11.1999

DSE-4106-T4

DEVELOPMENT OF RECRYSTALLIZATION AND THIN-FILM
SOLAR CELL PROCESSES

Final Report for October 1, 1977–September 30, 1978

By
Stanley J. Solomon

May 1979

Work Performed Under Contract No. EG-77-C-01-4106

Spire Corporation
Bedford, Massachusetts

U.S. Department of Energy

Solar Energy

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

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."

This report has been reproduced directly from the best available copy.

Available from the National Technical Information Service, U. S. Department of Commerce, Springfield, Virginia 22161.

Price: Paper Copy \$11.00
Microfiche \$3.50

DEVELOPMENT OF RECRYSTALLIZATION
AND THIN-FILM SOLAR CELL PROCESSES

FINAL REPORT
FOR PERIOD OCTOBER 1, 1977 TO SEPTEMBER 30, 1978

STANLEY J. SOLOMON

MAY 1979

SPIRE CORPORATION
PATRIOTS PARK
BEDFORD, MA 01730

Prepared by: *Stan J. Solomon*
Principal Investigator

Approved by: *Allen R. Kishpatenk*
Program Manager

PREPARED FOR THE
U.S. DEPARTMENT OF ENERGY
SOLAR ENERGY
UNDER CONTRACT EG-77-C-01-4106

This document is
PUBLICLY RELEASABLE
Bang Steel
Authorizing Official
Date: 7-19-07

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

mg

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.

TABLE OF CONTENTS

<u>Section</u>	<u>Page</u>
ABSTRACT	viii
1 INTRODUCTION	1-1
1.1 Contract Statement of Work	1-1
1.2 General Approach	1-2
1.2.1 Silicon Program	1-2
1.2.2 III-V Program	1-4
1.3 Program Accomplishments	1-5
1.4 Report Outline	1-6
2 SILICON RECRYSTALLIZATION	2-1
2.1 Background Considerations	2-1
2.2 Directed Energy Cell Fabrication Sequence	2-1
2.3 Thin-Film Cell Consideration	2-3
2.4 Depth-Localized Heating	2-4
2.4.1 Thermal Analysis	2-5
2.4.1.1 Electron Energy Deposition in Solids	2-5
2.4.1.2 Analytic Development of Fast Pulse Heating	2-6
2.4.1.3 Computer Modeling of Fast-Pulse Heating	2-14
2.4.1.4 Scanned Beam Thermal Analysis	2-18
2.4.2 Equipment Considerations	2-26
2.5 Experimental Results	2-30
2.5.1 Film Deposition	2-31
2.5.2 First-Step Recrystallization Experiments	2-36
2.5.3 Second-Step Recrystallization Experiments	2-69
3 PROCESSING OF III-V MATERIALS	3-1
3.1 Program Objectives	3-1
3.2 GaAs Studies	3-1
3.2.1 Ion Implantation	3-2
3.2.2 Protective Capping	3-2
3.2.3 Antireflective Coating	3-3

TABLE OF CONTENTS (Concluded)

<u>Section</u>	<u>Page</u>
3.2.4 Pulsed Electron Beam Annealing (PEBA)	3-3
3.2.5 GaAs Solar Cells	3-3
3.2.6 GaAs on Germanium Substrates	3-4
3.2.7 Pulsed Electron Beam Annealing of GaAs	3-4
3.2.8 Surface Modification by High Dose Implants	3-10
 4 CONCLUSIONS	 4-1
4.1 Efforts on Silicon	4-1
4.2 Efforts on III-V Compounds	4-3
 REFERENCES	 R-1
 APPENDIX A Analytic Model for Depth Localized Heating	 A-1
 APPENDIX B Cline and Anthony Heating Analysis	 B-1

LIST OF FIGURES

<u>Figure</u>		<u>Page</u>
1	Directed Energy Approach to Thin-Film Silicon Solar Cell Fabrication	2-2
2	Energy Deposition Profile of 12-keV Electron Beam in Silicon	2-7
3	Energy Deposition Profile of 55-keV Electron Beam in Silicon	2-8
4	Surface Normalized Temperature As a Function of Reduced Depth for $t \gg t_L$	2-11
5	Gaussian and Spencer Electron Energy Deposition Profiles in Aluminum	2-12
6	Fluence Per Degree Increase in Surface Temperature As a Function of Electron Energy	2-13
7	Ratio of Peak Pressure to Peak Temperature As a Function of Electron Energy	2-15
8	VXTEMP Calculation for the Time Dependence of Front Surface Temperature for a 0.3- μm Si Layer on Mo	2-16
9	Temperature Profiles at Various Times for the Calculation in Figure 8	2-17
10	Temperature Parameter, f , as a Function of X/R at $Y/R = 0$ for $RV/D = 1$ at Selected Values of Z/R	2-27
11	Selected Surface ($Z/R=0$) Values of f on the X-Y Half-Plane for $RV/D = 1$	2-28
12	Experiment A-4,1: As-Deposited 0.4- μm -Thick 800°C SiH_2Cl_2 Film on (111) Silicon	2-34
13	Experiment A-4,1: As-Deposited 1.3- μm -Thick 800°C SiH_2Cl_2 Film on (111) Silicon	2-34
14	Experiment A-4,2: As-Deposited 1.0- μm -Thick 790°C SiH_4 Film on (100) Silicon	2-35
15	Experiment A-4,2: As-Deposited 1.0- μm -Thick 790°C SiH_4 Film on (111) Silicon	2-35
16	SPI-PULSE 5000 Pulsed Electron Beam System	2-39

LIST OF FIGURES (Continued)

<u>Figure</u>		<u>Page</u>
17	SPI-PULSE 5000 Four-Position Sample Chamber	2-40
18	Experiment A-4,2: S3T1F4 Film	2-44
19	Experiment A-4,2: S4T2F4 Film	2-44
20	Experiment A-4,3: S1T4F0 Film	2-48
21	Experiment A-4,3: S1T2F2 Film	2-48
22	Experiment A-4,3: S2T4F0 RHEED Pattern	2-49
23	Experiment A-4,3: S1T4F2 RHEED Pattern	2-49
24	Experiment A-4,3: S1T2F0 RHEED Pattern	2-50
25	Experiment A-4,3: S1T2F2 RHEED Pattern	2-50
26	Experiment A-4,4: Surface Morphology Change of an S1T1 Film with Pulsed Beam Fluence	2-53
27	Experiment A-4,4: Surface Morphology Change of an S1T2 Film with Pulsed Beam Fluence	2-54
28	Experiment A-4,4: Surface Morphology Change of an S1T4 Film with Pulsed Beam Fluence	2-55
29	Experiment A-4,4: Detached S1T4F2 Film from "Thread" Area	2-57
30	Experiment A-4,4: RHEED Patterns for S1T1F0 and S1T1F2 Films	2-59
31	Experiment A-4,4: RHEED Patterns for S1T2F0 and S1T2F2 Films	2-60
32	Experiment A-4,4: RHEED Patterns for S1T3F0 and S1T3F2 Films	2-61
33	Experiment A-4,5: S1T1F0 Film	2-63
34	Experiment A-4,5: S1T1F1 Film	2-63
35	Experiment A-4,5: S2T1F0 Film	2-64
36	Experiment A-4,5: S1T1F1 Film	2-64

LIST OF FIGURES (Concluded)

<u>Figure</u>		<u>Page</u>
37	Experiment A-4,5: S1T2F0 Film	2-65
38	Experiment A-4,5: S1T2F1 Film	2-65
39	Experiment A-4,5: S2T2F0 Film	2-67
40	Experiment A-4,5: S2T2F1 Film	2-67
41	Experiment A-4,5: S2T2F1 Film After Six Anodic Oxidation-Strip Cycles	2-68
42	Experiment A-4,5: S1T1F1 RHEED Pattern	2-70
43	Experiment A-4,5: S2T1F0 and S2T1F1 RHEED Patterns	2-71
44	Experiment A-4,5: RHEED Patterns for Anodic Oxidized and Stripped S1T2F1 and S2T2F1 Films	2-72
45	Experiment A-4,6: VXTEMP/ELTRAN Output of Film Temperature As a Function of Time at Various Depths for an F2 Pulse in an S2T2 Film	2-75
46	Experiment A-4,6: VXTEMP/ELTRAN Output of Film Temperature As a Function of Depth at Various Times for an F2 Pulse in an S2T2 Film	2-76
47	Experiment A-4,6: S2T1F3 Film Surface Showing a 0.5-mA Slow-Scan Line	2-78
48	Experiment A-4,6: 1000X Metallographic Section of an S2T1F2 Film Through the Center of a 0.5-mA Slow-Scan Line	2-80
49	Experiment A-4,6: 1000X Metallographic Section of the Region to the Left of That Shown in Figure 48	2-80
50	Experiment A-4,6: RHEED Pattern From a Fast-Scan Region on an S2T1F2 Film That Was Scanned at ~55 mA	2-82
51	I-V Curve for Shallow Implanted GaAs on Ge As a Function of Anodic Oxidation and Stripping	3-6

LIST OF TABLES

<u>Table</u>		<u>Page</u>
1	Fast-Scan Heating Beam Parameters	2-20
2	α -Independent Beam Parameters for Fast-Scan Heating a Silicon Film	2-21
3	α -Dependent Beam Parameters for Fast-Scan Heating a 0.15- μ m Silicon Film	2-22
4	α -Dependent Beam Parameters for Fast-Scan Heating a 30- μ m Silicon Film	2-24
5	Film Deposition Parameter Summary	2-32
6	A-4,1 Experimental Details	2-38
7	A-4,1 Epitaxial Recrystallization Observations	2-41
8	A-4,2 Experimental Details	2-43
9	A-4,3 Experimental Details	2-45
10	A-4,3 RHEED Analysis	2-46
11	A-4,4 Experimental Details	2-51
12	A-4,4 RHEED Analysis	2-52
13	A-4,5 Experimental Details	2-62
14	A-4,5 RHEED Analysis	2-62
15	A-4,6 Experimental Details	2-73
16	Comparative Cell Performance	3-5
17	Summary of PEBA Results - Best Solar Cells	3-8
18	Summary of PEBA Results - Lowest V/I	3-9

ABSTRACT

This final report for Contract EG-77-C-01-4106, "Development of Silicon Recrystallization and Thin-Film Solar Cell Processes", covers the 12-month period, 1 October 1977 through 31 September 1978. The program had two thrusts: (1) based upon electron-beam thermal treatment of deposited silicon films, to increase crystallite sizes to the range thought to be useful for polycrystalline, thin-film cell fabrication; and (2) to explore the feasibility of applying the directed-energy technologies of ion implantation and pulsed electron beam activation, previously developed for silicon cell fabrication, to junction formation in III-V compounds.

The culmination of the recrystallization effort was demonstrating grains broader than the 30- μm film in which they were regrown. This proof of principle was accomplished by means of two-step thermal process that consisted of large-area pulsed electron beam melting followed by small-area heating in a moving DC electron beam. The pulsed beam treatment reduced the three-dimensional disorder of the initial submicrometer crystallite silicon film to one characterized by submicrometer-cross-section, full-film-thickness, columnar crystallites. The swept beam treatment allowed coalescence of these columnar crystallites, through directional freezing, in the melt path of the beam. It is believed that this demonstration is the first evidence of greater-than-film thickness recrystallization of useful thickness silicon films other than by extended heat treatment at greater than 1350°C.

The results of the studies on junction formation in III-V materials, while not so dramatic, have shown that low-energy ion implantation is a potentially viable alternative to liquid or vapor phase epitaxy in the fabrication of GaAs solar cells. Further, the technical feasibility of pulsed electron beam activation of ion implanted junctions in GaAs has been demonstrated. Lastly, the concept of forming front-layer windows of GaP and AlGaAs on GaAs by high-dose ion implantation has been shown to be technically feasible.

SECTION 1

INTRODUCTION

This is the final report on work performed by Spire Corporation under ERDA/DOE Contract EG-77-C-01-4106 from October 1977 through September 1978. This study is an extension of work initiated in February 1976 under NSF Grant AER76-06096. The NSF program addressed two particular tasks:

1. An investigation of the applicability of directed energy techniques to recrystallization of silicon films
2. The development of specialized processing concepts for the fabrication of thin-film silicon solar cells on glass sheets

The overall objective of the NSF program was to identify technologies that could lead to practical thin-film silicon solar cells. While most of the processing sequence elements were established as feasible, the limitation on cell performance was found to be the "quality" of the deposited films. Although recrystallization techniques showed promise, the films that were subsequently processed into cells showed poor performance due to their fine grain structure.

As a consequence, the continuation of this work under ERDA/DOE support emphasized recrystallization. An added subtask was an investigation of the application of the directed energy processing techniques used in silicon cell fabrication to III-V compounds.

1.1 CONTRACT STATEMENT OF WORK

The following summarizes the statement of work addressed under this contract:

1. Analytical and experimental studies necessary to determining the recrystallization parameters for producing large-grain silicon films were to be conducted. The recrystallization approach was to involve two process steps.
2. The specialized silicon cell processing techniques that had been initiated under the NSF program were to be further investigated. These included release of a silicon film from its temporary substrate during electrostatic

bonding, ion implantation of the junction, and pulsed electron beam annealing of the implanted region.

3. Attempts were to be made to fabricate, for feasibility demonstration, thin-film silicon solar cells using the techniques developed in the previous tasks. The goal for these cells was to be a conversion efficiency of at least 10% (AM1).
4. Studies were to be performed on III-V compounds to determine the applicability of ion implantation and pulsed electron beam annealing to these materials as they would be used for thin-film solar cells. The technical feasibility of ion beam epitaxy of thin-film III-V materials was also to be examined.

Roughly 85% of the effort was to be devoted to silicon studies. Of this effort, the predominant activity was to be recrystallization related.

1.2 GENERAL APPROACH

The central theme of this program was the application of directed energy processing to the requirements of solar cell fabrication. The specific techniques that were utilized were ion implantation, pulsed electron beam annealing and pulsed and scanned electron beam heating. Because of differences in the state-of-the-art and in material processing requirements, the silicon effort must be considered separately from the III-V effort.

1.2.1 Silicon Program

As noted earlier, the performance-limiting feature of the developmental cells fabricated under the NSF program was grain size of the silicon films. Because no reported single-step technique has demonstrated a capacity for forming the type of large-grain silicon film that will be required for a cost-effective cell, a two-step thermal process was selected.

The proposed two-step process begins with the deposition of a silicon film onto a temporary substrate. Since the crystallinity of this initial film is not of concern, it may be deposited from any process that is convenient. Low temperature CVD of polysilicon from silane was used here. The choice of deposition technique interacts with the choice of temporary substrate in that the latter must not degrade the transport properties of

the film during deposition. Again for convenience, silicon wafers and silicon wafers covered with a grown oxide were used.

