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PHOTOVOLTAIC MECHANISMS IN
POLYCRYSTALLINE THIN FILM
SOLAR CELLS

Quarterly Technical Progress Report No. 4

July 1, 1979 - September 30, 1979

Solarex Corporation
1335 Piccard Drive
Rockville, Maryland 20850

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REP

ABSTRACT

A more detailed model of the "vertical" junction effect was generated which investigates both the increase in light generated current due to enhanced collection at the grain boundary and the increase in dark current due to the increased junction area. Results show that there is an overall increase in the cell's maximum power; however, the increase in power is negligible for grain widths exceeding a few tenths of a millimeter. Solar cells were fabricated on a longitudinal section of cast polysilicon which was analyzed crystallographically by means of x-ray diffraction patterns. Special crystallographic orientation relationships are identified for the relative orientations of adjacent grains and for the alignment of their boundary interfaces along certain planar segments. The dark I-V characteristics of the polysilicon cells were dominated by recombination within the space-charge region. Scanning photoresponse patterns are matched with the microstructural information to show, in the absence of any detectable impurity effects, that an insignificant or reduced photoresponse measurement is associated with certain boundaries depending on their structural character. The special orientations of grains are indicated on the basis of a model example to be derived from single or multiple twinning relationships on $\{111\}$ systems.

DESCRIPTION OF PROJECT

This study is designed to increase the understanding of the mechanisms in thin film polycrystalline silicon solar cells that limit the photovoltaic conversion efficiency under solar illumination conditions. Theoretical models will be generated to relate the photovoltaic conversion efficiency to the chemical, physical, and electrical characteristics of polycrystalline thin film solar cells; and measurement techniques will be developed to test and update the proposed models. Finally, theoretical and experimental investigations of grain boundary effects will be conducted.

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I. INTRODUCTION

Considerable progress has been made during the past year in investigating the effects of grains and grain boundaries on the photovoltaic response and the task of characterizing the loss mechanisms in polysilicon solar cells. This report concentrates specifically on the relationship between the structural characteristics of the polysilicon material and the electrical characteristics of solar cells fabricated on the polysilicon material. In order to investigate the specific effect of individual grains and grain boundaries on the photovoltaic properties of the cell, the crystallographic orientation relationships of several grains and the positions of their boundary interfaces within the microstructure of a cast polysilicon section were determined and then matched with scanning photoresponse measurements obtained for cells fabricated within these same regions of the polysilicon section.

Section II summarizes the theoretical modeling work done on the "vertical" junction effect. - Section III details the development of measurement techniques and the structural and electrical measurements made on the cast polysilicon section. Finally, Section IV summarizes the results of the past year and the major effects which limit efficiency in polysilicon solar cells.

II. THEORETICAL MODELING

The "vertical" junction effect in polysilicon solar cells is being investigated using a two-dimensional model. "Vertical" junctions, due to the diffusion of dopant along grain boundaries, show an increased photoresponse as compared to adjacent grains. Previous analysis of this effect examined only the increase in short-circuit current as a function of grain radius (cylindrical grain model)¹. This analysis investigates the increase in both the light and dark generated current as a function of grain size due to the "vertical" junction. The results are used to estimate the change in the output power of the cell as a function of wavelength and grain size.

The model shown in Figure 1A can be divided into two basic regions: one where the generated carriers are collected by the surface planar junction and the other where carriers are collected by the vertical junction along the grain boundary. These two regions can further be subdivided into five sub-regions for the convenience of analysis as shown in Figure 1B. Sub-regions I, II, and III generate carriers which are collected by the vertical junction and sub-regions IV and V generate carriers which are collected by the surface junction. The grain width is W and the vertical penetration depth of the junction is Y_J .

Figure 1A. Vertical Junctions Along Grain Boundaries

Figure 1B. Subdivision of Grain for Analysis

The contribution of each sub-region to the overall short-circuit current can be calculated with the following expression:

$$(1) \quad \Delta I_L^{(i)} = (z) \iint g(\alpha, y) e^{-x/L} dx dy$$

where

$$(2) \quad g(\alpha, y) = \phi \alpha e^{-\alpha y} = \text{carrier generation rate}$$

α = absorption coefficient

ϕ = incident photon flux (photons/area/time)

L = minority carrier diffusion length

$e^{-x/L}$ = fraction of carriers collected at junction

In general, x is written in terms of y and Y_j depending on the particular sub-region (Figure 1B) when performing the integration for I_{sc} . The total short-circuit current is given by the sum of the contributions from the five sub-regions:

$$(3) \quad I_L = \sum_{i=1}^5 \Delta I_L^{(i)}$$

The fractional increase in short-circuit current over a planar junction is:

$$(4) \quad \frac{\Delta I_L}{I_L^P} = \frac{\sum_{i=1}^5 I_L^{(i)} - I_L^P}{I_L^P}$$

where I_L^P is the short-circuit current from a planar junction (i.e. no vertical junction).

