DETERMINATION OF PSEUDOGAP STATE DENSITY AND CARRIER MOBILITY
IN r.f. SPUTTERED AMORPHOUS SILICON

QUARTERLY TECHNICAL PROGRESS REPORT
FOR THE PERIOD
January 1980 - March 31, 1980

William Paul, Principal Investigator
David A. Anderson, Staff Scientist
Richard L. Weisfield, Graduate Student

DISCLAIMER

This book was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

June 1980

Work Performed under Contract DE-AC03-79ET23037

HARVARD UNIVERSITY
DIVISION OF APPLIED SCIENCES
CAMBRIDGE, MASSACHUSETTS 02138

MASTER

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency Thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

NOTICE

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States nor any agency thereof, nor any of their employees, makes any warranty, expressed or implied, or assumes any legal liability or responsibility for any third party's use or the results of such use of any information, apparatus, product or process disclosed in this report, or represents that its use by such third party would not infringe privately owned rights.

DETERMINATION OF PSEUDOGAP STATE DENSITY AND CARRIER MOBILITY
IN r.f. SPUTTERED AMORPHOUS SILICON

QUARTERLY TECHNICAL PROGRESS REPORT
FOR PERIOD JANUARY 1, 1980 - MARCH 31, 1980

WILLIAM PAUL
Principal Investigator

DAVID A. ANDERSON
Staff Scientist

RICHARD L. WEISFIELD
Graduate Student

JUNE 1980

HARVARD UNIVERSITY
DIVISION OF APPLIED SCIENCES
CAMBRIDGE, MASSACHUSETTS 02138

PREPARED FOR THE
U.S. DEPARTMENT OF ENERGY
SOLAR ENERGY
UNDER CONTRACT DE-AC03-79ET23037

ABSTRACT

The effect of a variety of plasma cleaning procedures on the level of bulk and interfacial contaminants in our films is analyzed by Secondary Ion Mass spectrometry. Bulk levels of O have been reduced considerably by N_2 plasma cleaning, but no reproducible reductions in interfacial contamination have been achieved. A method is described of determining the gap state density $N(E)$ of a-Si:H from field effect, in which no assumptions are made about the form of the band bending in the semiconductor. The problem is reduced to three successive integrals over an assumed $N(E)$ by change of variable from distance to applied voltage and the best fit to the experimental data is obtained by iteration of the assumed state density. The method is shown to be no less rigorous and considerably more economical than the recent analysis of Goodman, Fritzsche and Ozaki (1). In addition, we demonstrate an experimental means of determining the flat-band voltage to within 5% of the maximum gate voltage V_g used, by finding the value of V_g for which $(kT/e)d \log I_{SD}/dV_g$ is independent of temperature.

DESCRIPTION OF PROJECT

The purpose of this project is (a) to investigate the density of states in the gap of a-Si:H as a function of the r.f. sputtering deposition parameters by means of field effect experiments and (b) to study the drift mobility of excess carriers in the bands of the material by a time of flight technique.

TABLE OF CONTENTS

<u>Section</u>	<u>Page</u>
ABSTRACT.....	i
DESCRIPTION OF PROJECT.....	ii
INTRODUCTION.....	1
EXPERIMENTAL.....	1
FIELD EFFECT ANALYSIS.....	2
FLAT-BAND VOLTAGE DETERMINATION.....	13
SUMMARY AND FUTURE PLANS.....	17
REFERENCES.....	17
DISTRIBUTION LIST.....	18

LIST OF FIGURES AND TABLES

Figure 1.	Bulk impurity levels of N, O, and C.....	4
Figure 2.	Negative band bending in a-Si:H.....	6
Figure 3.	Conductance vs. gate voltage: Experimental data and calculated fits from Harvard and Chicago.....	11
Figure 4.	Density of states yielding fits in Figure 3,.....	12
Figure 5.	$(kT/e)d \log I_{SD}/dV_g$ vs. $10^3/T$, assuming uniform $N(\epsilon) = 10^{18} \text{ eV}^{-1} \text{ cm}^{-3}$	15
Figure 6.	Experimental $T(d \log I_{SD}/dV_g)$ vs. $10^3/T$ in Teflon geometry.....	16
Table I.	Pre-Sputtering Cleaning Procedures.....	3