The first-step thermal treatment is intended to convert the as-deposited, randomly oriented, small-grain film into a film characterized by full-film-thickness, small-cross-section, columnar grains. This was to be accomplished by full-surface exposure of the film to a properly tailored pulsed electron beam. The characteristic of this heating procedure is the extremely rapid deposition of a small quantity of energy into a thin layer at the front of the target. (Pulsed laser heating has a similar characteristic.) For a 10- μm film exposed to a 10- μs electron (or phonon) pulse, thermal energy cannot diffuse from its absorption volume during the pulse time. As a consequence, the film's thermal profile is congruent with the absorption profile of the incident electrons (or phonons). Since absorption depth is a function of the energy of the incident electron and heating is a function of the beam current (and film composition), pulsed electron beam heating allows the controlled melting of the film down to a preselected depth. Within the treated area, the temperature gradient, during and shortly after the pulse, is essentially unidirectional, into the substrate. As a consequence, the molten front layer can be expected to resolidify, by directional freezing, as columnar crystallites that were nucleated on sites at the melt depth limit. While this thermal geometry is consistent with the requirements for growth propagation of large grains, the multiplicity of nucleation sites at the melt depth limit would be expected to result in small- rather than large-cross-section columnar grains. Because the energy necessary to melt the film, 0.2-0.3 cal/cm², is small compared to the thermal mass of sensible deposition substrates, the latter remain at essentially room temperature throughout this step of the recrystallization process. The rationale for anticipating this type of recrystallization behavior was the extensive work being done on laser and electron beam annealing of ion implanted regions.

The second step thermal treatment must convert this small-cross-section, columnar grain film into a large-cross-section (100-200 μm) columnar film. Since full-area remelting could, at best, only be expected to replicate the starting film, the second-step heating must be confined, at least instantaneously, to small areas that contain a limited number of columnar crystallites. This can be done with a scanned, continuous electron (or laser) beam. The objective is to establish a local temperature gradient such that the instantaneous molten zone can crystallize on the previously solidified region immediately behind (and, after the first scan, beside) it on the beam path. This type of scanned, continuous electron (or laser) beam melting can, at least in

principle, be operated in two scan-rate modes. A sufficiently fast scan, if it can be realized with the required power density in an appropriate beam spot size, would simulate pulsed-beam heating. This would produce a tilted, unidirectional temperature gradient. As the scan speed is reduced, the resultant temperature gradient becomes more three-dimensional. There is still no definitive argument for predicting which scan-rate mode is likely to produce a larger grain film.

Analytic developments of the heat flow associated with both the first- and second-step thermal treatments were used as a guide for the actual recrystallization experiments. A computer model of the first-step treatment was also used.

Junction formation by ion implantation avoids the grain-boundary effects that are associated with diffused junctions. The applicability of this approach has been widely demonstrated with Wacker "Silso" and similar materials. Similarly, pulsed electron beam annealing for activation of the implanted species was expected to eliminate the grain boundary segregation effects that are associated with conventional furnace annealing. Electrostatic bonding was to be used for sealing the cell's front surface to a protective coverslip. During cooldown from electrostatic bonding, the thermal expansion differential between the glass superstrate and the deposition substrate was expected to cause the film to shear from the deposition substrate. Following this, the cell's back surface field was to be implanted and annealed and the back contact applied.

1.2.2 III-V Program

Because the III-V program was to be concerned with junction formation technology, no loss of generality would result from confining the studies to GaAs and, further, to single crystal GaAs. The intended thrust of this program was threefold:

1. Determine the feasibility of using ion implantation to form very shallow junctions in GaAs for potential use in solar cells. The rationale was that a sufficiently thin (and conductive) emitter layer would obviate the need for the AlGaAs "window" that is normally required for surface recombination velocity control in the thicker emitter layers that can be obtained from LPE structures.

2. Investigate the feasibility of using pulsed electron beam heating for capless annealing of implanted regions. The rationale was, primarily, process economics.
3. Attempt to form AlGaAs and GaAsP emitter windows by high dose implantation of Al and P into GaAs. Beyond the potential scientific importance of this work, the ultimate rationale was again process economics.

1.3 PROGRAM ACCOMPLISHMENTS

The most significant accomplishment achieved under this program can be summarized as follows:

1. Comprehensive analytical modeling was performed to determine directed energy beam processing parameters for the recrystallization of silicon grains. The development encompassed pulsed as well as scanned lasers and electron beams. Thermal histories, damage thresholds and resulting thermo-physical effects were addressed. (Because of the extensive nature of this analysis, it is fully reported in Appendix A.)
2. A computer code, VXTEMP, was developed for solving the time-dependent thermal diffusion equation. This code can accept temperature-dependent thermal properties, multilayer structures and time-dependent energy deposition profiles that cannot be treated by the analytic model.
3. Pulsed and scanned electron beams were used to demonstrate the potential of the two-step recrystallization process. Silicon grains broader than the 30- μm -thick film in which they were formed were achieved. This is believed to be the first evidence of greater-than-film-thickness silicon recrystallization other than by long-term heat treatment above 1350°C.
4. Ion implantation and pulsed electron beam annealing were shown to be technically feasible for forming shallow-junction single crystal GaAs cells. Mesa diode structures with V_{oc} 's up to 875 mV were obtained.
5. Ion beam epitaxy was demonstrated to be technically feasible by greater than 10% implantation of Al into GaAs.

1.4 REPORT OUTLINE

Section 2 of this report is the largest and reflects the extensive effort expended on the recrystallization tasks. The requirements for the films are discussed, the rationale behind two-step recrystallization is presented, the experiments described, and the results presented. The results indicate the potential of carrying the two-step recrystallization to large areas contingent upon availability of appropriate directed energy sources. Section 3 describes efforts toward applying directed energy processing techniques to III-V compounds. The experiments conducted, the results of these experiments and an indication of the potential of this technology are presented here. Conclusions and recommendations are presented in Section 4.

SECTION 2

SILICON RECRYSTALLIZATION

2.1 BACKGROUND CONSIDERATIONS

It is generally accepted that DOE's post-1986 goals for photovoltaic power costs and manufacturing-energy effectiveness can only be achieved through the development of thin-film cell structures. It is further anticipated that, while near-term requirements could be satisfied by silicon cells, long-term requirements would require compound-semiconductor cells.

To this end, Spire Corporation reports here on the demonstration of a concept for recrystallization of previously deposited silicon films. This concept, founded on regrowth through directional control of thermal gradients and implemented through the application of specialized electron beams, was initially funded by NSF under grant AER76-06096 for the period 1 February 1976 through 30 June 1977. The initial program succeeded in establishing the principle of the recrystallization concept that is being reported upon. This final report presents evidence of the feasibility of this recrystallization concept.

2.2 DIRECTED ENERGY CELL FABRICATION SEQUENCE

A plausible thin-film cell fabrication sequence is shown in Figure 1. With the exception of the recrystallization operation, all the necessary process steps have been previously demonstrated. The state-of-the-art with respect to these other process steps is, however, quite varied. At one extreme, ion implantation for junction formation, even in polycrystalline silicon, is a universally recognized process that requires no additional technical development. Pulsed electron beam annealing is at an intermediate position. While it is an established practice at a few laboratories, full acceptance of this process requires refinements in the design of the necessary equipment and the commercial availability of the equipment.

At the other extreme, electrostatic bonding (ESB) with simultaneous release of the bonded film from its deposition substrate is a developmental process at this time. While ESB for monocrystalline cells is under intensive investigation⁽¹⁾, its practical application to recrystallized polycrystalline films cannot be assured until a reproducible supply of such films is available. Further, transfer of the recrystallized film from its deposition substrate to an ESB glass superstrate, a process based on differential thermal

FIGURE 1. DIRECTED ENERGY APPROACH TO THIN-FILM SILICON SOLAR CELL FABRICATION

expansion between the superstrate/film composite and the film's deposition substrate during the ESB cycle, is dependent upon definition of the recrystallization process itself, the requirements imposed upon the deposition substrate by the recrystallization process, and the details of the film deposition process.

An additional "unknown" at this time is the exact nature of allowable front contacts to polycrystalline cells. As a consequence of these considerations, the sequence shown in Figure 1 cannot be taken as definitive, since it depicts a sequence of operations, all of which have not been reduced to routine practice.

2.3 THIN-FILM CELL CONSIDERATION

A decade ago, the thickness of a thin-film cell could be uniquely optimized because the structure under consideration was a monocrystalline cell and the trade-off consideration was power-to-weight ratio. Within the context of DOE's present thin-film cell program, the concept of an optimized cell thickness is considerably more complicated and, perhaps more to the point, not a primary design parameter. The bottom line figure for the present scenario is dollars per installed peak watt, a discriminant that is related to cell thickness in two distinct ways.

The first consideration is that installed cost is the summation of the various panel fabrication costs. One component of this total is the cost of the silicon, a cost that is proportional to cell thickness. Since it must be anticipated that, even for a polycrystalline cell, silicon cost will be a significant component of total cost, thickness minimization consistent with optimized cell output is a clear direction.

The second cell thickness interaction is, of course, with conversion efficiency. In a monocrystalline cell, conversion efficiency, for given front-layer and contact parameters, is a well-behaved function of insolation spectrum, absorption coefficient, cell thickness and the base-layer minority-carrier diffusion length⁽²⁾. The functional relation become more complex in a polycrystalline cell, since diffusion length is not necessarily invariant with thickness and grain size must be consistent with the effective diffusion length. It is in these two areas, diffusion length and grain size, that the technology of the fabrication process becomes of prime importance.

Since it is hard to imagine a grain boundary that is not a significant recombination surface, the polycrystalline grains must extend at least from the active depth limit of the cell to some point beyond the junction. While the continuation of these columnar grains to the cell's front surface may be necessary to achieve the desired front-layer

conductivity, this continuation is not intrinsically necessary to a reasonably high-performance thin-film cell. Similarly, the practical necessity for these columnar grains to extend from the cell's active depth limit to its back surface is only a function of achieving the requisite conductivity for this layer.

Given, as a minimum, this necessary columnar structure region, the question of grain cross section can be addressed. Since a light-generated minority carrier will recombine at the nearest recombination surface, a reasonable collection efficiency requires that the lateral grain boundaries be remote as compared to the distance to the collecting junction. For a right-cylindrical grain of radius R and height L , the lateral surface area is $2\pi RL$ and the end (junction) area is πR^2 . For a 10% loss of minority carriers to the lateral grain boundary, the most simplistic analysis require a 10-1 area ratio, i.e., $(R^2/2RL) = 10$, or for a 10- μm film, 200- μm columnar grains.

Considerably more refined analyses have been made by Hiborn and Lin⁽³⁾, by Hovel⁽⁴⁾ and by Soclof and Iles⁽⁵⁾. An engineering consensus is that a 10% (AM1) cell could be realized from 10- μm -thick columnar grains that have 100-200- μm cross sections in an n^+p-p^+ (BSF) structure, if the grains had a 10- μm effective diffusion length.

Since CVD of polysilicon onto thermal SiO_2 at temperatures as high as 1100°C⁽⁶⁾ gives grain sizes of less than 10 μm and PVD of silicon films onto polycrystalline foreign substrates gives even smaller crystallite sizes, it is generally conceded that large-grain silicon films can only be achieved through a postdeposition process for grain size enhancement. Long-term bulk heat treatment at temperatures in excess of 1300°C is, however, required for grain growth to the range of interest, even under favorable substrate conditions^(7,8). This range of process temperatures is too high for retention of electrical transport properties in silicon films deposited to foreign substrates. A variety of recrystallization concepts utilizing a third component to reduce the liquidus temperature of the silicon film have also turned out to be insufficient to this task. A recrystallization approach based upon depth-localized heating would appear to be consistent with the cell requirements.

2.4 DEPTH-LOCALIZED HEATING

If a pulse of incident energy is absorbed in a layer that is thin compared to the total thickness of the absorber and if the width of the energy pulse is small compared to the time necessary for thermal energy to diffuse out of the absorbing region, the

absorbing layer can be raised to an arbitrarily high temperature without significantly raising the temperature of the absorber as a whole. The temperature of the absorbing layer is determined by the fluence (energy density) and absorption depth of the incident radiation, since no heat is lost to the underlying region of the absorber during the heating pulse. The temperature excursion of the region that is not directly heated is proportional to the energy deposited and to the thermal mass ratio of the two regions.

Depth-localized heating produces an instantaneous temperature profile that is congruent with the absorber's depth-dose curve. Because photon absorption follows Beer's law, the depth-dose curve for laser heating is exponential and the peak temperature occurs at the surface. Consequently, depth-localized laser heating can only be realized for very thin films. Heating of thicker films necessitates the diffusion of thermal energy from the absorbing region and thus violates the principle of depth-localized heating.

Electron absorption occurs through random scattering in the absorber and for normal beam incidence gives a subsurface temperature maximum. As the incidence angle decreases, the random scattering causes the temperature peak to move nearer the surface. As a consequence beam incidence angle gives a third variable for control of electron beam heating.

The preceding has outlined the basic arguments that govern depth-localized heating. The following subsection provides quantitative models. The development is restricted to electron beam heating.

2.4.1 Thermal Analysis

2.4.1.1 Electron Energy Deposition in Solids

An energetic electron interacting with a solid absorber loses energy through radiative and ionizing collisions and, additionally, is scattered without energy loss in elastic collisions. The importance of the various interaction mechanisms is dependent upon initial electron energy and the absorber's atomic number (Z). For silicon and electron energies below 100 keV, as used in experiments reported here, the fraction of incident energy lost to radiative collisions (bremsstrahlung) is less than 10^{-3} and, hence, may be ignored. As a consequence, almost all the energy lost by incident electrons is through ionizing collisions that are characterized by a relatively small change in energy and scattering angle.

This absorption process can be statistically modeled to obtain an accurate calculation of the depth-dose profile. Monte Carlo techniques and certain simplifying assumptions are required. The validity of this approach has been confirmed by Everhart and Hoff⁽⁹⁾. One of the standard programs for this calculation is ELTRAN⁽¹⁰⁾. Two ELTRAN produced depth profiles for electron energy spectra characteristic of Spire's pulsed electron beam systems are shown in Figures 2 and 3. The ordinate is the normalized energy dose (calories per gram of material) deposited at the given depth by the electron beam for unit incident fluence (calorie per square centimeter). The integral of the curves in Figures 2 and 3 is slightly less (5%) than unity since the effect of backscattered electrons, which escape the surface of the material, has been subtracted from the total absorbed dose. Note the change in scales between these two beams. The near surface peak in Figure 2 is due to nonnormal incidence that results from self-focusing in the lower energy beam.

Returning to the physics of electron absorption, since the ultimate fate of electrons freed in ionizing encounters is excitation of some other atom, the absorption of electrons produces excited atoms that must decay to their ground state through radiationless transitions. According to the quantum theory of solids, however, the energy levels of the absorber atoms are broadened into bands and the incident (and secondary) electrons interact with the absorber electrons in these bands. Further, these interactions are quantized such that one or more phonons is involved in each interaction. Since the emission of a phonon is formally equivalent to a change in lattice vibrational energy, classically identified as thermal energy, absorption of electrons corresponds to heating the absorber within the electron absorbing region. As a consequence, classical thermodynamic considerations can be used to predict the magnitude and location of the temperature changes that are associated with electron absorption.

2.4.1.2 Analytic Development of Fast Pulse Heating

As was just shown, the result of absorbing energetic electrons in a solid is localized heating. If this heating occurs within a period that is short in comparison to the time required for phonons to diffuse from the heated region, i.e., the heating is adiabatic, the rapid thermal expansion of the heated region generates shock waves that are transmitted through the (unheated) body of the absorber. If the transient pressure due to these shock waves exceeds the absorber's yield strength, the latter will crack.

FIGURE 2. ENERGY DEPOSITION PROFILE OF 12-keV ELECTRON BEAM IN SILICON

FIGURE 3. ENERGY DEPOSITION PROFILE OF 55-keV ELECTRON BEAM IN SILICON

The first of the following subsections deals with the calculation of thermal effects in the absorber; the second treats the necessary limitation on energy deposition due to shock wave generation. (This theory is fully developed in Appendix A.)