Because of the junction penetration along the grain boundary into the bulk, there is additional collection of thermally generated carriers (saturation current). The thermal generation rate, G , is a function of temperature and the silicon energy gap. The contribution of each sub-region to the overall saturation current can be calculated using equation (1) with the substitution of G for $g(\alpha, y)$. The total saturation current is then found from the sum of the contributions from the five sub-regions:

$$(5) \quad I_S = \sum_{i=1}^5 I_S^{(i)}$$

The fractional increase in saturation current over a planar junction is:

$$(6) \quad \frac{\Delta I_S}{I_S^P} = \frac{\sum_{i=1}^5 I_S^{(i)} - I_S^P}{I_S^P}$$

where I_S^P is the saturation current from a planar junction (i.e. no vertical junction).

Using a minority carrier diffusion length of 50 μm , Figure 2 shows a plot of $\Delta I/I$ versus grain width, W , for boundary junction penetration depths of $Y_J = 10 \mu\text{m}$ (Figure 2A)

Figure 2A

Figure 2B

Figure 2. FRACTIONAL INCREASE IN LIGHT AND DARK CURRENT VERSUS GRAIN SIZE

and $Y_J = 50 \mu\text{m}$ (Figure 2B) where $\Delta I_L^P / I_L^P$ is calculated for $\lambda = 800 \text{ nm}$ and 1100 nm (solid lines) and $\Delta I_S^P / I_S^P$ is denoted by dashed lines. For $Y_J = 10 \mu\text{m}$, the fractional increase in saturation current exceeds the fractional increase in light current for all wavelengths, and the fractional increase in both the light and dark generated current is less than 1 percent for grain widths exceeding 0.7 mm . For $Y_J = 50 \mu\text{m}$, $\Delta I_L^P / I_L^P$ exceeds $\Delta I_S^P / I_S^P$ only at a wavelength of 1100 nm , however, both increases are less than 1 percent for grain widths exceeding 6 mm . Thus, even for large junction penetration depths ($50 \mu\text{m}$) the fractional increase in saturation current, which decreases V_{OC} , is generally greater than the fractional increase in light generated current, which increases cell efficiency. The overall effect on the cells' maximum power is calculated below.

The increase in short-circuit current, which increases the efficiency, is accompanied by an increase in the saturation current which lowers the open-circuit voltage and decreases the efficiency. The overall fractional change in maximum power due to both effects can be calculated as follows:

$$(7) \quad P_M = (F.F.) (I_L) (V_{OC})$$

$$(8) \quad V_{OC} \text{ (mV)} \approx 25.9 \ln (I_L / I_S) \text{ at } T = 25^\circ\text{C}$$

The increase in power is:

$$(9) \quad P_M + \Delta P = (F.F.) (25.9) (I_L + \Delta I_L) \ln \left[\frac{I_L + \Delta I_L}{I_S + \Delta I_S} \right]$$

Solving the above equations for the fractional increase in maximum power yields:

$$(10) \quad \frac{\Delta P}{P_M} = \frac{\Delta I_L}{I_L} + \left[\frac{25.9 (1 + \Delta I_L/I_L)}{V_{oc}} \right] \ln \left[\frac{1 + \Delta I_L/I_L}{1 + \Delta I_S/I_S} \right]$$

The fractional change in maximum power is a function of W , Y_J , α , L and V_{oc} .

Using equation (10), there will be a fractional increase in maximum power ($\Delta P/P_M \geq 0$) if:

$$(11) \quad \frac{(V_{oc}) (\Delta I_L/I_L)}{(25.9) (1 + \Delta I_L/I_L)} \geq -\ln \left[\frac{1 + \Delta I_L/I_L}{1 + \Delta I_S/I_S} \right]$$

The ratio $(V_{oc}/25.9)$ is relatively insensitive to V_{oc} for V_{oc} in the range of 500 - 600 mV so a value of $V_{oc}/25.9 = 22$ was used for evaluation (corresponding to $V_{oc} = 570$ mV).