INTRODUCTION

This quarterly report continues an account of our investigation of the density of states in the pseudogap of a-Si:H alloys through measurement of the field effect. In the previous two reports we have discussed the background to this investigation, the argument for field effect measurements and the difficulties, both experimental and analytical, in using the data to obtain a reliable bulk state distribution. In particular, we ended our last report with the conclusion that the interfacial regions between either film and substrate or film and atmosphere, the regions of the sample probed in the field effect experiment, were not representative of the bulk film. In the case of the film-atmosphere interface this is related partly to water vapor adsorbed on the sample surface and partly to intrinsic surface states, but the problem at the substrate interface has not yet been identified. In this report we will describe additional experiments we have performed in order to try to resolve this question. It is our view that it is important to establish to what extent this problem is specific to the sputtering deposition process, or whether the problem for field effect is universal, differing only in degree between different methods of deposition.

We have also devised a new method of analyzing the field effect data which we will describe in full in this report. This new method removes the need for any assumptions regarding the potential distribution in the sample $V(x)$, and the flat band voltage V_{FB} , but has the practical advantage over the earlier method of Goodman and Fritzsche [1] that the computation can be handled easily by a DEC PDP/11-03 minicomputer, whereas their method required a much larger machine.

EXPERIMENTAL

During the last quarter we have been engaged in a joint project with Charles Evan Associates to examine by SIMS analysis the effect of a variety of plasma cleaning procedures on the bulk and interfacial contamination in the films [2]. The need for such a study was suggested by earlier SIMS analyses which had shown not only disturbingly high concentrations of contaminants such as oxygen, carbon and nitrogen in the bulk of the samples, but also a very high level of contaminant at the interface with the substrate. We had earlier identified the primary source of oxygen as the water vapor in our base vacuum of 5×10^{-7} Torr and demonstrated that, by taking a number of simple precautions, the base vacuum could be reduced to $< 3 \times 10^{-7}$, and the oxygen content of the films decreased accordingly. The source of other contaminants, however, is probably on the walls of the sputtering system itself and the stainless steel shielding used to contain the plasma. When exposed to the plasma, adsorbed species on these walls will be sputtered off and some of them will find their way to the substrate. In time, as the supply of contaminant atoms dries up and also as the walls become coated with Si, the contaminant level seen in the sample will decay to a relatively constant bulk level. This is exactly what is observed (see Fig. 1 in last report).

By exposing the walls of the system to a plasma while the substrates are covered, we hoped to clean the surfaces before beginning deposition and reduce the levels of contamination in the sample. It had been our practice to do this using an argon plasma, applying power to the Si target, for about 5 to 10 mins., before every deposition. This was followed by a very brief substrate etch of about 30 secs at much lower power (≈ 50 watts) to sputter clean the substrate surface. The purpose of the present investigation was to examine how effective or detrimental these cleaning procedures were. We particularly set out to study the effect of using N_2 gas for the sputter cleaning rather than Ar, since nitrogen has the advantage that it forms gaseous species with all the principal contaminants, and therefore might be more effective in removing them entirely from the system, while argon was suspected of simply redistributing the contaminants on different surfaces.

The results of the first part of this investigation, the study of plasma cleaning treatment on the bulk level of impurity, are shown in Figure 1. The samples are identified by number, and Table I lists the cleaning procedures used. Sample 104 is included for comparison as an earlier sample which, from IR measurements, appeared to be oxygen free.

Two results are most immediately evident: (i) the bulk oxygen level has been reduced considerably by the nitrogen plasma pre-clean and (ii) the nitrogen content has increased, despite an equal argon sputter clean following the nitrogen clean. Adjustment of the sequence in which target and substrate cleaning treatments were performed appears to make little real difference to the level of bulk contamination. It is not clear that the *substrate* clean makes any difference at all to the bulk; in fact, the evidence suggests that too vigorous a substrate treatment can deposit contaminant onto, rather than remove it from, the substrates. (See sample 146.) We interpret this as the sputtering off of contaminant from the stainless steel substrate platform during the reverse sputtering process.