Thermal Considerations:

Consider the electron absorber to be a thick slab that extends from the plane $z = 0$ to the plane $x = L$, where the slab thickness, L , is sufficient that the slab appears to be infinitely thick within the time domain under consideration. If the isotherms within the slab are planes parallel to the plane $z = 0$, the problem can be reduced to one-dimensional form. For large diameter, uniform electron beams, neglecting edge effects, this one-dimensional approximation is valid.

The defining heat transport relation can be reduced to:

$$K(\partial^2 T / \partial z^2) - \rho C_p (\partial T / \partial t) = -\rho (\partial D / \partial t) \quad (1)$$

$$\dot{F} \equiv \partial F / \partial T = \rho \int_0^L [\partial D(Z, t) / \partial t] dz \quad (2)$$

where $T(z, t)$ is the temperature; t is time; D is the dose (energy/volume); F is the beam fluence (energy/area); and ρ , C_p and K are, respectively, the absorber's density, heat capacity and thermal conductivity. In this development, ρ , C_p , and K are assumed to be temperature independent constants. While this is a poor assumption (particularly for K), the potential error is reduced by using averages for the temperature range of interest (300-1685°K); these are:

$$\begin{aligned} \rho &= 2.33 \text{ g/cm}^3 \\ C_p &= 0.92 \text{ J/g-K}^0 \\ K &= 0.48 \text{ W/cm-K}^0 \end{aligned}$$

Equations (1) and (2) can be solved for the boundary condition that implies no heat flow across the surface at $z = 0$. This is a reasonable approximation if radiative heat loss from the front is negligible on the time scale of interest and if the heating pulse is

very short compared to the characteristic thermal diffusion time for a distance on the order of the energy deposition depth. The characteristic thermal diffusion distance is defined by

$$\theta(t) = (4\kappa t)^{1/2} \quad (3)$$

where $\kappa = K/\rho C_p$ is the thermal diffusivity. Figure 4 shows the temperature profile normalized to the surface temperature as a function of normalized depth, $z/\theta(t)$. Note that the shape of the curve is independent of both fluence and pulse width.

For this computation, the depth-dose profile for a monoenergetic electron beam is assumed to be Gaussian for ease of calculation. The exact profile is given by Spencer⁽¹¹⁾. The two profiles are compared in Figure 5. Using the Spencer depth-dose curve allows explicit recognition of the electron beam pulse width. The result given in Figure 6 expresses the fluence, ΔF , required per degree increase in maximum surface temperature, $\Delta T_{\max}$, as a function of pulse width and electron energy. For example, the average electron energy for the beam used to generate Figure 2 is 12 keV. It has an effective heating time of ~ 50 ns. Therefore, $6-8 \times 10^{-5} \text{ cal/cm}^2$ are required per degree increase in $T_{\max}$, or to reach melt temperature (1690°K) from room temperature requires $\sim 0.1 \text{ cal/cm}^2$. Actual melting of the surface requires the addition of heat of fusion energy, 392 cal/g. Since this development does not account for phase changes, the additional energy can be equated to an additional temperature rise by

$$\Delta T \approx H_f/C_p \approx 1782^\circ\text{K} \quad (4)$$

Referring to Figure 6 for this set of beam parameters and using $T_{\max} = 1690 - 293 + 1782 = 3179^\circ\text{K}$ gives $\Delta F = 0.26 \text{ cal/cm}^2$.

Hydrodynamic Considerations

Using the Gaussian deposition profile of Figure 5 and the pulse width dependent calculations which generated Figure 6, the temperature induced shock wave can be calculated from the Grueneisen parameter, γ , and the relation:

$$\gamma = V(\partial p / \partial U)_V \quad (5)$$

Note: Functions defined in Appendix A.

FIGURE 4. SURFACE NORMALIZED TEMPERATURE AS A FUNCTION OF REDUCED DEPTH FOR $t \gg t_L$

Note: Functions defined in Appendix A.

FIGURE 5. GAUSSIAN AND SPENCER ELECTRON ENERGY DEPOSITION PROFILES IN ALUMINUM

Note: Functions defined in Appendix A.

FIGURE 6. FLUENCE PER DEGREE INCREASE IN SURFACE TEMPERATURE AS A FUNCTION OF ELECTRON ENERGY

where V is volume, p is pressure and U is internal energy. The subscript V implies constant volume which holds away from the heated front surface and is approximately true at the surface, too. The results (see Appendix A) are presented in Figure 7. For the previous example, with 12-keV electrons and 50-ns pulse width, the peak pressure for a 3179°K rise in temperature (melting the surface) is less than the 100-bar yield strength of silicon. For experiments using the deep heating 55-keV beam (see Figure 3), the expected pressure peak is 1.5 kilobar for a 40-ns pulse width. This exceeds the silicon fracture threshold. For a 200-ns pulse width at the same electron energy, the peak pressure is about 300 bar, which is below the fracture threshold. Experiments performed at these average electron energies and approximate pulse widths confirm these calculations.

2.4.1.3 Computer Modeling of Fast-Pulse Heating

In the analytic model for pulsed electron beam heating, as applied to fast-pulse heating, we were constrained to employing temperature-independent thermal properties for the absorber because closed-form solutions could not be obtained for temperature-dependent thermal properties. Prior work at Spire, using a simple computer code for pulse heating, suggested that use of temperature-independent parameters could introduce a fluence error of up to a factor of two. As a consequence, a generalized computer code, VXTEMP, was developed for predicting pulsed heating effects.

Because early VXTEMP runs, done for other programs, gave fluence-to-melt values that compared favorably with the predictions of the analytic model, VXTEMP was run for an $0.3\text{-}\mu\text{m}$, polycrystalline silicon layer on a $250\text{-}\mu\text{m}$ molybdenum substrate. This structure, typical of what may be required eventually, cannot be easily treated by the analytic model. VXTEMP utilizes the finite element approach to solve the time-dependent diffusion equation. It has provisions for temperature-dependent thermal properties, multilayer structures, and time-dependent energy deposition profiles.

The results of this VXTEMP run are shown in Figures 8 and 9. Figure 8 displays the time dependence of the sample's front-surface temperature when exposed to a 0.26-cal/cm^2 Gaussian electron pulse centered at 50 ns and having a FWHM of 21 ns, a close approximation to the actual first-step pulse. In distinction to results obtained from VXTEMP for $0.3\text{-}\mu\text{m}$ of polysilicon on silicon, where this fluence causes front-layer melting, thermal relaxation through the high conductivity molybdenum substrate

Note: Functions defined in Appendix A.

FIGURE 7. RATIO OF PEAK PRESSURE TO PEAK TEMPERATURE
AS A FUNCTION OF ELECTRON ENERGY

FIGURE 8. VXTEMP CALCULATION FOR THE TIME DEPENDENCE OF FRONT SURFACE TEMPERATURE FOR A 0.3-μm Si LAYER ON Mo

FIGURE 9. TEMPERATURE PROFILES AT VARIOUS TIMES FOR THE CALCULATION IN FIGURE 8

precludes the availability of heat of fusion at the surface. Figure 9 gives the temperature profiles of this sample at 50, 70, 100, 150, and 200 ns. This figure shows the clamping of the surface at the melting point and an unusual interface phenomenon. For this pulse, the molybdenum at the interface rises above silicon's melting point, causing melting of a thin silicon layer at the interface. Since this beam is required for recrystallization of a 0.3- μm layer, the first-step treatment must not extend to the interface if the lifetime of the silicon layer is to be preserved.

2.4.1.4 Scanned Beam Thermal Analysis

As indicated in the Introduction, there are two scanned beam heating modes. In the first mode, the beam's "dwell" time over any small surface area is short as compared to the time required for thermal relaxation of the temperature profile that is produced by absorption of the incident energy. In the second mode, the converse is true. For fixed beam energy, current and diameter, the operative heating mode is a function of scan velocity; large scan velocities give heating in the first mode, while small velocities can only heat in the second mode. It should also be noted that the transition from one mode to the other is continuous. Scanned beam heating in the second mode is not depth-localized.

The effective pulse width for scanned heating is the time required for the beam spot to move one diameter. This is given by the ratio of the beam diameter, D , to the scan velocity, V . Another consideration is the ratio of beam diameter to heated depth, z_h . If D/z_h is not large, the resulting thermal gradient will be three-dimensional in both scan modes because lateral thermal diffusion can no longer be ignored. For slow-scan heating, z_h is the sum of the absorption depth and the thermal diffusion distance. Consequently D/z_h can readily be less than unity for this mode.

Fast-Scan Analysis

The analytic solution given in Appendix A and summarized in Section 2.4.1.2 is directly applicable to fast-scan DC beam heating if V/D is substituted for t_p . The one-dimensional heat flow restriction used in this development requires that $D/z_h \gg 1$, a condition that is satisfied for practical high-power beams. Using the silicon thermal parameters that have been previously listed and rearranging the equations of Appendix A allows the beam parameters for fast-scan heating to be expressed in terms of the film

thickness, z_1 , that is to be heated. The pertinent parametric equations are listed in Table 1. With the exception of the last relation, all symbols are as defined in Appendix A. In the last relation, $\Delta\tau$ is the temperature rise for a 15-mil, thermally isolated substrate of area A_0 and length L_1 that has been subjected to n scans in the L_1 direction.

Note that for a given z_1 and fixed α : E , I/D^2 and V/D are fixed. As a consequence, selection of I , V or D establishes a unique set of beam conditions. Since α is the ratio of the pulse width (D/V) to silicon's characteristic thermal diffusion time, these relations break down as $\alpha \rightarrow 1$.

Table 2 lists the α -independent beam parameters for a range of z_1 values. Table 3 lists the α -dependent beam parameters for $z_1 = 0.15 \mu\text{m}$ and a range of α and D values. Table 4 lists similar data for $z_1 = 30 \mu\text{m}$. In these last two tables, the subscripts 2 and 3 denote heating to the melt temperature and melting, respectively. Also, $\Delta\tau^*$ is the substrate temperature increase from a single 1-cm scan.

Slow-Scan Analysis

At slow-scan velocities, neither the analytic development presented in Appendix A nor VXTEMP is applicable, since the thermal gradient is now three-dimensional. Although the electron beam is still absorbed "in depth", the domination of the temperature profile by thermal diffusion allows the "in-depth" absorption to be physically replaced by "surface" absorption. As noted previously, "surface" energy absorption is characteristic of photon (laser) heating. Lax⁽¹²⁾ has given a general (closed-form) solution for laser heating. Cline and Anthony⁽¹³⁾ have analyzed scanned laser heating. Their development is examined in Appendix B.

Since the Cline and Anthony solutions are graphical, they cannot be discussed without reference to their figures. In the Cline and Anthony analysis, the beam is assumed to have a Gaussian fluence cross section that is characterized by a radius R between the peak and e^{-1} fluence points. Also, Z is depth in the absorber, X is the surface coordinate in the scan direction, Y is the surface coordinate orthogonal to X , V is the scan velocity, D is the absorber's diffusivity, and f is a distribution function that is proportional to temperature. Their analysis is also constrained to the use of temperature invariant thermal properties and does not explicitly consider heat of fusion.

TABLE 1. FAST-SCAN HEATING BEAM PARAMETERS

	<u>Units</u>
$[L_1] = \text{cm}$	$[T], [\Delta T], [T_{\max}], [\Delta \tau] = \text{K}^\circ$
$[z_1], [z_0], [a], [D] = \mu\text{m}$	$[E] = \text{V}$
$[A_0] = \text{cm}^2$	$[I] = \text{A}$
$[t_0], [t_p] = \text{s}$	$[J_0] = \text{A/cm}^2$
$[V] = \text{cm/s}$	$[F] = \text{J/cm}^2$
$[r_0] = \text{mg/cm}^2$	$[\dot{F}] = \text{W/cm}^2$

Functions

$$A = B/B_0 \quad \lim_{B_0 = \alpha \rightarrow 0} \left\{ \alpha / [(1 + \alpha)^{1/2} - 1] \right\} = 2$$

$$B = \alpha / [(1 + \alpha)^{1/2} - 1] \quad \alpha = t_p/t_0$$

$$q_1 = (z_1)^{1/1.73} \quad s_1 = [(z_1)^{2.73}]^{1/1.73}$$

Relations

$$y_0 = 4.85 \times 10^{-1} z_1; \quad z_0 = 2.08 z_1; \quad a = 1.18 z_1; \quad t_0 = 1.54 \times 10^{-8} z_1$$

$$F = 2.43 \times 10^{-4} T_{\max} A z_1$$

$$\dot{F} = 1.45 \times 10^4 \Delta T (A/\alpha) / z_1$$

$$E = 1.22 \times 10^4 q_1$$

$$J_0 = 1.19 \Delta T (A/\alpha) (1/s_1)$$

$$I/D^2 = 1.35 \times 10^{-8} \Delta T (A/\alpha) (1/s_1)$$

$$V/D = 6.48 \times 10^3 (1/\alpha) (1/z_1^2)$$

$$(\Delta \tau / L_1) / A_0 = n \times 2.74 \times 10^{-7} A \Delta T D z_1$$

TABLE 2. α -INDEPENDENT BEAM PARAMETERS FOR FAST-SCAN HEATING A SILICON FILM

	z_1 (μm)								
	0.10	0.15	0.20	0.25	0.30	1.0	10	30	50
r_0 (mg/cm^2)	4.85×10^{-2}	7.28×10^{-2}	9.71×10^{-2}	1.21×10^{-1}	1.46×10^{-1}	4.85×10^{-1}	4.85×10^0	1.46×10^1	2.43×10^1
a (μm)	1.18×10^{-1}	1.76×10^{-1}	2.35×10^{-1}	2.94×10^{-1}	3.53×10^{-1}	1.18×10^0	1.18×10^1	3.53×10^1	5.88×10^1
z_0 (μm)	2.08×10^{-1}	3.12×10^{-1}	4.17×10^{-1}	5.21×10^{-1}	6.25×10^{-1}	2.08×10^0	2.08×10^1	6.25×10^1	1.04×10^2
t_0 (ns)	1.54×10^{-1}	3.47×10^{-1}	6.17×10^{-1}	9.64×10^{-1}	1.39×10^0	1.54×10^0	1.54×10^3	1.39×10^4	3.85×10^4
E (kV)	3.21	4.06	4.78	5.45	6.06	1.22×10^1	4.60×10^1	8.68×10^1	1.17×10^2