Since equation (11) is transcendental, a set of solutions is found by plotting both the left hand side and the right hand side of equation (11) versus $\Delta I_L/I_L$ for various values of $\Delta I_S/I_S$. Such a graph is shown in

Figure 3 where the L.H.S. of eq. (11), which depends only on $\Delta I_L/I_L$, is denoted by a dashed line and the R.H.S. of eq. (11), which depends on both $\Delta I_L/I_L$ and $\Delta I_S/I_S$, is denoted by solid lines. Thus, $\Delta P/P_M \geq 0$ for all points lying on the dashed line which are greater than points on the solid lines. Figure 3 shows only the relationship between $\Delta I_S/I_S$, $\Delta I_L/I_L$ and $\Delta P/P_M$ and does not explicitly contain any information about grain size, W , or vertical junction penetration depth, Y_J . For example, using Figure 3, if $\Delta I_S/I_S = 0.5$ (upper right hand corner of Figure 3), then $\Delta P/P_M \geq 0$ for all values of $\Delta I_L/I_L \geq 0.018$. Thus, even a large fractional increase in the dark current is offset by a small increase in the light generated current.

The fractional increase in maximum power summed over the AM0 spectrum was calculated by partitioning the solar spectrum (Thekaekara) into eight components, calculating $\Delta I_L/I_L$ for each component and summing, then using equation (10). This calculation was done for two cases using $L = 50 \mu\text{m}$: (1) $Y_J = 10 \mu\text{m}$, $W = 0.1 \text{ mm}$ and (2) $Y_J = 50 \mu\text{m}$, $W = 0.1 \text{ mm}$. The results are summarized in Table 1.

Figure 3. Condition for $\Delta P / P_M \geq 0$

Table 1

Fractional Increase in Light Current, Dark Current
and Maximum Power for AM0 Illumination ($L = 50 \text{ } \mu\text{m}$, $W = 0.1 \text{ mm}$)

$Y_J \text{ (}\mu\text{m)}$	$\Delta I_S / I_S$	$\Delta I_L / I_L$ (TOTAL)	$\Delta P / P_M$
10	.069	.018	.016
50	.45	.098	.084

For the two cases shown in Table 1, which are for small grain sizes, there is a noticeable fractional increase in maximum power only for $Y_J = 50 \text{ } \mu\text{m}$. As the grain size increases by an order of magnitude (i.e. 1 mm) the fractional increase in power will decrease by almost an order of magnitude making it much less than 1 percent. The fractional increase in maximum power is greater than zero for all cases considered; however, it is negligible for grain sizes exceeding a few tenths of a millimeter. Hence, the "vertical" junction effect is most beneficial for small grain size material.

III. MEASUREMENTS

A. Development of Measurement Techniques

Deep Level Transient Spectroscopy (H. C. Lin and C. D. Wang)

The calibration of the DLTS system has been completed by measuring the thermal emission rate of the midgap in a gold doped p^+n diode. The data indicates good agreement with the value published by NBS.

Conventional DLTS techniques employ (a) a lock-in amplifier or (b) the double-boxcar method. The original measurement effort utilized the lock-in amplifier technique. However, choosing the phase between the capacitance transient signal and the reference signal is very critical with this method. In order to remove this difficulty, a CMOS switch was used to suppress all but the exponential part of the transient signal so that it was more suitable for analyzing. After studying the mechanism of the lock-in amplifier in detail, another method was developed to filter out the noise and to improve the signal-to-noise ratio of the detected thermal recovery signal of the junction capacitance after pulsing, i.e., the exponential signal.

The measurement of trap levels as a function of distance from a grain boundary using DLTS is planned. The method will utilize a point contact Schottky diode which is moved along the surface of the grain towards the grain

boundary to measure the capacitance transient effect. However, when such a small point contact is used, the signal is small and the signal-to-noise ratio suffers. Therefore, the signal from the capacitance meter will first be correlated to improve the signal-to-noise ratio so that the signal can be more accurately measured.

Optical Scanning System

The fine light spot scanning system is fully operational. The circuitry needed to interface the scanning tables and measurement apparatus with a PDP 11/03 microcomputer is completed and the software needed to control the tables, acquire and output the data to the x-y recorder was developed and implemented. Figure 4 shows a schematic of the system with all the components identified.

Monochromatic light incident on the vertical illuminator of the microscope is focused onto the solar cell which is mounted on a brass block fixed to the precision x-y positioning tables. The short-circuit current is measured with a picoammeter. The microscope and positioning tables are mounted inside a light-proof box.

The optical scanning of the solar cell is controlled via the microcomputer. The microcomputer digitally steps the x-y tables (the size of the scanned area, x and y step

Figure 4. Optical Scanning System Schematic

sizes, and starting location are inputs to the program), reads the short-circuit current at each position (A/D conversion), and outputs I_{sc} versus position to the x-y recorder (D/A conversion). Currently the spot size has a 60 μm diameter and work is being done to reduce it to 5 μm . Additionally, software is being developed to allow an on-line analysis of the spatial dependence of I_{sc} at different wavelengths. Optical scanning results are presented in the following sections.