The second part of the investigation, that of studying the effect of the plasma cleaning treatment on the level of contamination at the interface, was very much less conclusive because of the indeterminate and possibly large level of contamination on the surfaces of the substrates used for the investigation. This work is continuing and early indications are that the interfacial contamination may be confined to a narrower region of the film by the plasma treatment but the peak level is not reduced appreciably.

FIELD EFFECT ANALYSIS

The field effect is governed by a set of nonlinear equations which relate the change in source-drain current with gate voltage to the gap state density $N(\epsilon)$. While these equations are relatively simple to derive, their rigorous solution has eluded workers until a recent paper by Goodman and Fritzsche [1]. Previous attempts at deriving a state density have involved three major assumptions: the shape of the band-bending $V(x)$, zero-temperature statistics, and an arbitrarily determined flat-band voltage V_{FB} . We have

TABLE I

Pre-Sputtering Cleaning Procedures (numbers indicate order)

Sample	Target Sputter (N_2)	Target Sputter (Ar)	Substrate Backsputter (N_2)	Substrate Backsputter (Ar)
Si 144	1. 2×10^{-2} torr 350 W 30 min	2. 2×10^{-2} torr 350 W 30 min	none	none
Si 142	1. 2×10^{-2} torr 350 W 30 min	2. 2×10^{-2} torr 350 W 30 min	none	3. 2×10^{-2} torr 50 W 15 sec
Si 146	2. 2×10^{-2} torr 300 W 30 min	3. 2×10^{-2} torr 300 W 30 min	1. 2×10^{-2} torr 200 W 2 min	4. 2×10^{-2} torr 200 W 2 min
Si 147	2. 2×10^{-2} torr 300 W 30 min	3. 2×10^{-2} torr 300 W 30 min	1. 2×10^{-2} torr 200 W 2 min	none
Si 148	1. 2×10^{-2} torr 300 W 30 min	3. 2×10^{-2} torr 300 W 30 min	2. 2×10^{-2} torr 200 W 2 min	none

Figure 1. Bulk levels of O, N, and C for a-Si:H samples identified in Table I.

implemented a method of analysis which is free of these assumptions, which we will derive below. Moreover, we will show that by analyzing field effect measurements made on the same sample at different temperatures, it is possible to deduce the flat-band voltage V_{FB} . This parameter may produce dramatic changes in $N(\epsilon)$, as we demonstrated in the last quarterly report, but to our knowledge, no one has previously proposed a precise criterion for determining V_{FB} experimentally.

The magnitude of the field effect depends on the extent of band-bending induced in a sample through the application of a transverse gate voltage V_g . An example of negative band-bending is schematically represented in Figure 2. If we denote the source-drain current I_{SD} under flat-band conditions as I_0 in a sample of thickness t , then the field effect current is expressed by

$$I_{SD}(V_g) = \frac{I_0}{t} \int_0^t \exp[eV(x)/kT] dx \quad (1)$$

Inside the integral is a Boltzmann factor $\exp[eV(x)/kT]$ which expresses the relative number of conduction electrons at a distance x from the sample-insulator interface. The band-bending $V(x)$ depends both on $N(\epsilon)$ and on the size of the field E_0 at $x=0$, being large and positive when V_g is large and positive. In this case, a surplus of conduction electrons accumulates in the sample near the interface with the insulator, and the field effect current is thereby enhanced. Conversely, when a large and negative V_g is applied at the gate, the band-bending is large and negative. This depletes the interfacial region of electrons, and I_{SD} is diminished. We can view the field effect, therefore, as indicating the degree to which an applied V_g can produce a given band-bending $V(x)$ in the material. This quantity is uniquely and self-consistently related to the state density distribution $N(\epsilon)$, as we show below.

The band-bending $V(x)$ is an electrostatic potential distribution which is governed by Poisson's equation

$$\frac{d^2V}{dx^2} = - \frac{\rho(x)}{\kappa_s \epsilon_0} \quad (2)$$

Here, ρ is the induced charge density and κ_s is the dielectric constant of the sample. This equation must be solved with the appropriate boundary conditions

$$V(t) = - \frac{dV}{dx}(t) = 0 \quad (3)$$

and

$$- \frac{dV}{dx}(0) = E_0 \quad (4)$$

Figure 2. Potential inside semiconductor surface under conditions of negative band bending (electron accumulation).