TABLE 3. α -DEPENDENT BEAM PARAMETERS FOR FAST-SCAN HEATING
A 0.15- μ m SILICON FILM

		D (μ m)						
		0.3	0.75	1.5	15	25	50	100
2-22	$\alpha=0.01$							
	I_2 (A)	3.37 -3	2.1 -2	8.42 -2	8.42 0	2.34 +1	9.35 +1	3.74 +2
	I_3 (A)	7.74 -3	4.84 -2	1.94 -1	1.94 +1	5.38 +1	2.15 +2	8.6 +2
	V (cm/s)	0.65 +6	2.16 +7	4.32 +7	4.32 +8	7.21 +8	1.44 +9	2.88 +9
	$\Delta\tau_2^*$ (K ⁰)	1.71 -5	4.27 -5	8.54 -5	8.54 -4	1.42 -3	2.85 -3	5.7 -3
	$\Delta\tau_3^*$ (K ⁰)	3.93 -5	9.83 -5	1.97 -4	1.97 -3	3.28 -3	6.55 -3	1.31 -2
	$\alpha=0.05$							
	I_2	6.8 -4	4.25 -3	1.7 -2	1.7 0	4.72 0	1.89 +1	7.55 +1
	I_3	1.56 -3	9.77 -3	3.91 -2	3.91 0	1.09 +1	4.34 +1	1.74 +2
	V	1.73 +6	4.32 +6	8.65 +6	8.65 +7	1.44 +8	2.88 +6	5.76 +8
	$\Delta\tau_2^*$	1.73 -5	4.31 -5	8.63 -5	8.63 -4	1.44 -3	2.88 -3	5.75 -3
	$\Delta\tau_3^*$	3.97 -5	9.92 -5	1.98 -4	1.98 -3	3.31 -3	6.61 -3	1.32 -2
	$\alpha=0.1$							
	I_2	3.44 -4	2.15 -3	8.6 -3	8.6 -1	2.39 0	9.56 0	3.82 +1
	I_3	7.91 -4	4.94 -3	1.98 -2	1.98 0	5.49 0	2.2 +1	8.79 +1
	V	8.65 +5	2.16 +6	4.32 +6	4.32 +7	7.21 +7	1.44 +8	2.88 +8
	$\Delta\tau_2^*$	1.75 -5	4.37 -5	8.73 -5	8.73 -4	1.46 -3	2.91 -3	5.82 -3
	$\Delta\tau_3^*$	9.02 -5	1.0 -4	2.01 -4	2.01 -3	3.35 -3	6.69 -3	1.34 -2
	$\alpha=0.25$							
	I_2	1.42 -4	8.89 -4	3.56 -3	3.56 -1	9.88 -1	3.95 0	1.58 +1
	I_3	3.27 -4	2.04 -3	8.18 -3	8.18 -1	2.27 0	9.09 0	3.63 +1
	V	3.46 +5	8.65 +5	1.76 +6	1.76 +7	2.88 +7	5.76 +7	1.15 +8
	$\Delta\tau_2^*$	1.81 -5	4.51 -5	9.03 -5	9.03 -4	1.5 -3	3.01 -3	6.02 -3
	$\Delta\tau_3^*$	4.15 -5	1.04 -4	2.08 -4	2.08 -3	3.46 -3	6.92 -3	1.38 -2

TABLE 3. α -DEPENDENT BEAM PARAMETERS FOR FAST-SCAN HEATING
A 0.15- μ m SILICON FILM (Concluded)

		D (μ m)									
		0.3		0.75		1.5		15		25	
2-23	$\alpha=0.5$	I_2	7.47 -5	4.67 -4	1.87 -3	1.87 -1	5.19 -1	2.08 0	8.3 0		
		I_3	1.72 -4	1.07 -3	4.29 -3	4.29 -1	1.19 0	4.77 0	1.91 +1		
		V	1.73 +5	4.32 +5	8.65 +5	8.65 +5	1.44 +7	2.88 +7	5.76 +7		
		$\Delta\tau_2^*$	1.9 -5	4.74 -5	9.48 -5	9.48 -4	1.58 -3	3.16 -3	6.32 -3		
		$\Delta\tau_3^*$	4.36 -5	1.09 -4	2.18 -4	2.18 -3	3.63 -3	7.27 -3	1.45 -2		
	$\alpha=0.75$	I_2	5.2 -5	3.25 -4	1.3 -3	1.3 -1	3.61 -1	1.44 0	5.78 0		
		I_3	1.2 -4	7.47 -4	2.99 -3	2.99 -1	8.3 -1	3.32 0	1.33 +1		
		V	1.15 +5	2.88 +5	5.76 +5	5.76 +6	9.61 +6	1.92 +7	3.84 +7		
		$\Delta\tau_2^*$	1.98 -5	4.95 -5	9.9 -5	9.9 -4	1.65 -3	3.3 -3	6.6 -3		
		$\Delta\tau_3^*$	4.55 -5	1.14 -4	2.28 -4	2.28 -3	3.79 -3	7.59 -3	1.52 -2		
	$\alpha=1.0$	I_2	4.05 -5	2.53 -4	1.01 -3	1.01 -1	2.81 -1	1.13 0	4.5 0		
		I_3	9.32 -5	5.83 -4	2.33 -3	2.33 -1	6.47 -1	2.59 0	1.04 +1		
		V	8.65 +4	2.16 +5	4.32 +5	4.32 +6	7.21 +6	1.44 +7	2.88 +7		
		$\Delta\tau_2^*$	2.06 -5	5.14 -5	1.03 -4	1.03 -3	1.71 -3	3.43 -3	6.86 -3		
		$\Delta\tau_3^*$	4.73 -5	1.18 -4	2.37 -4	2.37 -3	3.94 -3	7.89 -3	1.58 -2		

TABLE 4. α -DEPENDENT BEAM PARAMETERS FOR FAST-SCAN HEATING
A 30- μ m SILICON FILM

		D (μ m)				
		60	150	300	600	1000
$\alpha=0.01$	I_2 (A)	3.15 -2	1.97 -1	7.87 -1	3.15	8.75
	I_3 (A)	7.24 -2	4.53 -1	1.81	7.24	2.01 +1
	V (cm/s)	4.32 +4	1.08 +5	2.16 +5	4.32 +5	7.21 +5
	$\Delta\tau_2^*$ (K ⁰)	6.84 -1	1.71	3.42	6.84	1.14 +1
	$\Delta\tau_3^*$ (K ⁰)	1.57	3.93	7.86	1.57 +1	2.62 +1
$\alpha=0.05$	I_2	6.36 -3	3.97 -2	1.59 -1	6.36 -1	1.77
	I_3	1.46 -2	9.14 -2	3.66 -1	1.46	4.06
	V	8.65 +3	2.16 +4	4.32 +4	8.65 +4	1.44 +5
	$\Delta\tau_2^*$	6.9 -1	1.73	3.45	6.9	1.15 +1
	$\Delta\tau_3^*$	1.59	3.97	7.94	1.59 +1	2.65 +1
$\alpha=0./1$	I_2	3.22 -3	2.01 -2	8.04 -2	3.22 -1	8.94 -1
	I_3	7.4 -3	4.62 -2	1.85 -1	7.4 -1	2.06
	V	4.32 +3	1.08 +4	2.16 +4	4.32 +4	7.21 +4
	$\Delta\tau_2^*$	6.99 -1	1.75	3.49	6.99	1.16 +1
	$\Delta\tau_3^*$	1.61	4.02	8.03	1.61 +1	2.68 +1
$\alpha=0.25$	I_2	1.33 -3	8.32 -3	3.33 -2	1.33 -1	3.7 -1
	I_3	3.06 -3	1.91 -2	7.65 -2	3.06 -1	8.5 -1
	V	1.73 +3	4.32 +3	8.65 +3	1.73 +4	2.88 +4
	$\Delta\tau_2^*$	7.22 -1	1.81	3.61	7.22	1.2 +1
	$\Delta\tau_3^*$	1.66	4.15	8.3	1.66 +1	2.77 +1

TABLE 4. α -DEPENDENT BEAM PARAMETERS FOR FAST-SCAN HEATING
A 30- μ m SILICON FILM (Concluded)

		D (μ m)				
		60	150	300	600	1000
$\alpha = 0.5$	I_2	6.99 -4	4.37 -3	1.75 -2	6.99 -2	1.94 -1
	I_3	1.61 -3	1.0 -2	4.02 -2	1.61 -1	4.46 -1
	V	8.65 +2	2.16 +3	4.32 +3	8.65 +3	1.44 +4
	$\Delta\tau_2^*$	7.59 -1	1.9	3.79	7.59	1.26 +1
	$\Delta\tau_3^*$	1.74	4.36	8.72	1.74 +1	2.91 +1
$\alpha = 0.75$	I_2	4.86 -4	3.04 -3	1.22 -2	4.86 -2	1.35 -1
	I_3	1.12 -3	6.99 -3	2.8 -2	1.12 -1	3.11 -1
	V	5.76 +2	1.44 +3	2.88 +3	5.76 +3	9.61 +3
	$\Delta\tau_2^*$	7.92 -1	1.98	3.96	7.92	1.32 +1
	$\Delta\tau_3^*$	1.82	4.55	9.11	1.82 +1	3.04 +1
$\alpha = 1.0$	I_2	3.79 -4	2.37 -3	9.48 -3	3.79 -2	1.05 -1
	I_3	8.72 -4	5.45 -3	2.18 -2	8.72 -2	2.42 -1
	V	4.32 +2	1.08 +3	2.16 +3	4.32 +3	7.21 +3
	$\Delta\tau_2^*$	8.23 -1	2.06	4.12	8.23	1.37 +1
	$\Delta\tau_3^*$	1.89	4.73	9.46	1.89 +1	3.15 +1

Figure 10 is a plot of f as a function of the reduced distance, X/R , along the center ($Y/R = 0$) of the scan line with reduced depth, Z/R , as a parameter for a scan velocity of $RV/D = 1$. This scan velocity is appropriate to a slow scan with electron absorption within a depth that is small compared to R . (RV/D is on the order of 20 for a fast-scan beam.) Note that the maximum lags the center ($X/R = 0$) of the beam and that the magnitude of the lag increases with increasing depth (Z/R). As a consequence, the solidification interface would be curved. (For melting of a doped silicon film, this curved interface could give rise to resistivity gradients in the Z -direction.) Figure 11 shows some surface ($Z/R = 0$) values of f in the X - Y half-plane. Peak f is not shown. The rapid decrease in surface f in the Y direction is evident. The distribution function behaves similarly at $Z/R = 1$. This figure clearly indicates the three-dimensionality of the temperature gradient.

The actual temperature is given by

$$T = P (C_p D R)^{-1} f$$

where P is the incident power, C_p is the heat capacity per unit volume and the other symbols are as defined above. For $D = 0.224 \text{ cm}^2/\text{s}$, $C_p = 0.92 \text{ J/g-K}^\circ$, $\rho = 2.33 \text{ g/cm}^3$ and $RV/D = 1$, this equation gives $P/R = 4.8 \times 10^3 \text{ W/cm}$ to bring the surface to melt temperature and $P/R = 11.6 \times 10^3 \text{ W/cm}$ to melt the surface (using the temperature equivalent of the heat of fusion, as was done previously).

2.4.2 Equipment Considerations

Completion of the thermal analysis for both first- and second-step melting allowed a definition of the electron beam parameters required for realizing these operations. This evaluation pointed to a set of interrelated equipment limitations and a processing problem. As a consequence, a number of compromises were necessary.

Spire Corporation's standard pulsed electron beam heating equipments are optimized for annealing of shallow ion implants. As a result, the average electron energy and beam incidence angle are such as to allow melting of silicon films in the thickness range of $0.1 - 0.3 \mu\text{m}$. A survey of organizations supplying continuous electron beam equipments and/or services indicated that for films of this thickness range and, hence, electron energy, the beam power requirements for fast-scan melting could not be realized by several orders of magnitude. At the relatively low electron voltages

FIGURE 10. TEMPERATURE PARAMETER, f , AS A FUNCTION OF x/R AT $y/R = 0$ FOR $RV/D = 1$ AT SELECTED VALUES OF z/R

FIGURE 11. SELECTED SURFACE ($Z/R = 0$) VALUES OF f ON THE X - Y HALF-PLANE FOR $RV/D = 1$

required, perveance limitations preclude obtaining the necessary current in small diameter beams, and brightness limitations preclude obtaining the required current in large diameter beams.

Since perveance is inversely proportional to the $3/2$ power of the beam voltage, higher beam energies would allow obtaining the required power density. This, of course, would necessitate working with significantly thicker silicon films. Because of the physical limitation on the current density obtainable from low-energy continuous electron beams, there was no other choice. Further work with suppliers of continuous electron beam equipments and/or services revealed that Leybold-Herzeus (Enfield, Connecticut) had an electron beam welder that could approach the fast-scan current density requirements for silicon films in the range of $30\text{ }\mu\text{m}$ thick. No other suitable equipment was available at anything approaching rational cost.

The problem then devolved to obtaining a pulsed electron beam configuration suitable to first-step processing of $30\text{-}\mu\text{m}$ silicon films. To this end, a very significant internal effort was applied to modifying a developmental pulsed electron beam system (MBS) to be applicable to this task. This effort was not successful. The principal problem was that the pulse width of the MBS system was so short that hydrodynamic effects (see Section 2.4.1.2 and Appendix A) literally destroyed the film. Lengthening the pulse width of a pulsed beam system requires redesign of the energy storage capacitor, a task that clearly was not within the financial or temporal scope of this program. As a consequence, the internal effort turned to modifying the plasma diodes on operational systems so as to obtain higher average electron energies.

This effort was partially successful. An experimental complication inherent to electron emitting plasma diodes is that electron energy is a critical function of diode geometry and further that the magnetic field associated with the electron pulse self-focuses (Bennet pinch) the propagating beam such that its incidence angle onto the target (film) is not necessarily normal. As a consequence, obtaining a high average energy pulsed beam required an extensive series of trial and error experiments. The resulting optimized beam, with average electron energy of 55 keV and normal beam incidence, would melt only approximately $13.5\text{ }\mu\text{m}$ of the $30\text{-}\mu\text{m}$ film.

That the full $30\text{-}\mu\text{m}$ film thickness could not be melted is not, at this time, that important for two reasons. The first is the simple point that if the deposited film is melted to the silicon-substrate interface, deleterious film substrate interaction will occur. As a consequence, it is desirable to limit the melt depth of the first-step

treatment such that the silicon-substrate interface does not experience a temperature excursion above some preselected value. For a film on grown SiO_2 , a maximum temperature of 850°C would appear to be reasonable. Although VXTEMP could be used to specify the required beam parameters quite accurately, no calculation was made for this particular case, since the available pulsed beam would not produce any significant thermal excursion at the interface.

The second reason for accepting the limitation on first-step melting depth is that the as-deposited CVD films were essentially columnar. Since the purpose of the first-step treatment is to convert an equiaxed random grain film to a full-film-thickness, columnar grain film, the pre-existence of a columnar grain film obviated the necessity of the first-step treatment. This point will be discussed more fully in Sections 2.5.1 and 2.5.2.

Based on the observations that polysilicon CVD films deposited from SiH_4 at temperatures as low as 790°C already had a columnar structure and that low film deposition rates were obtained from low-temperature SiH_4 polysilicon, the films used for the full two-step treatment were deposited from SiCl_4 at high temperature. As explained in the preceding paragraph, this did not have any appreciable effect on the experimental results.

Lastly, the high power density of the continuous electron beam precluded any attempt to measure beam diameter in the sense that this parameter is used in the thermal analysis. What was possible was an estimate of beam diameter based on "hot spot" size for a stationary beam. This point will be discussed in Section 2.5.3. The consequence of this limitation was simply that the second-step treatment would have to be run as a function of beam current. Anticipating results presented in Section 2.5.3, this was no problem for slow-scan second-step treatments. The maximum current available from the electron beam welder was, however, insufficient to give visible indication of melting in the fast-scan experiments. As a consequence, it is not possible to estimate accurately how closely melt temperature was approached in the fast-scan experiments.

2.5 EXPERIMENTAL RESULTS

Six experimental series were run. The first five sets of experiments investigated only first-step processing. These experiments employed thin polysilicon films that could be easily obtained and first-step processed in readily available pulsed beam systems. The

complication of a pre-existing columnar film necessitated considerably more activity with first-step processing than had been planned.

