to measurements on undoped glow discharge deposited a-Si:H films. It is found that high temperature annealing as well as strong illumination raise the density of states near midgap by about one order of magnitude.

Introduction.— Field effect has widely been used to determine the density of localized gap states in a-Si. A variety of methods has been proposed for an analysis of the experimental data. Neudeck and Malhotra¹ used an ansatz for $N(E)$ to fit their data. Spear et al. started with a crude step method² but later improved their analysis and applied finite temperature statistics³. More accurate methods published recently^{4,5} are still failing in calculating the density of states $N(E)$ in a straight forward way free from "predictor corrector" loops. In this paper we present a new scheme which allows a direct evaluation of at least the excess charge density from the experimental $I(V_F)$ data. The method is applied to experimental results obtained on undoped a-Si:H films deposited by glow discharge technique.

Method of Evaluation.— The field effect modulates the conductance by varying the band bending $eV(x)$ in the semiconductor by an applied transverse field voltage V_F . Neglecting interface effects and assuming a homogeneous semiconductor, the current is given by

$$I(V_F) = I_0 \frac{1}{l} \int_0^l e^{\beta V(x)} dx \quad (1)$$

$\beta = \frac{e}{kT}$, l thickness of the semiconductor, I_0 flat band current. For simplicity we assume n-type conduction. However, all formula can easily be extended to the bipolar case. The excess charge density $\rho(V)$ can be written as

$$\rho(V) = e \int_{-\infty}^{+\infty} dE N(E) [f(E - eV) - f(E)] \quad (2)$$

where $f(E)$ is the occupation probability for a state at energy E . From Poisson's equation one readily finds with $F(V) = \int_0^V dV' \rho(V')$ and $R^2 = \frac{1}{\epsilon_0 \epsilon_s}$

$$\frac{d}{dx} V(x) = - R \sqrt{2F(V)} \quad (3)$$

Substituting eq. (3) into eq. (1), thus avoiding explicit solution of Poisson's equation, we get with $V_0 = V(0)$

$$\frac{I}{I_0} - 1 = \frac{1}{Rl} \int_0^{V_0} \frac{e^{\beta V} - 1}{\sqrt{2F(V)}} dV \quad (4)$$

Our aim is to express the charge density $\rho(V)$ in terms of the experimental quantities only⁶. We differentiate eq. 4 with respect to V_F and insert eq. 3 for $x=0$ together with the boundary condition $dV(x)/dx|_0 = -V_F/a$, $a = d\epsilon_s/\epsilon_d$, where d is the thickness of the dielectric and ϵ_s , ϵ_d denote the dielectric constants. This leads to a differential equation which can be integrated immediately:

$$\frac{1}{\beta} (e^{\beta V_0} - \beta V_0 - 1) = \frac{1}{a} \frac{1}{I_0} [V_F I(V_F) - \int_0^{V_F} I(\tilde{V}_F) d\tilde{V}_F] \quad (5)$$

On the other hand, by differentiating eq. 3 at $x=0$ with respect to V_0 and using again the boundary condition, we find

$$\rho(V_0) = \frac{V_F}{(aR)^2} \left(\frac{dV_0}{dV_F} \right)^{-1} \quad (6)$$

Finally, to deconvolute eq. (2) we differentiate this expression with respect to eV and arrive at

$$\frac{1}{e} \frac{d\rho(V)}{e dV} \Big|_{eV=E} = N_0(E) = \int_{-\infty}^{+\infty} \frac{dE' N(E')}{4kT \cosh^2 \frac{(E'-E)}{2kT}} \quad (7)$$

The meaning of $N_0(E)$ is that of a density of states function with $T=0$ statistics. $N_0(E)$ contains all information necessary to calculate the density of states $N(E)$ at $T \neq 0$. The following points have to be stressed: (1) The charge density can be obtained directly from the experimental data using eqs. 5 and 6. (2) If there is initial band bending, V_F has to be shifted by the flat band voltage V_{FB} . (3) Single particle statistics has been applied, i.e. $f(E)$ is the Fermi function. Actually, results concerning the density of states may be altered if correlation effects are considered⁷.