The first condition states that in the bulk of the film, the bands are assumed to be flat and the transverse electric field $-dV/dx$ vanishes. This necessitates using a sufficiently thick film, i.e., $t \gtrsim 1 \mu\text{m}$. The second condition requires the electric field at the sample-insulator interface to have the value

$$E_0 = \frac{\kappa_i}{\kappa_s} \frac{V_g - V_{FB}}{d}, \quad (5)$$

where κ_i and d are, respectively, the dielectric constant and thickness of the insulator. A nonzero flat-band voltage takes into account any fixed surface charge density residing at $x=0$. With V_{FB} as an unknown parameter, we know E_0 only within an additive constant. Later, we will show how V_{FB} can be determined experimentally.

The induced charge density $\rho(x)$ can be expressed as a function of $N(\epsilon)$ and $V(x)$ by

$$\rho(x) = -e \int_{-\infty}^{\infty} N(\epsilon) [f(\epsilon - eV(x)) - f(\epsilon)] d\epsilon \quad (6)$$

The quantity $f(\epsilon)$ is the Fermi-Dirac distribution function. In the limit of zero-temperature statistics, where $N(\epsilon)$ does not change significantly over an energy range kT , the expression for $\rho(x)$ reduces to the more simple form

$$\rho(x) \approx -e \int_{\epsilon_F}^{\epsilon_F + eV(x)} N(\epsilon) d\epsilon + O(kT)^2 \quad (7)$$

In this limit, the only states affected by the application of a gate voltage are residing in energy between the bulk Fermi level ϵ_F and $\epsilon_F + eV(x)$. At higher temperatures, the demarcation of filled and empty states is not as sharp, and thus, contributions to the charge density can occur from states a few kT above or below the limits of integration in equation (7). In either case, we note that ρ depends explicitly only on the potential V , with the position x appearing simply as a parameter. Indeed, we can suppress the implicit x dependence of ρ and V and rewrite equation (6) to read

$$\rho(V) = -e \int_{-\infty}^{\infty} N(\epsilon) [f(\epsilon - eV) - f(\epsilon)] d\epsilon \quad (8)$$

Combining equations (2) and (8), we generate an integrodifferential equation for $V(x)$:

$$\frac{d^2V}{dx^2} = + \frac{e}{\kappa_s \epsilon_0} \int_{-\infty}^{\infty} N(\epsilon) [f(\epsilon - eV) - f(\epsilon)] d\epsilon \equiv - \frac{\rho(V)}{\kappa_s \epsilon_0} \quad (9)$$

The conventional approach to solving for $V(x)$ has been either to assume ρ is a constant up to a fixed depth in the film, yielding a parabolic, Schottky barrier for $V(x)$; or to assume that $N(\epsilon)$ is constant, yielding an exponentially decaying $\rho(x)$ and $V(x)$. Goodman and Fritzsche, on the other hand, have recently solved this problem numerically by guessing a tabulated $N(\epsilon)$, calculating $\rho(V)$ by equation (8), and then solving equation (9) by iteration in order to achieve consistency with boundary conditions 3 and 4. Once they know $V(x)$ for a given gate voltage, the expected field effect current is calculated by equation (1) and then compared with the value measured. The function $N(\epsilon)$ is then adjusted point by point, $\rho(V)$ and $V(x)$ recalculated, in order to reduce the deviation between theoretically and experimentally derived field effect response to within experimental error. Their iterative method is valid, in principle, for analyzing samples with varying $N(\epsilon)$ distributions, even at finite measurement temperatures. Since their numerical analysis requires the use of a powerful IBM 360 computer, it would be excessively time-consuming if implemented on a laboratory minicomputer. However, we now show that, with a simple change of variable, we can calculate the field effect response for a given state density distribution much more efficiently, so that the entire computation can be carried out on our DEC PDP/11-03 minicomputer, without loss of rigor.