The sixth experimental set, done on 30- μm polysilicon films, was processed through both first- and second-step treatment. The exhaustion of both program funding and time precluded more extensive investigation.

2.5.1 Film Deposition

It is to be noted that the thrust of this program was to be a demonstration of the effectiveness of the proposed two-step thermal treatment in converting a randomly oriented, small-grain, polycrystalline silicon film that was deposited onto a foreign, polycrystalline substrate into a full-film-thickness, columnar grain structure with a grain cross section of 100-200 μm . As a consequence, the method used for obtaining the initial films is not germane at this point so long as these films are pure silicon and can be deposited in a manner that minimizes film-substrate interaction.

Primarily for convenience, but with some thought for ultimate economics, a CVD approach to film deposition was adopted for this program. Physical vapor deposition (evaporation, sputtering) approaches were rejected because the extreme vacuum conditions required for obtaining oxide-free silicon films by these methods were not thought to be consistent with ultimate solar photovoltaic goals. Also, with PVD deposition rates for silicon being comparatively low, the ultimate requirement for a 10- μm film suggests that PVD methods may not be cost effective. A third consideration is that thick PVD films of nonductile metals are normally highly stressed. Further, the energy required for obtaining a silicon film from a silicon chemical is expected to be less than the energy required for obtaining a silicon film from silicon "metal". A final justification of the CVD approach is that in a large-scale operation, CVD processes can be operated in a continuous mode with recovery and recycling of unreacted feedstock. This would be particularly easy for CVD polysilicon deposited from SiH_4 in H_2 or N_2 .

A variety of CVD processes was used in this program for the following reasons: (1) difficulty in depositing reasonably smooth (continuous) films from SiH_2Cl_2 at low temperatures, (2) the slow deposition rates obtained from SiH_4 at low deposition temperatures, (3) the fact that all CVD film deposited with an essentially columnar morphology, and (4) the necessity for obtaining 30- μm films in a reasonable time. The deposition parameters for the six sets of films are summarized in Table 5.

TABLE 5. FILM DEPOSITION PARAMETER SUMMARY

Experiment Number	Deposition Gas	Carrier Gas	Deposition Temperature (°C)	In Situ Cleaning	Substrate Details	Film Thickness (μm)
Setup	SiH ₂ Cl ₂	H ₂	850	H ₂ at 1150°C	(111) oxidized wafers	~ 0.2
A-4,1	SiH ₂ Cl ₂	H ₂	800	H ₂ at 1250°C	(111) oxidized wafers	0.14, 0.24, 0.40, 1.3
A-4,2	SiH ₄	H ₂	790	HCl	(100), (110), & (111) wafers	0.10, 0.20, 0.50, 1.0
A-4,3	SiH ₄	H ₂	790	None	(100) wafers	0.09, 0.19, 0.46, 1.5
A-4,4	SiH ₄	N ₂	900	None	(100) wafers	0.14, 0.25, 0.40, 0.80
A-4,5	SiH ₄	N ₂	800	None	(100) oxidized wafers	0.10, 1.0
A-4,6	SiCl ₄	H ₂	1190	None	(100) oxidized wafers	30, 50

Setup runs were made to check out the general details of the intended deposition procedure. While only the first setup run is listed in Table 5, a number of such runs were required before continuous films could be deposited from SiH_2Cl_2 at 800°C . In these and in the A-4,1 run the substrates were furnace oxidized prior to the CVD step, and the oxide was removed by high-temperature reaction with H_2 immediately prior to the start of deposition. The in situ cleaning was found to be necessary because this system tended to deposit as isolated islands rather than as a continuous film. Further, in reducing the deposition temperature from 850 to 800°C , it was found that the reactor had to be operated at a large SiH_2Cl_2 supersaturation. Even in this limit, the surface of the resulting films was extremely rough. Figure 12 is a 25,000X SEM photograph of a $0.4\text{-}\mu\text{m}$ film. Figure 13 is a 2000X photograph of a $1.3\text{-}\mu\text{m}$ film. The latter shows the rather high density of dendritic growth that was characteristic of all A-4,1 films. The area shown in Figure 12 is between the dendrites. This local roughness was also characteristic of all A-4,1 films.

Because the projecting surface dendrites would interfere with RHEED analysis and because of the extreme surface roughness, the A-4,2 runs were made from SiH_4 in H_2 at 790°C . (The reactor's temperature control system would not operate at lower temperatures.) Seven different substrate types, to cover possible orientation, type and resistivity effects, were used in the A-4,2 run. The resulting films were characterized by both dendrites and projecting crystallites, as illustrated in Figures 14 and 15. The former is a 10,000X SEM photograph of the fractured edge of a $1.0\text{-}\mu\text{m}$ film on (100) silicon. In addition to the obvious dendrites, the structure of the fractured film edge suggests that the film deposits as a columnar grain structure. Figure 15 is a 20,000X SEM photograph of the surface of a $1.0\text{-}\mu\text{m}$ film on (111) silicon. The high density of surface crystallites is notable.

Because of the poor surface morphology, flow conditions were modified for run A-4,3. While some improvement in surface quality was obtained, dendritic projections were still observed. An SEM photograph of a typical A-4,3 film surface can be seen in Section 2.5.2, Figure 20.

In a further attempt to eliminate as-deposited film structure, the deposition was made from an N_2 carrier for the A-4,4 run. This change indeed produced acceptable surface morphology. Scanning electron microscope photographs of the surfaces of these films can be found in Section 2.5.2, Figures 26, 27 and 28. The A-4,4 run concluded deposition directly onto monocrystalline silicon wafers.

FIGURE 12. EXPERIMENT A-4,1: AS-DEPOSITED 0.4- μm -THICK 800°C SiH_2Cl_2 FILM ON (111) SILICON

FIGURE 13. EXPERIMENT A-4,1: AS-DEPOSITED 1.3- μm -THICK 800°C SiH_2Cl_2 FILM ON (111) SILICON

FIGURE 14. EXPERIMENT A-4,2: AS-DEPOSITED 1.0- μm -THICK 790°C SiH_4 FILM ON (100) SILICON

FIGURE 15. EXPERIMENT A-4,2: AS-DEPOSITED 1.0- μm -THICK 790°C SiH_4 FILM ON (111) SILICON

For the A-4,5 run, the deposition temperature was lowered to 800°C, to minimize the columnar structure of the as-deposited films. Both bare and oxide covered (50-nm) substrates were used in this run. The surface morphology of these films was quite good. Scanning electron microscope photographs of these surfaces are also shown in Section 2.5.2.

The observation that film deposited from SiH₄ in N₂ at temperatures as low as 800°C still had an essentially columnar structure, coupled with the low deposition rates obtainable from CVD under these conditions and the need for thick films for the scanned beam experiments, prompted the decision to go to a high-temperature SiCl₄ process for the A-4,6 run. The surface morphology of these films was quite good, as would be expected. An SEM photograph of a typical surface is shown in Section 2.5.3. Deposition was made onto both bare and oxide covered (100-nm) wafers.

In retrospect, the selection of a CVD process for obtaining the necessary starting films was far from as convenient as had been anticipated. As a consequence, obtaining the starting material for this investigation consumed more time and effort than had been planned for. In view of the problems associated with depositing thick PVD films, the choice of CVD was, however, appropriate. The only technical limitation associated with this choice was that the pre-existence of a columnar granularity precluded any definitive evaluation of the necessity for the first-step thermal treatment in the recrystallization of CVD polysilicon.

2.5.2 First-Step Recrystallization Experiments

The a priori objective of the first-step thermal treatment was to convert a randomly oriented, small-grain-polycrystalline, silicon film on a foreign, polycrystalline substrate into a full-film-thickness, columnar-grain film by a method that does not subject the film-substrate interface to temperature excursions that would cause deleterious metallurgical interaction or degrade the film's minority carrier transport properties. While it is well demonstrated that pulsed electron beam heating can provide the requisite depth-localized heating, it had not previously been demonstrated that this technique was capable of causing columnar recrystallization of a polycrystalline silicon layer on either a foreign or silicon substrate. As a consequence, a necessary prerequisite to the goal was a demonstration that a pulsed electron beam treatment could cause the epitaxial regrowth of a polycrystalline layer that had been deposited directly onto a monocrystalline silicon substrate.

To this end, the first four experimental series were concerned only with the regrowth of a homoepitaxial silicon layer. The fifth experimental series then was used to demonstrate that pulsed electron beam melting would indeed produce a columnar grain structure in a polycrystalline layer on a foreign (amorphous) substrate. The results of the sixth recrystallization series were not examined prior to second-step processing. These latter results are discussed in Section 2.5.3.

As discussed in the previous section, unanticipated difficulties with respect to CVD deposition of silicon films caused the effort devoted to a demonstration of epitaxial silicon regrowth to exceed initial estimates. Moreover, the columnar tendency of the as-deposited films precluded a rigorous demonstration of conversion to a columnar grain film. A minimum conclusion from this phase of the study is, however, that pulsed electron beam melting of a columnar silicon film on a foreign amorphous substrate returns a columnar film.

The initial first-step recrystallization experiment, A-4,1, was primarily intended to experimentally bracket pulsed electron beam heating parameters and to evaluate the operational problems that would be encountered with the proposed analytic techniques, RHEED and SEM. Details of the A-4,1 film deposition were previously given in Table 5. Details of the experiment itself are given in Table 6. This experiment consisted of one substrate, four film thicknesses and five pulsed beam fluences plus untreated controls. The surface morphology of typical films from this experiment was previously shown in Figures 12 and 13. Pulsed electron beam heating was done in the system shown in Figure 16. This system is normally used for annealing ion implants. Figure 17 shows the four-position sample chamber, allowing four samples to be processed in a single pumpdown. Because the surface dendrites precluded meaningful RHEED on these films, analysis was confined to microscopic observation. These observations are summarized in Table 7. The lowest pulsed beam fluence, F1, produced no observable change in surface morphology on any A-4,1 films. The highest fluences, F4 and F5, caused substrate cracking in all A-4,1 films. The two intermediate fluences, F2 and F3, produced observable changes in surface morphology for all film thicknesses. This was rather unexpected since annealing of amorphous implanted layers is normally done at approximately the F4 fluence. Moreover, the average beam energy for this test should only melt $\sim 0.3 \mu\text{m}$ of silicon. As a consequence, the T3 and T4 films would not be expected to show substrate damage in F4 treatment. That changes in surface morphology were observed at lower than expected fluences (F2 and F3) has been ascribed to the thermal isolation of the projecting dendrites. No other conclusions were drawn from this experiment.

TABLE 6. A-4,1 EXPERIMENTAL DETAILS

Nomenclature: Each film is designated by a six-character alphanumeric, $S_{\alpha} T_{\beta} F_{\gamma}$, where S, T and F represent, respectively, substrate, film thickness and pulsed beam treatment fluence and α , β and γ are identifying numerics, as listed below.

Substrates: S1 (111), n-type, 0.01 ohm-cm

Preclean: Chemical; furnace oxidation in dry O_2 (900°C)

In Situ Clean: H_2 at 1250°C

Deposition: SiH_2Cl_2 in H_2 at 850°C

Film Thickness:

T1	0.14 μm
T2	0.24 μm
T3	0.40 μm
T4	1.3 μm

Pulsed Beam Fluence:

F0	None
F1	0.11 cal/cm ²
F2	0.15 cal/cm ²
F3	0.20 cal/cm ²
F4	0.26 cal/cm ²
F5	0.32 cal/cm ²

R77009P

FIGURE 16. SPI-PULSE 5000 PULSED ELECTRON BEAM SYSTEM

FIGURE 17. SPI-PULSE 5000 FOUR-POSITION SAMPLE CHAMBER

TABLE 7. A-4,1 EPITAXIAL RECRYSTALLIZATION OBSERVATIONS

Pulsed Electron Beam Fluence	Polycrystalline Layer Thickness			
	T1	T2	T3	T4
F1	No effect	No effect	No effect	No effect
F2	Structural change	Structural change	Structural change	Structural change
F3	Structural change	Structural change	Structural change	Structural change
F4	Substrate damage	Substrate damage	Substrate damage	Substrate damage
F5	Substrate damage	Substrate damage	Substrate damage	Substrate damage

The experimental details for the next epitaxial regrowth experiment, A-4,2, are listed in Table 8. Films of four thicknesses were deposited on each of seven substrates. Each substrate-film thickness combination was exposed to four electron beam fluence levels. Following normal cleaning procedures, one wafer from each substrate was loaded into the deposition reactor, along with an oxide-coated thickness measurement sample, and the wafers were in situ HCl etched immediately prior to film deposition. No difficulty in obtaining continuous films was experienced with this deposition system.

The objective in using the multiplicity of substrates was, primarily, to determine if there was an orientation, resistivity, or doping effect on pulsed electron beam recrystallization of the deposited films and, secondarily, to assess the effect of these substrate parameters on the film deposition process itself. The results of this experiment were disappointing in that optical and electron microscope inspection showed the as-deposited films to be nearly epitaxial, as was previously shown in Figure 14. Moreover, the film surfaces contained many projecting crystallites (see Figure 15). Surface views of S2 and S3 films showed the crystallites of Figure 15 to have the square cross section expected from deposition on a (100) face. In general, the crystallite density of (111) substrates was higher than either (110) or (100) substrates. Comparative evaluation of all 28 as-deposited substrate-thickness suggested only that film crystallinity was "worse" on the (111) substrates than on (110) or (100). This is in accord with the normal observation that it is hardest to grow epitaxial layers on the (111) face. In any case, the films were deemed to be far too crystalline for instrumental analysis of pulsing results.

Figures 18 and 19 are typical of results obtained from pulsing at higher fluence levels. Figure 18 is a 500X photomicrograph of an S3T1F4 film. This picture is reasonably characteristic of the appearance of all F4 treatments. The density of the "folding" pattern decreases with decreasing fluence and increasing film thickness. This latter effect is seen in Figure 19, a 500X photomicrograph of an S4T2F4 film. Substrate effects, except on film growth morphology, did not appear to be important. That no substrate cracking was observed in the A-4,2 films treated at the F4 fluence while severe substrate cracking was observed in A-4,1 films treated at lower fluences is ascribed to a systematic error in the A-4,2 fluence calculations. No further work was done with these samples.

The third experimental set, A-4,3, aimed at demonstrating epitaxial recrystallization and was considerably more successful. The experimental details are listed in Table 9 and the RHEED results are listed in Table 10.

TABLE 8. A-4,2 EXPERIMENTAL DETAILS

Nomenclature: Each film is designated by a six-character alphanumeric, $S_{\alpha} T_{\beta} F_{\gamma}$, where S, T and F represent, respectively, substrate, film thickness and pulsed beam treatment fluence and α , β and γ are identifying numerics, as listed below.