Experimental results and analysis.— The measurements were performed in a conventional arrangement. As substrate material and field electrode highly n-type doped crystalline Si was used on which SiO_2 was grown thermally with a thickness of $0.2 \mu\text{m}$. The $I(V_F)$ -characteristic was measured by stepwise variation of the field potential. For each step the current was recorded to ensure saturation. In some cases, in particular when other dielectrics were used, saturation was not completely attained; hysteresis effects then prevented a reasonable analysis of the data.

Fig. 1 presents a typical $I(V_F)$ curve together with the calculated density of states N_0 ($T=0$ approximation) for various values of the flat band voltage. When the flat band voltage V_{FB} is shifted from negative to positive values, $N_0(E_F)$ near the Fermi level decreases strongly and the structure near 0.5 eV becomes much less pronounced. This example demonstrates how sensitive structures in the field effect density of states depend on the assumptions about V_{FB} . In order to find a reasonable value for V_{FB} we have investigated the temperature dependence of the field effect between 300 and 480 K. The $N(E)$ calculated for the different $I-V_F$ -curves are expected to coincide if the correct value of V_{FB} is used. This method is not too sensitive but indicates that V_{FB} here should be near -2 V.

Further uncertainties arise when the density of states $N(E)$ is calculated from these data with finite temperature statistics. If the band tails are steep, a large contribution to the charge density at E may be due to regions far up in energy. The result therefore is strongly affected by the extrapolation of $N_0(E)$ to high energies. Generally, if we observe some structure in $N_0(E)$, it will be more pronounced in $N(E)$. This is especially true if this structure is located near a steep band tail. It is important to note, that already small changes in the slope

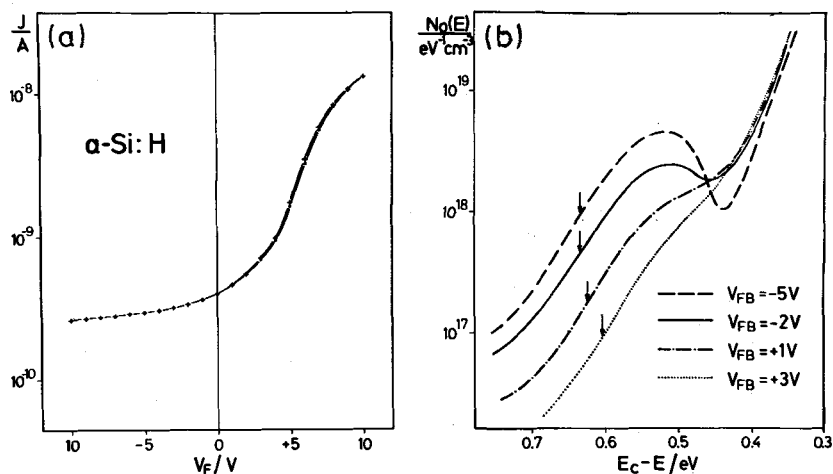


Fig. 1: (a) $I(V_F)$ characteristic of an undoped a-Si:H film taken at 353 K with increasing and decreasing V_F .
 (b) Density of states $N_0(E)$ ($T=0$ statistics) using various values for the flat band voltage V_{FB} . The arrow indicates the position of the bulk Fermi level.

of the tail lead to changes in the depth of the minimum of $N(E)$.

The properties of a-Si:H films change by annealing at temperatures where the hydrogen effuses⁸ and by illumination with light⁹. Whereas hydrogen effusion is known to create defect states near midgap, the situation in case of the Staebler-Wronski effect is not that clear. By annealing the conductivity decreases, the $I(V_F)$ -characteristic becomes more flat for $V_F < 0$ (Fig. 2). In principle, the extension of the flat part can be caused by a much higher density of states or alternatively by a shift of the flat band voltage to about +3 V. This value would correspond to a depletion region with a band bending around 0.35 eV which is unreasonably high. For