We first rewrite Poisson's equation by changing the independent variable from x to V :

$$E(V) \frac{dE}{dV} = - \frac{\rho(V)}{\kappa_s \epsilon_0} \quad (10)$$

This can be integrated with respect to V , yielding

$$\frac{1}{2} \kappa_s \epsilon_0 E^2(V) \Big|_{V'=0}^{V'=V} = - \int_0^V \rho(V') dV' \quad (11)$$

Using boundary condition 3 that E vanishes when V does, we obtain the result that

$$E(V) = \pm \left[- \frac{2}{\kappa_s \epsilon_0} \int_0^V \rho(V') dV' \right]^{1/2} \quad (12)$$

We choose E to have the same sign as V . Now we can solve directly for $V(x)$ without the need for iteration, since we know the field $E(V) = -dV/dx$, which when integrated gives

$$x(V) = - \int_{V_0}^V \frac{dv'}{E(V')} \quad (13)$$

Here, $V_0 = V(0)$ is determined by boundary condition 4 that $E(V_0) = E_0$.

Knowing $V(x)$ explicitly is not necessary, however, in order to calculate the field effect response. We first slightly alter equation (1) to read

$$\frac{I_{SD}(V_g)}{I_0} - 1 = \frac{1}{t} \int_0^t [\exp(eV(x)/kT) - 1] dx \quad (14)$$

In this form, we can transform the independent variable of integration from x to V , yielding

$$\frac{I_{SD}(V_g)}{I_0} - 1 = \frac{1}{t} \int_0^{V(V_g)} \frac{\exp(eV/kT) - 1}{E(V)} dV \quad (15)$$

Now we have eliminated any explicit reference to x in calculating $\rho(V)$, $E(V)$, and $I_{SD}(V_g)$.

The calculation of the field effect is now reduced to successively integrating equations (8), (12), and (15). We first calculate accumulation data by incrementing the upper limit of integration V_0 , continuously increasing $E(V)$ and noting when it equals values of E_0 determined by equation (5) for the experimental values of V_g . We then calculate depletion data by decreasing V_0 below 0, sweeping $E(V)$ through values of E_0 corresponding to gate voltages $V_g < V_{FB}$. This procedure represents considerably less numerical work than solving for $V(x)$ and integrating equation (1) over the entire thickness of the sample each time a new gate voltage is chosen. Nevertheless, the integrity of the solution is retained, so that for any given $N(\epsilon)$ and choice of V_{FB} , a unique field effect response can be calculated for any temperature.

We have found it convenient to represent $N(\epsilon)$ by fitting its logarithm to an m -th order polynomial in $\epsilon - \epsilon_F$:

$$\log N(\epsilon) = a_0 + a_1(\epsilon - \epsilon_F) + a_2(\epsilon - \epsilon_F)^2 + \dots \quad (16)$$

usually retaining no more than three terms. Due to the inaccuracies found in most experimental field effect data, it is unlikely that any structure in $N(\epsilon)$ derived from field effect would not be modeled adequately by this smoothly varying functional form. While such a parameterization restricts the class of state density distributions available for analysis, the optimization

of the determination of $N(\epsilon)$ is quite straightforward. By having our analysis program graphically display both the experimental and computed field effect response curves, it is a simple matter to manually adjust the parameters which define $N(\epsilon)$ in order to bring the theoretical field effect into close visual agreement with experiment. This process is tedious, however, and so efforts have been made to optimize $N(\epsilon)$ automatically with the help of the computer.

A good criterion for determining the correct density of states distribution is to find that $N(\epsilon)$ which minimizes

$$\chi^2 = \frac{1}{N-m-1} \sum_{n=1}^N \frac{[I_{SD}^{\text{expt}}(V_g^n) - I_{SD}^{\text{cal}}(V_g^n)]^2}{\sigma_{I_{SD}}^2(V_g^n)^2}, \quad (17)$$

where m is the number of parameters used to fit $N(\epsilon)$ for an experiment with N measured values of I_{SD} with estimated errors $\sigma_{I_{SD}}$. To minimize χ^2 we have tried several nonlinear least-squares fitting routines. These procedures fine-tune the choice of parameters which determine $N(\epsilon)$ with varying degrees of efficiency. They all suffer by converging slowly, if at all, when $N(\epsilon)$ is far from the true distribution. We have found it convenient to use an earlier routine set up to calculate $N(\epsilon)$ assuming an exponential barrier $V(x)$, in order to obtain an approximate density of states which is close enough to the true density of states to be used as an initial guess for the more rigorous calculation we have outlined above. This ensures much more rapid convergence.