Substrates:

S1	(110), p-type, 5 - 10 ohm-cm
S2	(100), p-type, 1 ohm-cm
S3	(100), p-type, 10 ohm-cm
S4	(111) 2° off, n-type, 0.05 ohm-cm
S5	(111), p-type, 0.2 ohm-cm
S6	(111), n-type, 0.75 ohm-cm
S7	(111), n-type, 0.01 ohm-cm

Preclean: Chemical

In Situ Clean: HCl at 790°C

Deposition: SiH₄ in H₂ at 790°C

Film Thickness:

T1	0.1 μ m
T2	0.2 μ m
T3	0.5 μ m
T4	1.0 μ m

Pulsed Beam Fluence:

F0	None
F1	0.17 cal/cm ²
F2	0.22 cal/cm ²
F3	0.28 cal/cm ²
F4	0.35 cal/cm ²

FIGURE 18. EXPERIMENT A-4,2: S3T1F4 FILM

FIGURE 19. EXPERIMENT A-4,2: S4T2F4 FILM

TABLE 9. A-4,3 EXPERIMENTAL DETAILS

Nomenclature: Each film is designated by a six-character alphanumeric, $S_{\alpha} T_{\beta} F_{\gamma}$, where S, T and F represent, respectively, substrate, film thickness and pulsed beam treatment fluence and α , β and γ are identifying numerics, as listed below.

Substrates: S1 (100), p-type, 10 ohm-cm

Preclean: Chemical

In Situ Clean: None

Deposition: SiH_4 in H_2 at 790°C

Film Thickness: T1 0.09 μm
T2 0.19 μm
T3 0.46 μm
T4 1.5 μm

Pulsed Beam Fluence: F0 None
F1 0.15 cal/cm^2
F2 0.26 cal/cm^2

TABLE 10. A-4,3 RHEED ANALYSIS

Sample	Analysis
S1T1F0	Minor random poly-Si; possible (400) single crystal; twins
S1T1F1	Crystals in epitaxy; possible (400) single crystal; twins
S1T1F2	Crystals in epitaxy; possible single crystal
S1T2F0	Strong random poly-Si; crystals in (400) epitaxy; twins
S1T2F1	Similar to T2F0
S1T2F2	Very weak random poly-Si; many crystals in (400) epitaxy; twins
S1T4F0	Mostly random poly-Si
S1T4F1	Mostly random poly-Si; many crystals in (400) epitaxy parallel to surface; twins
S1T4F2	Epitaxy with (400) parallel to surface; twins; unidentified polycrystalline phase
S1T5F0	Many random poly-Si crystals in (400) epitaxy; twins
S1T5F1	Similar to T5F0
S1T5F2	Similar to T5F0

Figure 20 is a 3,000X SEM photograph of the surface and fractured edge of an S1T4F0 sample. The prominent surface features are triangular dendrites from the CVD operation. They did not appear to influence the results of this experiment. The striations on the fractured film edge are interpreted as conchoidal fracture lines, as might be expected from a randomly oriented, small-grain film. As-deposited films of the other thicknesses appeared to be qualitatively similar to Figure 20. Figure 21 is a 3,000X SEM photograph of an S1T2F2 film. The lower density of surface dendrites, as compared to Figure 20, is accidental. While the features visible on the fractured edge appear to be different from those observed on untreated films, no more than this observation is claimed.

Table 10 provides a variety of information. Examining the F0 data as a function of film thickness, it appears (1) that CVD of polysilicon from SiH_4 in H_2 at 790°C produces close to epitaxial deposits near the interface, and (2) that this organization first decreases and then increases with increasing film thickness. On examining the T2 and, particularly, the T4 films as a function of treatment fluence, the improvement in film organization with increasing fluence is quite evident. This change is illustrated by the comparison between Figures 22 and 23 and Figures 24 and 25. Figure 22 is the S1T4F0 film. The multiplicity of spots and the residual (random) ring pattern are to be compared to the much simpler spot pattern of the S1T4F2 sample shown in Figure 23. (Note that in Figure 23 the weak spots occurring at one-third the lattice spacing are due to twins and that the faint ring structure is an unidentified second phase that is not pure silicon.) Figure 24, the S1T2F0 sample, is qualitatively similar to the S1T4F0 (Figure 22) sample in that it displays a complicated spot pattern and a random ring pattern. The S1T2F2 sample shown in Figure 25 has a simple spot pattern and only very faint ring patterns.

Because of the highly organized structure of the as-deposited film used in the A-4,3 experiment, the essential points of this experiment were repeated on films deposited from SiH_4 in a N_2 carrier. It was anticipated that this deposition would give a significantly "poorer" as-deposited film structure. The experimental details of the A-4,4 experiment are listed in Table 11 and the RHEED results are presented in Table 12.

Figure 26 is a SEM photograph of the S1T1F0, S1T1F1 and S1T1F2 films at 50,000X. A distinct change in surface morphology is evident on the S1T1F2 sample. Figure 27 displays the same phenomena at 20,000X for the S1T2 samples. Similar changes were observed in the S1T3 films. By contrast, the S1T4 samples shown in Figure 28 at 20,000X did not exhibit this change in surface morphology. This is as

FIGURE 20. EXPERIMENT A-4,3: S1T4F0 FILM

FIGURE 21. EXPERIMENT A-4,3: S1T2F2 FILM

FIGURE 23. EXPERIMENT A-4,3: S1T4F2 RHEED PATTERN

579053P

FIGURE 22. EXPERIMENT A-4,3: S1T4F0 RHEED PATTERN

FIGURE 24. EXPERIMENT A-4,3: S1T2F0 RHEED PATTERN

S79054P

FIGURE 25. EXPERIMENT A-4,3: S1T2F2 RHEED PATTERN

TABLE 11. A-4,4 EXPERIMENTAL DETAILS

Nomenclature: Each film is designated by a six-character alphanumeric, $S_{\alpha} T_{\beta} F_{\gamma}$, where S, T and F represent, respectively, substrate, film thickness and pulsed beam treatment fluence and α , β and γ are identifying numerics, as listed below.

Substrates: S1 (100), p-type, 10 ohm-cm

Preclean: Chemical

In Situ Clean: None

Deposition: SiH_4 in N_2 at 900°C

Film Thickness: T1 $0.14\mu\text{m}$
T2 $0.25\mu\text{m}$
T3 $0.40\mu\text{m}$
T4 $1.80\mu\text{m}$

Pulsed Beam Fluence: F0 None
F1 0.15 cal/cm^2
F2 0.25 cal/cm^2

TABLE 12. A-4,4 RHEED ANALYSIS

Sample	Analysis
S1T1F0	Random poly-Si with slightly preferred orientation, (100) perpendicular to surface, i.e., (100) texture
S1T1F1	Random poly-Si and crystals in epitaxy
S1T1F2	Complete epitaxy (100); Kikuchi lines visible
S1T2F0	Poly-Si with mixed (100) and (111) texture
S1T2F1	Mostly random poly-Si with some preferred orientation; mixed (100) and (111) texture
S1T2F2	Random poly-Si plus (100) epitaxy
S1T3F0	Poly-Si with mixed (100) and (111) texture; very faint (100) epitaxy
S1T3F1	Poly-Si with mixed (100) and (111) texture
S1T3F2	Random poly-Si plus (100) epitaxy
S1T4F0	Poly-Si with mixed (100) and (111) texture
S1T4F1	Poly-Si with mixed (100) and (111) texture; very faint (111) epitaxy
S1T4F2	Poly-Si with mixed (100) and (111) texture

S1T1F0

S1T1F1

S1T1F2

FIGURE 26. EXPERIMENT A-4,4: SURFACE MORPHOLOGY CHANGE OF
AN S1T1 FILM WITH PULSED BEAM FLUENCE
2-53

S1T2F0

S1T2F1

S1T2F2

FIGURE 27. EXPERIMENT A-4,4: SURFACE MORPHOLOGY CHANGE OF AN S1T2 FILM WITH PULSED BEAM FLUENCE

S1T4F0

S1T4F2

5790579

FIGURE 28. EXPERIMENT A-4,4: SURFACE MORPHOLOGY CHANGE OF AN S1T4 FILM WITH PULSED BEAM FLUENCE

expected, since the analytic model for pulsed beam heating predicted that the F2 beam parameters for this experiment would produce actual melting to a depth of approximately $0.35\text{ }\mu\text{m}$. Considering the accuracy of the model and the parameters, it can be supposed that the three thinner films, S1T1, S1T2 and S1T3, would be melted down to and, for the S1T1 film, into the substrate, while the S1T4 film would only be melted to approximately half its thickness. On cooling, the S1T1-S1T3 films would regrow from a monocrystalline substrate, while the S1T4 film would regrow from a small-grain, polycrystalline base. The change in surface morphology observed for the three thinner samples can then be correlated with epitaxial regrowth.

An anomaly was observed in small areas of the S1T4F2 sample. This effect is shown in Figure 29. The upper picture is a 500X view of a region in which film became detached from the substrate as a result of the F2 treatment. This phenomenon occurred in small, roughly circular areas that are thought to correspond to localized "threads" in the pulsed beam. These threads, due to anode contamination, are regions of high fluence. Film detachment in these areas is probably due to bending moments generated by differential thermal expansion. The lower photograph in Figure 29 is a 20,000X view of the edge and surface of a piece of film from one of these areas. The surface morphology of this sample is more characteristic of those samples that melted to the interface (see Figure 26, S1T1F2, and Figure 27, S1T2F2) than of the normal regions of the S1T4F2 film (see Figure 28). While the edge morphology of this sample is suggestive of the edge morphology of the monocrystalline substrate, there is no other evidence that the observed flakes are monocrystalline.

The RHEED analysis, Table 12, corresponds with the SEM observations. As was observed in the A-4,3 experiment (see Table 10), the F1 (0.15 cal/cm^2) treatment, as expected, was insufficient to produce full recrystallization while the F2 (0.25 cal/cm^2) treatment, again as is predicted by the analytic model, was sufficient. Also, as was observed in the A-4,3 experiment, the effectiveness of the F2 treatment decreased with increasing film thickness. The one abnormality in Table 12 is the lack of improved crystal organization in going from S1T4F1 to S1T4F2. This is explained on the following basis. Since the total energy of the pulsed beam is fixed, high energy "threads" imply lower energy density in the other parts of the beam. Since the film detachment shown in Figure 29 is thought to be due to threads, it is reasonable to suppose that the fluence in the "normal" regions of the beam used for the S1T4F2 sample was actually less than F1 fluence.

S1T4F2

S1T4F2

379058P

FIGURE 29. EXPERIMENT A-4,4: DETACHED S1T4F2 FILM FROM "THREAD" AREA

Figure 30 shows the RHEED patterns for the S1T1F0 and S1T1F2 samples. The presence of Kikuchi lines and the complete absence of ring patterns in the S1T1F2 sample is particularly noteworthy. Figure 31 shows the RHEED data for the S1T2F0 and S1T2F2 samples. The reduced perfection of the S1T2F2 sample, as compared to the S1T1F2 sample, is evident in the ring structure and the absence of Kikuchi lines on the S1T2F2 plate. This progression is completed with Figure 32, the RHEED plates for the S1T3F0 and S1T3F2 samples. It is to be noted, however, that the starting films are still more organized than is desired.

The results of experiments A-4,3 and A-4,4 conclusively demonstrated that an electron beam pulse will produce, at a minimum, columnar recrystallization of CVD polysilicon deposited on a monocrystalline silicon substrate. Moreover, the film thickness that can be treated is within 20% of that predicted by the analytic model.

Having conclusively demonstrated that pulsed electron beam melting was capable of recrystallizing a polycrystalline film deposited on a monocrystalline silicon substrate into an epitaxial film, the feasibility of converting a polycrystalline film on a foreign, noncrystalline substrate into a full-film-thickness, columnar film could be explored. This was done in experiment A-4,5. The experimental details are listed in Table 13. The RHEED analysis is summarized in Table 14.

Figures 33 through 40 are SEM photographs of the various films. These films do not appear to be different from previous thin polysilicon layers. Figure 33 shows the S1T1F0 film at 20,000X. Figure 34 shows this film after F1 pulsing. The change in surface morphology is evident and, in accord with previous experiments, indicates film melting. Figures 35 and 36 are SEM photographs of the S2T1 samples prior to (S2T1F0) and following (S2T1F1) pulsed beam treatment. The slight film cracking seen in Figure 35 is probably due to densification of the 850°C steam oxide. (A 1,000°C oxide would be more appropriate.) The cracking seen in the pulse-processed sample, Figure 36, is at least partially due to the relatively low temperature oxide but is also apparently due to a higher than expected pulsed beam fluence (see below). Areas within a cracked region, however, both before and after pulsed beam treatment, are comparable to the corresponding films that were deposited directly on silicon (S1) substrates.

Figures 37 and 38 are the SEM views of the S1T2 films before (F0) and after (F1) pulsing, respectively. Figure 37 is characteristic of previous films in this thickness range. The severe cracking of the film shown in Figure 38, along with the change in surface morphology, suggests that the pulsed beam fluence, for unknown reasons, was

FIGURE 30. EXPERIMENT A-4,4: RHEED PATTERNS FOR S1T1F0 AND S1T1F2 FILMS

37906CP

FIGURE 31. EXPERIMENT A-4,4: RHEED PATTERNS FOR S1T2F0 AND S1T2F2 FILMS

FIGURE 32. EXPERIMENT A-4,4: RHEED PATTERNS FOR
S1T3F0 AND S1T3F2 FILMS

TABLE 13. A-4,5 EXPERIMENTAL DETAILS

Nomenclature: Each film is designated by a six-character alphanumeric, $S_{\alpha} T_{\beta} F_{\gamma}$, where S, T and F represent, respectively, substrate, film thickness and pulsed beam treatment fluence and α , β and γ are identifying numerics, as listed below.

Substrates: S1 (100), p-type, 10 ohm-cm
S2 50-nm-grown SiO_2 on S1

Preclean: Chemical

In Situ Clean: None

Film Thickness: T1 $0.1\mu\text{m}$
T2 $1.0\mu\text{m}$

Pulsed Beam Fluence: F0 None
F1 0.25 cal/cm^2

TABLE 14. A-4,5 RHEED ANALYSIS

Sample	Analysis
S1T1F0	Not analyzed
S1T1F1	Complete epitaxy (100); twins
S2T1F0	Random poly-Si
S2T1F1	Random poly-Si
S1T2F0	Random poly-Si with preferred orientation
S1T2F1	As S1T2F0
S2T2F0	Random poly-Si
S2T2F1*	Random poly-Si and crystals in epitaxy

* After six anodize-strip cycles. (The unetched sample was lost in preparation.)

FIGURE 33. EXPERIMENT A-4,5: S1T1F0 FILM

FIGURE 34. EXPERIMENT A-4,5: S1T1F1 FILM

FIGURE 35. EXPERIMENT A-4,5: S2T1F0 FILM

FIGURE 36. EXPERIMENT A-4,5: S2T1F1 FILM

FIGURE 37. EXPERIMENT A-4,5: S1T2F0 FILM

FIGURE 38. EXPERIMENT A-4,5: S1T2F1 FILM

significantly higher than 0.25 cal/cm^2 , since this fluence had not previously caused cracking in films of this thickness range. (The actual pulsed beam fluence can only be determined by its effect on a target. Shot abnormalities can cause the "setup" fluence to be significantly higher or lower. While the reason for an abnormal shot can almost always be determined after its effect has been observed, such shots are sufficiently infrequent that it is not practical to attempt to preclude their occurrence by disassembly of the plasma diode for inspection prior to each shot.) Figures 39 and 40 show the S2T2 films before (F0) and after (F1) pulsing, respectively. Their similarity to Figures 37 and 38, respectively, is so great that no further discussion of the latter figures is necessary.