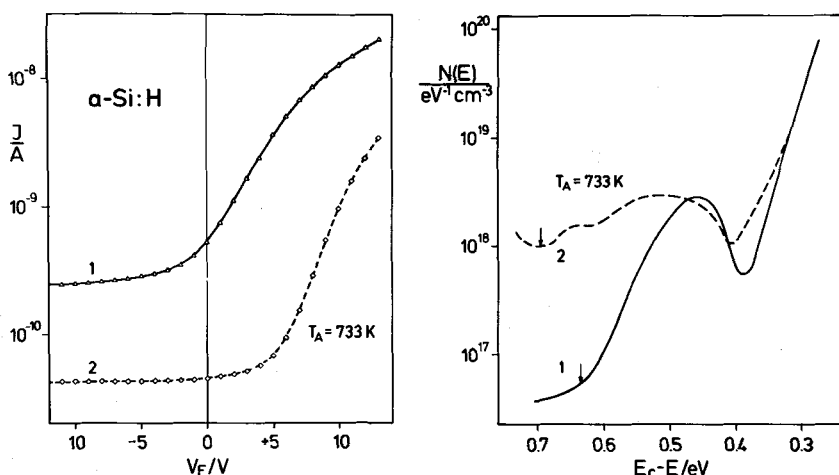


Fig. 2: $I(V_F)$ -characteristics and density of states $N(E)$ for an undoped film.
 (1) annealed at 170°C, (2) after annealing at 733 K. Calculation with $V_{FB} = -2$ V. The arrow indicates the position of E_F .

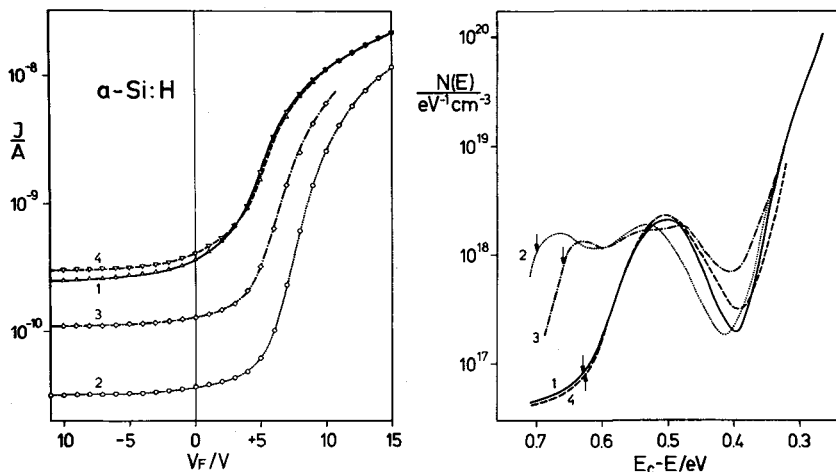


Fig. 3: $I(V_F)$ and $N(E)$ of undoped a-Si:H. (1) annealed at 170°C, (2) after strong illumination, (3) after 0.5 hour anneal at 170°C, (4) after 4 hours anneal at 170°C. Arrow indicates position of E_F .

the analysis it is assumed that V_{FB} does not change with annealing in this temperature range. Using $V_{FB} = -2$ V we find that annealing leads to a strong increase of $N(E)$ near the Fermi level to $10^{18} \text{cm}^{-3} \text{eV}^{-1}$ whereas above 0.5 eV no significant changes occur.

A similar trend is observed upon exposure of the films to light (Fig. 3). After illumination a similar $I(V_F)$ -characteristic (curve 2) is obtained as after H-effusion. Annealing at 170°C reproduces the original $I(V_F)$ -curve. These changes by illumination cannot be explained by a surface effect e.g. a reduction of an original accumulation layer by illumination as was proposed by Solomon et al.¹⁰. $N(E)$ is calculated assuming $V_{FB} = 0$ V. By light exposure $N(E_F)$ is raised to about $10^{18} \text{cm}^{-3} \text{eV}^{-1}$. This effect of light exposure on $N(E)$ is thus quite similar to that of high temperature annealing. This is in accordance with recent results of luminescence¹¹ and ESR-investigations¹² which suggests that in both effects dangling bond type defects are generated.

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