The complete finite-temperature Fermi-Dirac statistics embodied in Equation (8) are probably unnecessary in many cases. In order to streamline the computation further, we have taken into account finite-temperature statistics by expanding $\rho(V)$ in powers of kT and retaining the first temperature correction term:

$$\rho(V) = -e \left[\int_{\epsilon_F}^{\epsilon_F + eV} N(\epsilon) d\epsilon + \frac{\pi^2}{6} (kT)^2 \frac{dN}{d\epsilon} \bigg|_{\epsilon_F}^{\epsilon_F + eV} + O(kT)^4 \right], \quad (18)$$

which is valid provided $d \log N(\epsilon)/d\epsilon < kT$. This requirement can be checked *a posteriori* by observing how rapidly $N(\epsilon)$ varies with energy.

To test the reliability of our computer program, we have analyzed some of the field effect data published by Goodman and Fritzsche on glow discharge produced a-Si:H. In Figure 3 we show a plot of their field effect data and the best fits obtained by their analysis and by ours. The agreement is satisfactory in both cases. In Figure 4 we show the optimal state density distributions producing the fits seen in the previous figure. The region above the Fermi level ($\epsilon > \epsilon_F$) is reproduced by our analysis very well, especially near ϵ_p . The small bump 0.3 eV above ϵ_F is not reproduced by

Figure 3. Field effect data for a-Si:H, from Goodman et al. (1) Conductance vs. gate voltage, assuming equal electron and hole contributions at $V_{FB} = -450$ V.

Figure 4. Density of states $N(\epsilon)$ vs. $\epsilon - \epsilon_F$ giving calculated field effect curves in Figure 3.

our analysis, because the low order polynomial used to fit $\log N(\epsilon)$ does not possess sufficient fine structure. This is of no real consequence, since Goodman and Fritzsche do not claim that the bump can be substantiated by this set of field effect data. We, like them, obtained an equally good fit to the data without it. The density of states below the Fermi level ($\epsilon < \epsilon_F$) is not in such good agreement, though near ϵ_F the fits are rather close. The discrepancy may, in fact, be due to two problems. First, the data for V_g slightly below V_{FB} do not vary much from point to point, so that small errors in transcribing the data from their figure may produce large errors in $N(\epsilon)$ below ϵ_F . Secondly and more importantly, the state density they derived below ϵ_F varies rapidly with energy, decreasing by an order or magnitude in 0.1 eV. Such rapid variations in $N(\epsilon)$ bring the validity of our temperature expansion into question, and in these extreme circumstances, the exact finite temperature statistics of equation (8) should be used.

Flat-Band Voltage Determination

The one remaining parameter in our field effect analysis which has not received much attention is the flat-band voltage V_{FB} .

In physical terms, it marks the delineation between electron accumulation ($V_g > V_{FB}$) and depletion ($V_g < V_{FB}$). However, on a graph of I_{SD} versus V_g , the distinction between the two regimes seems quite arbitrary. Nevertheless, additional analysis can reveal an experimental means for determining V_{FB} , as we now demonstrate.

Experimentally, it is possible to measure the logarithmic derivative of the field effect response $d \log I_{SD} / dV_g$ at various gate voltages and temperatures. We can also calculate the logarithmic derivative theoretically, by differentiating equation (15) with respect to V_g :

$$\frac{d \log I_{SD}}{dV_g} = \frac{1}{I_{SD}} \frac{dI_{SD}}{dV_g} = \frac{I_0}{I_{SD}(V_g)} \frac{1}{t} \frac{\exp(eV_0/kT) - 1}{E_0} \frac{dV_0}{dV_g} \quad (19)$$

Combining equation (5) and (10), the above simplifies to

$$\frac{d \log I_{SD}}{dV_g} = \frac{I_0}{I_{SD}(V_g)} \frac{\kappa_1 \epsilon_0}{dt} \frac{\exp(eV_0/kT) - 1}{-\rho(V_0)} \quad (20)$$