B. Structural Studies
(R. W. Armstrong)

In order to investigate the specific effect of individual grains and grain boundaries on the photovoltaic properties of a polysilicon solar cell, it was planned to determine the crystallographic orientation relationships of several grains and the positions of their boundary interfaces within the microstructure of a section of a cast polysilicon ingot and, then, to match this crystallographic information with electrical measurements (specifically scanning photoresponse patterns) obtained for cells fabricated from different regions selected within the known microstructure of the sectioned ingot³. A longitudinal slice cut vertically through the cast polysilicon ingot which was chosen is shown in Figure 5 together with a sketch of the particular grains to be studied. Previously reported structural characterization of grains 1 and 2 will be repeated for completeness¹.

Figure 5. Optical Micrograph and Sketch of the Microstructure Within a Longitudinal Section of a Polysilicon Casting

In the longitudinal section in Figure 5, a main portion of the area is shown to be taken-up by a single grain. This large grain is designated as grain 1 in the sketch. Grain 1 has enveloped completely a second grain, designated as grain 2, which originated at the base of the ingot. The envelopment of grain 2 by grain 1 was confirmed by serial sectioning of the casting.

The boundary between grains 1 and 2 is indicated to have a planar morphology at two positions along its length corresponding to the linear traces which are observed at the upper left side and at the right sloping top of the mutual interface between the grains. Grains 3 and 5 are also marked in Figure 5. Near to the top of the casting, the roughly vertical boundary between grains 1 and 3 was observed to take on a wavy appearance. This type of boundary morphology has been categorized as a "sinuous" boundary because of its pronounced meandering nature⁴. Such boundaries are found to be particularly susceptible to localized chemical attack, say, by NaOH etching. "Sinuous" boundaries have exhibited an enhanced photo-response due to dopant penetration into the boundary^{1,5}. As indicated in the sketch in Figure 5, lamellar twins on {111} systems were observed to be present in each of the grains chosen to be studied.

The orientations of individual grains were determined first by x-ray diffraction employing Laue back-reflection photographs. By comparison of their orientations, the grains were found to exhibit special orientation relationships. The relative orientations of grains 1 and 2 are shown superposed in a stereographic projection in Figure 6. The final solidification direction of the casting is the top most direction along the vertical diameter of the basic circle in the Figure.

Grains 1 and 2 are shown in the second quadrant of Figure 6 to have a common $\langle 101 \rangle$ which is indicated as the $[10\bar{1}]_1$ for grain 1 by its subscript and by the particular $[\bar{1}0\bar{1}]_2$ indices chosen for grain 2. Other particular directions, each marked with its respective subscript for either grain 1 or 2 are shown in the stereographic projection. The misorientation of grains 1 and 2 is accounted for in Figure 6 by a rotation of approximately 35° around the common $\langle 101 \rangle$, say, between $[0\bar{1}0]_1$ and $[001]_2$, and this very nearly produces a coincidence between the $[111]_1$ and $[\bar{1}10]_2$ in the mutual $\{101\}$ traced by the coincident arcs of great circles containing these four directions.

The relative orientations of grains 1 and 3 are shown in a stereographic projection in Figure 7. These grains have a nearly coincident $\langle 112 \rangle$ rotation axis with the

Figure 6. Orientations of Grains 1 and 2 in Cast Silicon

Figure 7. Orientation Relationship for Grains 1 and 3 of 90° Rotation About Nearly Common $\langle 112 \rangle$ Axes

$[\bar{1}\bar{1}2]_1$ shown to be at about the same position as the $[\bar{1}\bar{1}2]_3$. A rotation of approximately 90° about the common $\langle 112 \rangle$ would bring the two crystal orientations into register, say, by matching the $[001]_1$ and $[001]_3$ as well as by matching the $[0\bar{1}0]_3$ and $[100]_1$.

Figure 8 shows the relative orientations of grains 3 and 5. In this case, though the grain appearances in Figure 5 give no obvious indication of any special relationship between themselves through the geometry of their interface morphology, they are found crystallographically to be in a twin orientation relationship. This follows because the $[111]_3$ is coincident with the $[111]_5$ and the grain orientations are related by a 180° rotation about the coincident $[111]$. The twin relationship is able to be described equally well in Figure 8 by a rotation of 70.5° about the coincident $[\bar{1}01]$ for both subgrains which is shown very near to the center of the stereographic projection.

The observation of special orientation relationships between the three pairs of grains which have been described, including the $\{111\}$ twinning relationship between grains 3 and 5, is in agreement with previous pioneering results reported for the special orientations of grains as a

Figure 8. (111) Twin Orientation Relationship of Grains 3 and 5

normal occurrence within the cast microstructure of germanium ingots⁶. When vertically solidified, the orientations of grains within germanium ingots were found to be related through multiple stages of twinning as if the grain structure came from a single nucleus. Previous results were reported some time ago, also, for the now well-known occurrence of only $\{111\}$ twinning being produced in silicon across the easily recognized coherent interfaces of twin boundaries⁷.