While the A-4,5 RHEED analysis that is given in Table 14 appears, at first glance, to be negative, this is not the case. Based on the known characteristics of the pulsed electron beam used in this experiment, full-depth recrystallization can only be expected for the T1 ($0.1 \mu\text{m}$) films. In the S1 film (polysilicon on monocrystalline silicon), epitaxial regrowth via directional freezing in the field of the unidirectional thermal gradient is possible and was observed. The RHEED analysis for film S1T1F1 (and corresponding films in earlier experiments) confirms this expectation. For the S2 films (polysilicon on a foreign noncrystalline surface), directional freezing under the unidirectional thermal gradient can, at best, be expected to produce full-film-thickness, columnar crystallites unless the density and orientation of the nucleation sites at the original liquid-solid interface is controlled. Because the density of growth propagation sites cannot be controlled, the cross section of the columnar crystallites and their rotational organization would be expected to be qualitatively similar to those of the starting CVD film. As a consequence, RHEED analysis of a recrystallized film would be expected to show a pattern that was similar to that of the starting film. This was observed for the S2T1F1 sample.

Confirming that S2T1F1 type films do indeed have a columnar structure is difficult. The simplest approach is to optically monitor the film's surface morphology as the surface is nonselectively removed. Assuming even a modest tendency for preferential reaction at grain boundaries, constancy of grain boundary contours could be taken as an indication of a columnar grain structure. To this end, one of the S2T2F1 films was subjected to repeated anodic oxidation and oxide stripping cycles. Because all S2T2F1 samples were cracked after pulsing, this attempt was unsuccessful. Figure 41 is a 2,000X SEM photograph of an S2T2F1 film after six anodize-strip cycles. The heavy substrate attack at the film cracks is evident. This localized attack precluded obtaining any meaningful information about the film structure.

FIGURE 39. EXPERIMENT A-4,5: S2T2F0 FILM

FIGURE 40. EXPERIMENT A-4,5: S2T2F1 FILM

FIGURE 41. EXPERIMENT A-4,5: S2T2F1 FILM AFTER SIX ANODIC OXIDATION-STRIP CYCLES

Figure 42 is the RHEED plate from the S1T1F1 sample. Except for the twinning, which may be due to residual oxide at the CVD interface, this pattern is as clean as the one shown in Figure 30, indicating that the pulsed beam was behaving as expected. Figure 43 shows the RHEED patterns for the S2T2 films before and after treatment. That these two patterns are essentially identical is, as was explained above, to be expected. It should be noted that the ring pattern in S2T1F1 indicates that the interfacial oxide is still present; if it had been consumed during the pulsed beam processing, a pattern like that shown in Figure 42 would have been observed. The RHEED patterns for all T2 films, as expected, are quite similar to the random polysilicon patterns observed on other thick films. Figure 44 shows RHEED patterns for an S1T2F1 film processed through three anodic oxidation/strip cycles and an S2T2F1 film processed through six thinning cycles. The spot and Kikuchi line structure seen on the S2T2F1 sample is due to the substrate; the ring pattern is due to the film.

This experiment completes the development work on the first step of the two-step recrystallization process.

2.5.3 Second-Step Recrystallization Experiments

The A-4,6 experiment was processed through the full two-step recrystallization cycle. Film deposition details were listed previously in Table 5. The other experimental details are listed in Table 15.

While the high-temperature SiCl_4 CVD process that was used in this experiment was expected to give a columnar structure film, it was anticipated that the SiCl_4 as-deposited film would be no more organized than the films obtained from the low-temperature processes used in the previous experiments. Because thick films were required, a high deposition rate CVD process was deemed to be appropriate.

The pulsed beam fluences listed in Table 15 cannot be directly compared to the values listed for the earlier A-4 experiments because, as has been noted previously, this beam was produced from a different plasma diode geometry. Experiment A-4,6 required a high average energy beam that could produce melting to a depth of 30-50 μm , as contrasted to the beams used in the previous A-4 experiment. The latter melted silicon to a depth of 0.3-0.4 μm . The equipment limitations that were discussed in Section 2.4.2 precluded obtaining a beam suitable for processing the T2 films within the time and resources available for the program. Indeed, the pulsed beam used for processing the T1 films was only capable of melting $\sim 13.5 \mu\text{m}$ of silicon. While this

S1T1F1

579068P

FIGURE 42. EXPERIMENT A-4,5: S1T1F1 RHEED PATTERN

9790697

FIGURE 43. EXPERIMENT A-4,5: S2T1F0 AND S2T1F1 RHEED PATTERNS

S79070P

FIGURE 44. EXPERIMENT A-4,5: RHEED PATTERNS FOR ANODIC OXIDIZED AND STRIPPED S1T2F1 AND S2T2F1 FILMS

TABLE 15. A-4,6 EXPERIMENTAL DETAILS

Nomenclature: Each film is designated by a six-character alphanumeric, $S_{\alpha} T_{\beta} F_{\gamma}$, where S, T and F represent, respectively, substrate, film thickness and pulsed beam treatment fluence and α , β and γ are identifying numerics, as listed below.

Substrates: S1 (100), p-type, 10 ohm-cm
S2 100-nm-grown oxide on S1

Preclean: Chemical

In Situ Clean: None

Film Thickness: T1 30 μm
T2 50 μm

Pulsed Beam Fluence: F0 None
F1 0.90 cal/cm²
F2 1.3 cal/cm²
F3 1.5 cal/cm²

Swept Beam Conditions:

Accelerating Voltage: 86.7 keV
Fast-Scan Velocity: 1×10^5 cm/s
Slow-Scan Velocity: 67 cm/s
Fast-Scan Current: 50, ~55 mA
Slow-Scan Current: 1.0, 0.5, 0.1 mA
Beam Diameter Estimate: 0.15 - 0.25 mm

limitation could be removed with an expanded effort, the columnar nature of the as-deposited film allowed a realistic demonstration of second-step recrystallization to be made on the output of a less than optimum first-step process.

The pulsed beam used in the A-4,6 experiment was characterized by an average electron energy of 55 keV and a pulse width of 200 ns. This beam is better characterized by the information displayed in Figure 45. This plot, temperature at selected depths in the film as a function of time, was calculated by using the pulse's actual I-t and V-t curves in ELTRAN (see Appendix A) to determine the depth-dose profile and inputting the ELTRAN output to VXTEMP. Note that because heat of fusion can only be considered through its temperature equivalent (see Section 2.4.1), temperatures above silicon's melting temperature indicate actual melting while melt temperature itself represents a solid at that temperature. From this explanation, it is seen that the liquid-solid interface for this pulse occurred somewhere between 10 and 15 μm into the film. Also note that because of surface radiation losses, the film surface did not actually melt. Figure 46 is a presentation of this calculation in terms of temperature as a function of depth into the film with time as a parameter. It shows that a liquid phase is present at an appreciable depth for more than 2000 but less than 8000 ns.

The swept beam parameters listed in Table 15 were established from the expected equipment capabilities and the analytic model. Because beam diameter can only be estimated (see Section 2.4.2), it was anticipated that achieving melting in the rapid-scan mode would be questionable. As will be discussed later, melting could not be attained in this mode.

The scanned-beam recrystallization experiment was performed in a large Leybold-Heraeus welder at their Enfield, Connecticut, facility. Since the welder did not have a raster-scanning beam-sweep circuit, only linear scanning of the samples was possible at this time. To this end, a one-shot oscillator was built to drive the beam's magnetic deflection coils. This circuit allowed a single scan across the sample. The maximum sweep velocity was limited by the frequency response of the deflection coils and system geometry. It should be pointed out the sweep velocity that was obtained, 10^5 cm/s, was due to the long focal length of the triode gun that is used in this system. This allows a long "throw arm" beyond the coils that could not be obtained from a diode gun system. Indexing between scans was obtained from a table motion in the chamber.

FIGURE 45. EXPERIMENT A-4,6: VXTEMP/ELTRAN OUTPUT OF FILM TEMPERATURE AS A FUNCTION OF TIME AT VARIOUS DETPHS FOR AN F2 PULSE IN AN S2T2 FILM

FIGURE 46. EXPERIMENT A-4,6: VXTEMP/ELTRAN OUTPUT OF FILM TEMPERATURE AS A FUNCTION OF DEPTH AT VARIOUS TIMES FOR AN F2 PULSE IN AN S2T2 FILM

Because the beam's power density, for the fast-scan experiments, was high enough to vaporize all materials when the beam was stationary, beam sweeps were started and stopped on beam dumps that were below the plane of the sample. The sample was also elevated above the table by a block that could not be seen by the incident beam. No "beam-splash" of foreign material was observed on the surface of any of the A-4,6 samples.

The vacuum in the welder chamber was on the order of 10^{-2} Pa. While this is considerably higher than would be desired, no significant amount of surface oxidation could be observed on any of the processed samples.

Prior to actual sample processing, the focus control settings that gave a constant beam diameter, 0.15-0.25 mm, as estimated from the "hot-spot" size of the nondeflected beam, were recorded for various beam currents. Since among beam diameter, scan velocity and beam current, there is only one independent variable, constant beam diameter and sweep velocity would allow the experiment to be run as a function of beam current. While in a triode gun, beam focus is almost independent of beam current at high beam currents, operation at low beam currents is rather unstable since the electron gun is biased to near cut-off. As a consequence, the current increments in the slow-scan experiments could not be as fine as would be desired. A diode gun system would be better suited to slow-scan melting.

Slow-Scan Experiments

The A-4,6 slow-scan experiments were performed at a beam voltage of 86.7 keV with currents of 1, 0.5 and 0.1 mA. The estimated beam diameter was 0.15-0.25 mm and the scan velocity was 67 cm/s. The beam currents that were used were determined by trial and error on setup films.

The 0.1-mA sweeps gave no surface or metallographic section evidence of having produced melting on any of the A-4,6 samples. By contrast, both the 0.5- and 1-mA sweeps gave distinct surface melt tracks on all A-4,6 samples. Considering the uncertainty in scanned beam diameter, this result is in satisfactory agreement with the Cline and Anthony analysis (see Appendix B).

Figure 47 is a 100X photomicrograph of an S2T1F3 film that has been both pulse beam and slow-scan melted. The scan beam moved from right to left, as is suggested by the solidification ripples. This view also shows the "boundary" of the pulse beam heated region. Pulse beam fluence decreased from left to right, as is suggested by the gradual

FIGURE 47. EXPERIMENT A-4,6: S2T1F3 FILM SURFACE
SHOWING A 0.5-mA SLOW-SCAN LINE

loss in contrast in that direction. This change in contrast at the radial limit of effective pulse beam heating is thought to be due to either grain boundary oxidation or orientation sensitive surface oxidation during pulse beam treatment, since, microscopically, there is no change in surface morphology between the F0 and the F1-F3 films. Since Figure 45 indicates the surface of the T1 films does not become liquid in the F2 treatment, the invariance of surface morphology is not unexpected. While not resolvable at this magnification, the surface displayed the faceted features that are characteristic of (100) texture⁽¹⁴⁾.

Figure 48 is a 1000X photomicrograph of a section through the center of a 0.5-mA slow-scan line. the central horizontal line is the 100-nm oxide layer. Its curvature indicates local substrate melting. The heavy vertical substrate feature is a crack. Film and substrate cracks were seen in all slow-scan melted films. A heavier slip pattern parallel to (100) and a lighter slip pattern parallel to (111) are evident in the substrate. While the regrown film, itself, is also heavily slipped, several central crystallites can be seen to have widths in excess of the film thickness. There is little doubt that a metallographic section parallel to the scan line would show very large crystals. The small crystallites at the film's surface are thought to be due to parasitic nucleation on surface oxides.

Figure 49 is a 1000X photomicrograph of the region to the left of that shown in Figure 48. The prominent vertical film feature is a crack at the edge of the slow-scan melt zone. The increasing tilt of the regrown crystallites in response to the increasing lateral component of the temperature gradient near the melt zone boundary is quite evident. The contrast between the crystallites in the melt region and outside its boundary is also marked. The region to the left of the crack is representative of all T1 films, both before and after pulsed beam treatment. This is not unexpected in view of the existence of a columnar structure in the as-deposited films and the depth limitation of the available pulse beam configuration. None the less, this experiment has demonstrated that the proposed two-step thermal treatment is capable of producing full-film-thickness columnar crystallites that have a cross section of at least $30\text{ }\mu\text{m}$ in a polysilicon film deposited on a foreign, noncrystalline substrate. This is believed to be the first demonstration of greater than film thickness recrystallization of silicon films except by prolonged heat treatment at temperatures in excess of 1300°C ^(7,8).

FIGURE 48. EXPERIMENT A-4,6: 1000X METALLOGRAPHIC SECTION OF AN S2T1F2 FILM THROUGH THE CENTER OF A 0.5-mA SLOW-SCAN LINE

S79072P

FIGURE 49. EXPERIMENT A-4,6: 1000X METALLOGRAPHIC SECTION OF THE REGION TO THE LEFT OF THAT SHOWN IN FIGURE 48

Fast-Scan Experiments

While the original intent in the fast-scan heating experiment was to examine this heating mode as a function of beam current, a setup sweep at a beam current of 50 mA produced no visual evidence of film melting. As a consequence, the beam current was raised to its limit, ~ 55 mA, and the setup scan was repeated. This beam did not give visible evidence of film melting either. If the beam diameter were at the upper side of its estimated range, this result would be in accord with the prediction of the analytic model.

A number of S1T1F2 and S2T1F2 and F3 films were processed in the ~ 55 -mA fast-scan beam. One S2T1F2 film was metallographically sectioned. Microscopic observation across this section did not reveal any regions having a distinctly different crystallite structure. A fractured section of an S2T1F2 film was then examined by RHEED. Except for two narrow regions, separated by the 0.100-in. distance between two successive fast scans, the RHEED pattern showed only the ring structure that would be expected from a randomly oriented polycrystalline film. In these two regions, however, the rather distinct spot pattern shown in Figure 50 was observed. It is obvious that significant solid-phase recrystallization had occurred in the ~ 55 -mA fast scan.

S79071P

FIGURE 50. EXPERIMENT A-4,6: RHEED PATTERN FROM A FAST-SCAN REGION ON AN S2T1F2 FILM THAT WAS SCANNED AT ~ 55 mA

SECTION 3

PROCESSING OF III-V MATERIALS

This section is concerned with studies on III-V materials. For simplicity, low-cost monocrystalline GaAs was taken as a representative demonstration vehicle.

3.1 PROGRAM OBJECTIVES

In addition to conventional two-layer p-n junction cells, the possibility of stacking thin films of different materials, each absorbing strongly in a different region of the solar spectrum, into a multiple junction solar cell so as to increase overall conversion efficiency is an attractive concept. It is, therefore, of technical interest to determine if the cell fabrication processes developed for silicon using the directed energy approaches of ion implantation and electron beam annealing are applicable to the III-V semiconductor compounds. These studies were carried out in anticipation of the development of an economical process for deposition of thin films of these compounds.

Among the III-V semiconductor compounds, GaAs is best known and most available. While it is more expensive than silicon, it has properties that make it superior to silicon for solar cell use. Consequently, GaAs was chosen as a representative of the III-V compounds for this work. Since the process technology is better developed for monocrystalline silicon, it was decided that similar work on GaAs should start with monocrystalline rather than polycrystalline material. It was also found appropriate, at this early stage, to work with the cheaper, lower-grade commercial GaAs single crystals. The approach was to establish a broad data base on implantation, annealing, fabrication and encapsulation of GaAs solar cells.