Now let us examine the behavior of this quantity near flat-band conditions, when V_0 is very small. In this limit the charge density becomes proportional to V_0 , that is $\rho(V) \approx -e^2 N_0 V$. To lowest order, $I_{SD} \approx I_0$ for V_0 small, so expanding equation (20) in powers of V_0 , we obtain

$$\frac{d \log I_{SD}}{dV_g} \approx \frac{\kappa_1 \epsilon_0}{dt} \frac{e/kT}{e^2 N_0} \left[1 + \frac{1}{2} \left(\frac{eV_0}{kT} \right) + O \left(\frac{eV_0}{kT} \right)^2 \right] \quad (21)$$

This formula allows us to determine which gate voltage makes $V_0 = 0$. If we plot $(kT/e)d \log I_{SD}/dV_g$ versus $1/T$ for various values of V_g , it is clear that only when $V_g = V_{FB}$ is this quantity independent of temperature. For gate voltages $V_g > V_{FB}$, V_0 is positive and $(kT/e)d \log I_{SD}/dV_g$ increases linearly with $1/T$, whereas for $V_g < V_{FB}$, this quantity decreases linearly with $1/T$. So, assuming that V_{FB} remains constant throughout a field effect experiment performed at several temperatures, we now can determine its value based on this experiment alone. In addition, we can estimate the state density at the Fermi level by noting the value of $(kT/e)d \log I_{SD}/dV_g$ when $V_g = V_{FB}$, because

$$N_0 = \frac{\kappa_i \epsilon_0}{4\pi e^2} \left[\frac{kT}{e} \frac{d \log I_{SD}}{dV_g} \right]_{V_g = V_{FB}}^{-1} \quad (22)$$

This method has been tested by calculating the theoretical response for field effect in a 1 μm thick sample using our typical .127 mm Teflon insulator. The field effect is calculated for temperatures from 25°C to 200°C, assuming a constant state density $N_0 = 10^{18} \text{ eV}^{-1} \text{ cm}^{-3}$ and $V_{FB} = 0 \text{ V}$. Numerically differentiating the data as one would do experimentally, the results are plotted versus $1000/T$ in Figure 5. Even for the relatively large state density chosen, for which the field effect response is rather moderate, one can easily see the fan-like trend in $(kT/e)d \log I/dV_g$, described above. For this set of data, the flat-band voltage, at which $(kT/e)d \log I/dV_g$ is independent of temperature, can be recovered within an accuracy of $\pm 100 \text{ V}$.

Now examining some real experimental data, we apply this analysis to the field effect measurements on sample Si 105-3, first presented in the last quarterly report. These measurements were made using the Teflon geometry at temperatures of 23°C, 53°C, and 110°C. The quantity $T(d \log I_{SD}/dV_g)$ is plotted versus $1000/T$ in Figure 6. Although there is some experimental scatter in these rather preliminary data, one can clearly distinguish a flat-band voltage $V_{FB} = -2000$ to within $\pm 250 \text{ V}$ accuracy. The simple "fan" seen in the previous figure is not nearly as evident here for at least two reasons. First, the density of states in a-Si:H is not constant in the gap, so only close to the flat-band voltage will the fan be evident. Second, in a real insulator there can be varying degrees of hysteresis in the flat-band voltage, and this hysteresis can be temperature-dependent as well. In fact, some of the time-dependent effects observed in the Teflon geometry may be attributed to shifts in V_{FB} as the gate voltage is changed. At this point, our experience with Teflon is limited. More extensive measurements of field effect as a function of temperature must be performed before we can say how important flat-band voltage hysteresis is in the Teflon geometry.

Figure 5. $(kT/e) d \log I_{SD} / dV_g$ vs. $10^3/T$ for a-Si:H, calculated assuming constant density of states $N(E) = 10^{18} \text{ eV}^{-1} \text{ cm}^{-3}$ and flat band voltage $V_{FB} = 0 \text{ V}$.

Figure 6. Experimental $T(d \log I_{SD}/dV_g)$ vs. $10^3/T$ for a-Si:H sample in Teflon insulator field effect geometry.