In Figure 9 is shown a model of the orientation relationship measured in the current investigation between grains 1 and 2. The results in the Figure are obtained if both grains are in a $\{111\}$ twin geometry relative to a third grain, thus giving what is termed a second order twinning relationship. The relative twinning geometry is indicated in the inset diagram. The original (third grain) crystal orientation was chosen as a $[111]$ standard projection which is represented by a small black triangle at the center of the projection encircled by three additional small black triangles representing the three remaining $\langle 111 \rangle$ symmetrically placed about the central one. The twinning operation for the orientation of grain 1 is represented by the large black triangles, and other accompanying black symmetry figures for $\langle 100 \rangle$ and $\langle 110 \rangle$, all rotated 180° about the central $[111]$. The separately

Figure 9. Second Order Orientation Relationship of Grains 1 and 2 in $\{111\}$ Twin Geometry Relative to a Third Grain

twinned orientation of grain 2 is obtained in turn by a 180° twinning rotation about the $[\bar{1}11]$ of the original crystal now represented by the open triangle at $[\bar{1}11]_2$ and by the accompanying open symbols shown for the various additional directions. The resultant relationship between the hypothetical grains 1 and 2 is then found to be given by their having a common $[01\bar{1}]$ axis and a rotation of 38.9° about this axis. This seems to be in reasonable agreement with the measured result which has been described for Figure 6. The difference between the hypothetical and measured misorientations might easily be taken up by the presence of dislocations in the boundaries between the grains.

Special orientations of grains within silicon material have been determined also for the method of forming ribbon material by the Edge-defined Film-fed Growth (EFG) process, for example, as shown by the description which has been given of 32° grain boundaries formed with a $[\bar{1}10]$ rotation axis aligned along the material growth direction⁸. Directional solidification of solar grade silicon material in a carbon crucible is reported to produce grains with preferred $\langle 110 \rangle$ orientations although some have preferred axes along $\langle 111 \rangle$ as well⁹. Most recently, particular dislocation structures have been described by the method of Transmission Electron Microscopy (TEM) for a number of special grain boundaries in sintered silicon bicrystals¹⁰.

In a number of instances, the boundaries between grains in polysilicon are observed to take-up a crystallographic appearance along certain segments of the interfaces. This has been described earlier in this report for a portion of the upper left and right sloping top edges of grain 2 in the sketch of Figure 5. The planar appearance of the boundaries was observed to carry through the thickness of serial sections cut through the casting and, from such observations, the positions of the boundaries have been roughly determined thus far. The orientations of the two boundary segments described for grains 1 and 2 are able to be described with respect to Figure 6. The reasonably straight boundary segment along the upper left edge of grain 2 was measured to run close to the dashed great circular arc drawn for the $(\bar{1}\bar{1}2)_1$. This boundary orientation, though only approximately planar, showed a changing orientation for different serial sections through the casting. The boundary alignment for the right sloping top segment of grain 2 was found to run very close to the essentially coincident $(111)_1$ and $(\bar{1}10)_2$ orientations of the grains.

Finally, along the vertical solidification axis of the casting, the boundary between grains 1 and 3 takes on an alignment near to the $(\bar{1}\bar{1}0)_1$ and $(111)_3$ being coincident within the grains. The grains each have an approximate alignment of $\langle 112 \rangle$ axes both in these coincident planes and

in the plane of the section of the casting. As the boundary progresses along the vertical growth direction for the grains, the boundary takes on a "sinuous" appearance. Scanning photoresponse measurements in this case have revealed an increased photoresponse in the regions of such boundaries. The positions of such boundaries within the casting leads to the conclusion that they form so as to allow excess solute to be incorporated into the material during the solidification process. Further structural characterization is discussed in the next section, together with the electrical properties of the solar cells which were fabricated within the known microstructure of the sectioned ingot.

C. Oriented Polysilicon Cells

Solar cells were fabricated on an adjacent serial section of the longitudinal section shown in Figure 5. Figure 10 is a tracing of the serial section showing the locations of the experimental cells. The dark strip on the cells indicates the main buss bar where electrical contact is made to the front of the cell.