SUMMARY AND FUTURE PLANS

We have found that there are significant bulk levels of oxygen, nitrogen and carbon in our sputtered films and that these levels can be reduced by a combination of nitrogen and argon sputter cleaning before film deposition. At the interface with the substrate there appears to be a significant increase in the level of all three contaminants above the bulk level and we find this is affected much less by the precleaning. In some instances backsputtering the substrates can actually result in more contaminant at the interface. Metallic impurities such as Al, Cr and Fe have also been found at a level of between 10^{17} cm^{-3} and 10^{18} cm^{-3} in a very sharp peak at the interface.

It has not been possible yet to positively identify the contamination as the source of the difficulties in making field effect measurements. To clarify the situation we have to do one of two experiments: either (i) measure the contamination profile in a sample which gives a large field effect or (ii) measure field effect in a sample with no increased interfacial contamination. To do the first we intend to study the impurity profiles of a-Si:H samples made by glow discharge in SiH_4 in this laboratory, some of which have given a very healthy field effect. The second requires further study into the sources of the contamination.

In an effort to study how representative the healthy field effect response of the glow discharge samples is of the bulk state density, we will be making greater use of capacitance-frequency measurements developed by P. Viktorovitch to compare the state densities derived from the two techniques. The use of a Teflon insulator to study field effect in the top surface of the sample has been found to be extremely limited by the presence of water vapor on the surface and also, apparently, by surface states intrinsic to the sputtered a-Si:H material. Work is continuing to try to encapsulate the film and to explore the feasibility of performing the measurement *in situ* inside the deposition system.

REFERENCES

1. N.B. Goodman, H. Fritzsche, and H. Ozaki, in Proceedings of 8th International Conference on Amorphous and Liquid Semiconductors, Cambridge, 1979 (W. Paul and M. Kastner, eds.), *J. Non-Cryst. Solids* 35-6, 599 (1980).
2. Work to be published in collaboration with Charles Evans Associates.

DISTRIBUTION LIST

L. Guttman
Argonne National Laboratory
Solid State Science Division
Argonne, IL 60493

Battelle Columbus Laboratories
Attn: Dr. Alfred E. Austin
505 King Avenue
Columbus, OH 43201

Brookhaven National Laboratory
Dept. of Energy & Environment
Attn: R.W. Griffith
Upton, NY 11973

JILA
University of Colorado
Attn: A. Gallagher
Boulder, CO 80309

Institute of Energy Conversion
University of Delaware
Attn: Dr. Vikram Dalal
1 Pike Creek Center
Wilmington, DE 19808

Duke University
Department of Mechanical Engineering
Attn: Dr. Franklin H. Cocks
Durham, NC 27706

EIC Corporation
Attn: Dr. R. David Rauh
55 Chapel Street
Newton, MA 02158

Harvard University
Division of Applied Sciences
Attn: Dr. William Paul
Pierce Hall
Cambridge, MA 02138

Lawrence Berkeley Laboratories
University of California
Attn: Dr. Nabil Amer
Berkeley, CA 94720

Lockheed Missiles & Space Co., Inc.
Research & Development Division
Attn: Art Jonath
3251 Hanover Street
Palo Alto, CA 94304

Massachusetts Institute of Technology
The Energy Laboratory
Attn: Dr. David Adler
Cambridge, MA 02139

Mobil Tyco
Attn: M. Cretella
16 Hickory Drive
Waltham, MA 02154

Nval Research Laboratory
X-Ray Optics Branch
Attn: D.A. Papaconstantopoulos
Washington, DC 20375

Naval Research Laboratory
Semiconductors Branch
Attn: C. Taylor
Washington, D.C. 20375

Naval Weapons Center
Michelson Laboratory
Attn: Dr. T.M. Donovan
China Lake, CA 93555

Pennsylvania State University
Attn: Dr. R.F. Messier
265 Materials Research Laboratory
University Park, PA 16802

RCA Corporation
Attn: Dr. David E. Carlson
P.O. Box 432
Princeton, NJ 08540

Xerox Corporation
Attn: R.A. Street
3333 Coyote Hill Road
Palo Alto, CA 94304

Jet Propulsion Laboratory
PV Data Center
Attn: Leau Ann Burrus
MS 50241
4800 Oak Grove Drive
Pasadena, CA 91103