Light and Dark I-V Characteristics

The light and dark I-V characteristics of the cells are summarized in Table 2. To eliminate the effect of series and shunt resistance the dark I-V characteristics

Figure 10. Tracing of the Longitudinally-Cut Cast Polysilicon Section Showing the Locations of the Fabricated Solar Cells

CELL #	AM1 Efficiency	CELL AREA (cm ²)	Grains Included	J _{SC} (mA/cm ²)	V _{OC} (mV)	J _{SCO} (mA/cm ²)	J _{QNO} (mA/cm ²)	n _{sc}	V _E (mV)
1-1	13.0	3.30	1, 2	29.7	580	3.52x10 ⁻⁴	8.81x10 ⁻⁹	2.25	495
1-2	13.1	3.99	1, 2	30.0	577	1.16x10 ⁻³	8.40x10 ⁻⁹	2.58	498
1-3	11.6	1.71	1, 2	28.6	567	1.77x10 ⁻³	7.91x10 ⁻⁹	2.48	532
1-4	13.3	3.04	1, 2	30.5	585	1.61x10 ⁻³	3.11x10 ⁻⁹	2.53	567
2-2	13.8	4.00	1, 3, 5	30.6	582	2.72x10 ⁻⁴	5.89x10 ⁻⁹	2.25	500

Table 2. Light and Dark I-V Characteristics
of Oriented Polysilicon Cells

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were determined by measuring $I_{sc} - V_{oc}$ at voltages above 400 mV (to eliminate series resistance) and subtracting out the shunt resistance contribution from the dark I-V below 400 mV. The dark current was separated into its two components - one originating from recombination in the space-charge region (J_{sc0} , n_{sc}) and the other from recombination in the quasi-neutral regions (J_{QNO} , $n = 1$). The voltage where the current contribution from the two regions are equal is denoted by V_E . The characteristics of the cells are very similar with the exception of cell 1-3 which has a lower efficiency. The lower efficiency is due mostly to the decreased open-circuit voltage which may be due to the larger percentage of front contact shadowing because of the smaller cell size (see Figure 10). The short-circuit current densities are also very similar for two apparent reasons: (1) the grain boundaries have little effect on the total short-circuit current because the grain sizes within the cells are large; and (2) the minority carrier lifetime within each grain is the same or very close (the diffusion length within a grain was determined to be 90 μm from spectral response measurements). Additionally, although there is variation in the components comprising the dark currents of the cells the dark I-V curves are all (except 1-3) very similar around the maximum power and open-circuit voltage regions (this was determined by superimposing the dark I-V curves).

Optical Scanning

In order to determine the effect of the various grains and grain boundaries on the short-circuit current scanning photoresponse "maps" of various regions were made. Figure 11 is an optical photoresponse scan of a 1.0 cm x 1.75 cm area in cell 1-1 at a wavelength of 900 nm. At 800 nm the extinction length, α^{-1} , is 10 μ which is much greater than the junction depth of approximately 0.4 μ m. Grains 1 and 2 are labelled in the Figure. The location (direction) of the main buss bar is shown and the scan lines are perpendicular to the buss bar (i.e. parallel with the arrow). The location of the cell within the longitudinal section is shown in Figure 10.

The boundary between grains 1 and 2 can be clearly seen. Additionally, there is a crack in the cell that runs parallel to the vertical axis in the left hand side of the figure which shows a decrease in photoresponse. The current response within each grain is very uniform (the random variations in current within the grains are due to material on the surface such as bits of metallization). The uniformity in photoresponse within the grains

Main Buss Bar

Expanded area shown in Figure 12

Figure 11. I_{sc} Versus Position of an Area in Cell 1-1
Showing Grains 1 and 2 ($\lambda = 800$ nm)

indicates that the minority carrier diffusion length is nearly constant throughout the cell with the exception of the small regions near electrically active grain boundaries. Thus the short-circuit current response can be modeled using a constant diffusion length within the grain and an effective minority carrier recombination velocity at electrically active grain boundaries and previous modeling results are applicable^{1,2}.

The pattern shows a reduced photoresponse at all points along the boundary interface except for an almost negligible effect at the upper region near to the top of grain 2 (to the right of the crack in the lower left hand corner of Figure 11) where the boundary interface takes up an alignment for the near coincidence of the $(111)_1$ and $(\bar{1}10)_2$. An enlargement of the photoresponse pattern of this area (the area designated in Figure 11) is shown in Figure 12 and a tracing of the grain boundaries which are seen optically in a microscope in this region is shown in Figure 13. Preliminary x-ray reflection topographs of this region of the juncture of the grains appear to show a locally changed orientation of grain 2 relative to the rest of its volume and this might be related to an absence of dislocations or a changed character for them within this region of the cell¹¹.

There are two further observations to be made. In the upper left hand corner of Figure 12 there is an electrically

Figure 12. Expanded Area Designated in Figure 11

Figure 13. Tracing of Grain Boundaries Seen Optically in the Area Shown in Figure 12

active grain boundary which is not optically visible (Figure 13) and appears to be a subgrain boundary contained in grain 1. Finally, in the lower left hand corner of Figure 12, there is a small included grain (see Figure 13) which exhibits recombination along only part of its boundary. As previously stated above, the change in photoresponse (i.e. no observable recombination) along a particular boundary may be related to an absence of dislocations or a changed character for them within this region.

Figure 14 is an optical photoresponse scan of a 1.0 cm x 1.75 cm area in cell 2-2 at a wavelength of 800 nm. The scanned area contains grains 1, 3, and 5. The main buss bar runs vertically along the left hand side of the pattern (note the reduced response). The location of the cell within this longitudinal section is shown in Figure 10. Figure 15 shows an enlargement of the area designated in Figure 14 and Figure 16 is a tracing of the grain boundaries seen optically in this area using a microscope.

The boundary between grains 1 and 3 and between grains 1 and 5 is clearly visible both electrically (Figure 14 and 15) and optically (Figure 16). No change in photoresponse is observed in crossing the boundary between grains 3 and 5. The approximately vertical boundary segment between grains 3 and 5 in the sketch

Figure 14. I_{SC} Versus Position of an Area in Cell 2-2
 Showing Grains 1, 3, and 5 ($\lambda = 800 \text{ nm}$)

Figure 15. Expanded Area Shown
in Figure 14

Figure 16. Tracing of Grain Boundaries Seen Optically
in the Area Shown in Figure 15.

in Figure 5, though not very planar, runs fairly close to the coherent (111) interface for the twinned grains as can be recognized in the stereographic projection in Figure 8. The absence of electrical response at this boundary is consistent with the previous observations that twin boundaries exhibit no electrical activity during optical photoresponse scanning.

A large disruption of the photoresponse is observed to occur within grain 1 to the left of the triple junction of it and grains 3 and 5. A careful examination of the optical micrograph in Figure 5 shows that several sub-grain boundaries are running nearly vertically through grain 1 into this region. The pronounced decrease in photoresponse in this case of a small misorientation of a region within a grain, though totally accountable in terms of dislocations, is interesting to compare with an absence of any change in photoresponse at the appreciable misorientation which occurs without the need for dislocations being present at the boundary between grains 3 and 5. More detailed measurements of the misorientations of particular grains and of the crystallographic character of the boundaries within the microstructure of grains in polysilicon should allow the specific dislocation content of boundaries to be determined so as to match their photoresponse characteristics with the electrical and optical properties predicted for individual dislocations as one-dimensional conductors¹².

IV. SUMMARY OF ACCOMPLISHMENTS/RESULTS

The next section summarizes the results of the previous four quarters of study on "Photovoltaic Mechanisms in Polycrystalline Thin Film Solar Cells". The summary is presented according to the three tasks: (1) Theoretical Modeling, (2) Development of Measurement Techniques, and (3) Theoretical and Experimental Investigations of Grain Boundary Effects. Finally, a summary of the major effects which limit efficiency in polysilicon solar cells is given.

(1) Theoretical Modeling

Two theoretical models were generated to investigate various properties of polysilicon solar cells: the cylindrical grain model and the "vertical" junction model.

Cylindrical Grain Model - The effect of grain size on short-circuit current density was investigated by approximating individual silicon grains as right circular cylinders and solving the diffusion equation within the base region. Two effects were investigated: the degradation in J_{SC} due to grain boundary recombination, and the effect of enhanced current collection at grain boundaries due to dopant penetration into the boundary creating a "vertical" junction. The results show that for grain radii exceeding a few tenths of a millimeter - which is the case for the polysilicon investigated in this program - the minority

carrier lifetime in a grain essentially determines the short-circuit photoresponse and neither recombination nor collection of minority carriers at the grain boundary will have a substantial effect.

"Vertical" Junction Model - A more detailed model of the "vertical" junction effect was generated which investigates both the increase in light generated current due to enhanced collection at the boundary and the increase in the dark current due to the increased junction area. Results show that although the fractional increase in dark current, which decreases V_{oc} and lowers cell efficiency, is generally greater than the fractional increase in light generated current, the fractional increase in cell maximum power increases due to the logarithmic dependence of V_{oc} on the dark current. However, the fractional increase in power is negligible for grain widths exceeding a few tenths of a millimeter.

(2) Development of Measurement Techniques

Optical Scanning System - The fine light spot scanning system is fully operational. The optical scanning of polysilicon cells is controlled with a PDP 11/03 micro-computer which allows for an on-line analysis of the spatial dependence of I_{sc} in the cell. Additionally, the use of a monochromator as an illumination source allows the evaluation of the wavelength dependence of I_{sc} (which can

be used to determine the minority carrier diffusion length). Results are discussed in sub-section 3.

Deep Level Transient Spectroscopy (DLTS) - The DLTS system is fully operational and the calibration of the system shows good agreement with a standard supplied by NBS. The DLTS technique will be used to determine defect concentrations, energy levels, capture cross-sections and emission rates of recombination centers within the band gap. Since theoretical modeling has shown that the short-circuit current is most sensitive to the minority carrier lifetime within the grain, for the polysilicon studied here, DLTS measurements are essential to determine the levels within the energy gap which are most detrimental to the lifetime.

(3) Theoretical and Experimental Investigations of Grain Boundary Effects

The emphasis of the latter half of the study has been the investigation of the relationship between the structural characteristics of the polysilicon and the electrical characteristics of the solar cell by: (1) measuring the spatial dependence of the dark I-V characteristics by fabricating small diodes on a polysilicon wafer; (2) optically scanning solar cells which were fabricated on a longitudinal section of polysilicon which has been analyzed crystallographically (x-ray

diffraction, SEM, electron channelling).

Spatial Dependence of I-V Characteristics - The spatial dependence of the dark I-V characteristics within a polysilicon wafer was investigated by fabricating small diodes on the wafer and then measuring their dark I-V characteristics. Illuminated I-V characteristics were generated by assuming a short-circuit current density and then using the shifting approximation. The dark current of the diodes was dominated by recombination within the space-charge region well past the one-sun maximum power point and although the dark I-V characteristics of the diodes varied considerably, the illuminated characteristics did not vary greatly. Measurements made on diodes containing grain boundaries and on diodes within boundary free regions showed little difference in their dark I-V characteristics. These measurements, together with the fact that the grain sizes are large, lead to the conclusion that the space-charge dominated dark current originates within the grains. Finally, the degradation of cell performance due to areal inhomogeneity was not observed for these diodes.

Oriented Polysilicon Cells - Solar cells were fabricated on a longitudinal section of a cast polysilicon ingot which was analyzed crystallographically. The relative orientations of adjacent crystal grains and the

nature of the boundaries between the grains were studied by x-ray diffraction, x-ray topography, electron channelling, optical microscopy, and scanning electron microscopy methods. Macroscopic cell characteristics (light and dark I-V characteristics) were measured; grain and grain boundary effects were investigated by optical photore-sponse scanning.

By means of x-ray diffraction and electron channelling patterns obtained from cast polysilicon material, special crystallographic orientation relationships are identified for the relative orientations of adjacent grains and for the alignment of their boundary interfaces along certain planar segments. Scanning photoresponse patterns are matched with this microstructural information to show, in the absence of any detectable impurity effects, that an insignificant or reduced photoresponse measurement is associated with certain boundaries depending on their structural character. The origin of "sinuous" grain boundaries, which show an increased photoresponse due to the diffusion of dopant into the boundary, is attributed to the incorporation of substantial impurities, even as micro-precipitates, at boundaries during the initial material solidification process.

The special orientations of grains are indicated on the basis of a model example to be derived from single or multiple twinning relationships on {111} systems. The

dislocation structure associated with the single or multiple incoherent twinning relationship and associated with the difference between the model orientation relationships as compared with the measured ones is proposed to be responsible for the photoresponse characteristics of particular boundaries, either directly through their own structural effect or through their cooperative effect with impurities, say, at "sinuous" boundaries.

Dark I-V characteristics of the cells were again dominated by recombination within the space-charge region. The short-circuit current density was very uniform between the cells for two apparent reasons: (1) the grain boundaries had little effect on the total short-circuit current because the grain sizes within the cells are large, and (2) the minority carrier lifetimes within the individual grains are very uniform. Optical photoresponse scanning showed that the current response within each grain is very uniform except in small regions around electrically active grain boundaries. These observations confirm the hypothesis that the lifetime is nearly constant throughout the grains and that the short-circuit current response can be modeled using a constant diffusion length within the grain and an effective recombination velocity at the grain boundary.

Major Effects Which Limit Efficiency in Polysilicon Solar Cells

The major effects which limit efficiency in polysilicon solar cells are summarized below¹:

Short Circuit Current - For grain radii exceeding a few tenths of a millimeter the short-circuit current is determined by the minority carrier diffusion length within the grain. Recombination at grain boundaries has a large effect only on small grain size material. Additionally, increases in short-circuit current occur at some grain boundaries due to dopant diffusion into the boundary and theoretical modeling indicates that the increase in dark current due to the increased junction area is not enough to decrease the overall efficiency of the cell.

Fill Factor and V_{oc} - The domination of the dark current by the space-charge component in the grains decreases the fill factor and the open circuit voltage.

Ohmic Shunts - Ohmic shunts are believed to be caused by dopant penetration along grain boundaries to the back contact of the solar cell. This effect is most often observed in cells containing "sinuous" grain boundaries.

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