3.2 GaAs STUDIES

Although GaAs is similar to silicon as a semiconductor material, it differs from it in several important ways that require special attention during certain processing steps. Unlike silicon, which consists of a single element, GaAs is a binary compound comprising the elements Ga and As in a 1:1 stoichiometric ratio. In high-temperature treatment, GaAs preferentially decomposes, leaving a nonstoichiometric surface. Hence, many processes that have proven successful with silicon cannot be transferred to GaAs without some modification or additional protective measure. The different lines of investigation on measures to circumvent these limitations are reported below.

3.2.1 Ion Implantation

Because GaAs is expensive vis-a-vis silicon, it makes economic sense to anticipate the need for thin-film solar cells. This would require the formation of a shallow p-n junction, a requirement that, in principle, is most easily achieved by ion implantation. In addition, the strong optical absorption by GaAs causes a significant fraction of the solar insolation to be absorbed with the emitter (front) layer, a region that is dominated by a high surface recombination velocity. As a consequence a substantial fraction of the photogenerated carriers are lost to surface recombination unless some special provisions are made. The latter have taken the form of "transparent" front windows of AlGaAs. An alternative approach is to ion implant a much thinner emitter layer.

Implantations in GaAs were carried out with Mg, Zn, Si, Se and Te ions at doses ranging from 10^{14} to 10^{15} ions/cm² and at energies ranging from 5 to 80 keV. The implantation voltage for each ion was selected to give a junction depth of 50 nm with the peak concentration at ~ 25 nm. In practice, a "tail" is obtained for the implant profile because of diffusion into the damaged region, channeling and other effects.

It has been reported that (deep) implanted n-type dopants give about an order of magnitude lower sheet resistance than p-type dopants, at low dose levels. This is probably due to the higher mobility of electrons. The initial work on very shallow implants of n-type dopants suggests that surface effects can dramatically reduce doping efficiency.

3.2.2 Protective Capping

To prevent the decomposition of GaAs during high-temperature treatment, the surface of GaAs cells are normally capped with a removable protective layer of inert material. Two methods were tried: spin-on Ga-doped glass and plasma-deposited silicon nitride.

The nitride capping was carried out on samples that were implanted with Zn at 10 keV and concentrations of 1×10^{15} ions/cm². Thermal annealing was performed in the range of 700 to 800°C. The spin-on glass capping was carried out for 3×10^{14} -ion/cm² Zn implants with annealing temperatures in the range of 800 to 900°C. Protective capping markedly improves cell V_{oc} . The major difference between the two caps is that the spin-on glass produces greater variability of results. Nitride capping is thought to be more suited to very shallow junctions.

3.2.3 Antireflective Coating

The use of an antireflective coating on GaAs can greatly improve cell current density. While some early work with vacuum deposited TiO_2 films produced a 20-30% I_{sc} improvement, V_{oc} degradation was also noted. More recent results with anodic oxidation have shown that this technique gives very satisfactory results; I_{sc} increases by 30-50%, while V_{oc} either remains the same or increases slightly. Both these phenomena have been reported by other experimenters.

Anodic oxidation is particularly interesting in that it helps in four simultaneous ways:

- a. It serves as an antireflection coating, thus increasing I_{sc} .
- b. It produces a shallower junction, thus increasing I_{sc} .
- c. It lowers the surface recombination velocity, thus reducing the dark current and improving both V_{oc} and I_{sc} .
- d. The anodic oxide is compatible with electrostatic bonding to a glass superstrate.

3.2.4 Pulsed Electron Beam Annealing (PEBA)

Annealing GaAs with a pulsed electron beam was studied with Zn implants done at 10 keV and 1×10^{15} ions/cm². Results show that implanted GaAs can be readily annealed in a pulsed electron beam. The required fluence, however, appears to be considerably lower than that for annealing implanted silicon. As a consequence, the optimum target geometry, beam voltage and fluence levels have not yet been completely determined. For best GaAs results, a new machine configuration may be necessary. The best pulse-annealed GaAs, to date, gave V_{oc} 's up to 500 mV and I_{sc} 's of 6 mA/cm², clearly inferior to results obtained from capped thermal annealing.

3.2.5 GaAs Solar Cells

Because PEBA technology for GaAs is not optimized, capped thermal annealing was used to fabricate implanted cells for performance comparison with the state-of-the-art GaAs cells.

The characteristics of our best cell as compared to the latter are shown in Table 16. The high V_{oc} of 1060 mV was a pleasant surprise. Unfortunately, this particular cell was accidentally destroyed, and efforts to duplicate its performance were unsuccessful. Subsequent best efforts gave V_{oc} 's in the neighborhood of 900 mV, a value respectable in itself.

In general, the results show that thermally annealed ion-implanted GaAs cells gave excellent open circuit voltage; their short circuit current, however, is still below that of state-of-the-art GaAs cells. The best explanation for the low current density is that the starting material is of poor quality and the junction may be too deep for good collection efficiency.

3.2.6 GaAs on Germanium Substrates

Germanium is a possible substrate for future thin-film cell technology. A preliminary evaluation of its potential was made by utilizing a commercially available L.E.D. substrate that had a 12- μ m GaAs (n-type, 2×10^{16} ions/cm²) layer on a germanium wafer.

Somewhat surprisingly, results were appreciably better than with the usual n-type bulk GaAs substrates (see Figure 51). These results suggest that further refinement would lead to higher efficiencies.

3.2.7 Pulsed Electron Beam Annealing of GaAs

Pulsed electron beam annealing has been found to give high-efficiency silicon cells. In theory, it would be expected that the extremely short times involved (~ 10 ns) would help in achieving high activation in GaAs without surface dissociation. In practice, a considerable amount of experimentation is required to optimize beam pulse parameters, since they differ from those used for silicon. While considerable progress has been made, an optimized annealing configuration has not yet been achieved. The major parameters that were investigated were beam fluence and depth of beam penetration into the wafer. Penetration depth is a strong function of the diode geometry, which in turn affects angle of incidence through self-pinch of the beam.

Present state-of-the-art for this technology is summarized below:

- a. A satisfactory degree of reproducibility has been achieved.
- b. Modest activation can be obtained without physical surface damage.

TABLE 16. COMPARATIVE CELL PERFORMANCE

	Investigator		
	Spire AM1	Fan AM0	Hovel AM0
V _{oc} (mv)	1060	970	1015
I _{sc} (mA/cm ²)	14.6	25.6	33.1
Cell Area (cm ²)	0.092	0.5	0.1
Cell Type	p/n	n/p	p/n
Technique	ion implant	vapor phase epitaxy (VPE)	liquid phase epitaxial (LPE)
Starting Material	40- μ m GaAs/Ge	p ⁺ bulk GaAs	laser diode n-GaAs
Base	same	VPE, p ⁺ , 2 μ m	p, GaAs, 2 μ m
Junction	Zn 10 keV 1 x 10 ¹⁵ ions/cm ² x _j = ?	VPE, n ⁺ , 0.5 μ m	AlGaAs, p ⁺ , 0.5 μ m
AR Coat	anodic oxidation	anodic oxidation	TiO ₂
Other	silicon nitride anneal cap	—	etchback regrowth
Top Metalliza- tion	aluminum dots	gold plated fingers	Pd-Al grid

FIGURE 51. I-V CURVE FOR SHALLOW IMPLANTED GaAs ON Ge AS A FUNCTION OF ANODIC OXIDATION AND STRIPPING

- c. The V/I of PEBA samples shows a broad minimum over the range 0.075 to 0.19 cal/cm². Below this range the samples are not annealed, and above this range surface damage frequently results. Activation with pulse annealing is about 20% of that obtained from thermal annealing at this time.
- d. With mesa diode cells, a V_{oc} of 500 mV and I_{sc} of ~5 mA/cm² (no AR coating) has been obtained.

Best Solar Cells

Table 17 shows the "best" solar cell results obtained, along with the various PEBA annealing conditions. The results, while not so good as obtainable from thermal annealing, indicate a good probability that a useful PEBA beam can be developed. An unannealed sample and a typical thermal anneal sample are included for comparison. The following qualitative results apply (decreasing magnitude to the right):

<u>Parameter</u>	<u>System Configuration</u>
PEBA beam depth	3, 2, 1
PEBA beam uniformity	3 and 2, 1 (at low fluence)
Highest I _{ss}	1, 2, 3

In general the results have reached a broad optimization and "something else" appears to be limiting progress. A major limitation on solar cell results may be the high V/I obtained from PEBA. This limitation is discussed below.

Lowest V/I

Table 18 summarizes the PEBA conditions found to give the lowest V/I for the Zn implanted layer. From Table 18 it can be concluded that for lowest V/I the configuration ranking is 1, 2, 3. Data scatter and some differences in V/I measurement technique make this a tentative conclusion at present.

The high V/I that has so far been obtained from PEBA processed cells is probably responsible for the low V_{oc} that has been observed. While for silicon one could conclude that the PEBA anneal was producing incomplete activation, the situation with GaAs is much more complex. Certain defects can act as dopant compensation centers. It is

TABLE 17. SUMMARY OF PEBA RESULTS - BEST SOLAR CELLS

Run Number	Best Cell Sample No.	Solar		V/I	PEBA			
		V _{oc} (mV)	I _{sc} (mA)		Setup	Depth	Charging Voltage (keV)	Beam Fluence
1371-I	4	500	350	150	3	D	136	0.15
1455-I	2	500	400	150	2	S	200	0.105
1171-IV	3 (bake)	500	450	200	2	S		0.075
1171-I	A	500	450	140	1	VS	90	Nonuniform
Zn Standard (Typical Thermal Anneal)		810	700	30				
Unannealed			50	10,000		(Rectifying Contacts)		

Note: All cells n-type GaAs, implanted with Zn at 10 keV and 1×10^{15} ions/cm², no AR coating.

TABLE 18. SUMMARY OF PEBA RESULTS - LOWEST V/I

Run Number	Best Cell Sample No.	V/I	PEBA	
			Setup	Beam Fluence
1371-I	4	150	3	0.15
	3	150	3	0.13
1455-II	2	150	3*	0.22
1455-I	2	120	2	0.105
	6	135	2	0.105
1171-IV	4	116	2	0.105
	3	200	2	0.075
1171-II		100	1**	Nonuniform

* Cracks observed below the surface.

** Setup No. 1 is used for silicon processing.

possible that while PEBA may have regrown the lattice, it may have left or caused a defect that not only influences carrier lifetime but also effectively counter dopes the Zn implant. As a consequence, it is important not to draw firm conclusions from this preliminary study.

3.2.8 Surface Modification by High Dose Implants

Spire now has the capability of implanting at sufficiently high dose levels to alter the chemical composition of surface layers. Of obvious interest would be the conversion of the surface layer of a GaAs solar cell to AlGaAs or to GaAsP.

The first experiment was to implant a GaAs wafer with a dose of 1×10^{18} ions/cm² P⁺ at 20 keV and another wafer with a dose of 1×10^{19} ions/cm² Al⁺ at 50 keV.

The wafers were then nitride capped and thermally annealed at 790°C for 15 min. Visually, neither wafer appeared to have sustained surface damage. The P⁺ implanted wafer was analyzed by electron microprobe and found to have a Ga-As-P atomic ratio of 1.1-1.3-2.0. This corresponds to a uniform distribution in about 0.5 μm of the substrate. No attempt was made to analyze the electrical activity of the implanted phosphorous. The Al implanted sample was not analyzed.

Analytical techniques that could be used to determine the lattice position of the implanted species are difficult. It is likely that some form of emission spectroscopy is required to detect the bandgap widening that would be due to this surface layer. A full study of this technique would also have to include characterization of the damage and an analysis of nonstoichiometry effects. Co-implants of Ga may also be required for low defect structures.

SECTION 4

CONCLUSIONS

4.1 EFFORTS ON SILICON

Despite a formidable number of constraints imposed by equipment and process limitations, the preponderance of the experimental evidence presented in Sections 2.5.2 and 2.5.3 appears to support the following conclusions:

- a. The proposed two-step thermal process for recrystallization of polycrystalline silicon on a foreign noncrystalline (or polycrystalline) substrate is, at a minimum, compatible with the long-term requirements imposed by thin-film silicon solar cell considerations.
- b. Large-area pulsed electron beam melting of CVD polycrystalline silicon films on monocrystalline silicon substrates leads to epitaxial regrowth; similar exposure of CVD polycrystalline silicon films on foreign noncrystalline substrates leads to full-film-thickness columnar regrowth.
- c. Electron beam melting in a small-area slow-scanned beam leads to regrowth of crystallites having a cross section that is at least equal to the film thickness.
- d. Electron beam heating in a small-area fast-scanned beam produces significant solid-phase recrystallization at temperatures that are an unknown fraction of silicon's melting temperature.
- e. Adequate modeling procedures for depth-localized analysis are now in existence and are capable of predicting required process parameters.
- f. Equipments necessary for practical realization of large-area silicon films for thin-film solar cells can be constructed, although this task would be neither easy nor inexpensive.
- g. Film cracking during second-step fast-scan melting may be as much of a problem as it has been observed to be in slow-scan melting.
- h. No further evaluation of the potential of the proposed two-step thermal recrystallization process is possible without a significant investigational effort.

While the tone of these conclusions is positive, the potential for cracking in fast-scan melting, a factor that cannot be evaluated on the basis of existing data, remains a major cautionary signal. In the slow-scan melting reported here, severe substrate and film cracking was always observed. J. Fan⁽¹⁵⁾ has indicated that similar cracking problems were encountered in scanned laser recrystallization of silicon films. While no cracking problems were encountered in the fast-scan heating experiments performed under this program, it must be emphasized that the maximum film temperature that was obtained was an unknown fraction of silicon's melting temperature and that the size of the crystallites that were obtained from fast-scan heating are well short of practical solar cell needs. As a consequence, the energy deposition in fast-scan heating would have to be increased, so as to bring the film temperature nearer to melt temperature.

Increased energy density may, however, lead to an increased probability for film and/or substrate cracking. For slow-scan heating, the prediction that cracking would occur is reasonable on the basis of the difference in density between liquid and solid silicon, silicon's rather narrow elastic deformation range and the high surface tension of liquid silicon. The consequence of these factors is that the cross section of the molten zone would be concave downward in slow-scan melting. Since the total time that a given small region could be kept liquid is small, raster scanning of the film surface could not be utilized to continuously keep one side boundary of the zone liquid if practical sized films were to be processed. As a consequence the molten zone would have to crystallize on both lateral boundaries as well as at the bottom boundary. Crystallization, under this three-boundary constraint, of a molten zone having a cross section that is not identical with that of the solid from which it was produced would inevitably seem to lead to cracking. This change in cross section on melting, and again on resolidifying, is the reason the melt path on the slow-scanned films was so evident. The parabolic surface "ripples" in the melt line may indeed be due to a periodic stress relief in the melt path through cracking.

Because the change of surface morphology with laser glazing limits the applications of this technique, Anthony and Cline⁽¹⁶⁾ have analyzed this problem. Their principal point is that the molten zone surface depression that is observed in laser glazing (and electron beam welding) is due to the vapor pressure of the molten material above the molten zone. They then show that for a sufficient laser scan velocity, the inertia of the material in the molten zone will be such as to preclude surface depression during the period the region is molten. The zone will then resolidify without change in cross section. It can be argued that this will lead to solidification without cracking.

While Anthony and Cline could approach these melting conditions with a laser on metals, the latter have a rather extensive elastic deformation range. By contrast, the conditions for depth-localized heating by a scanned electron beam require a scan velocity that is more than adequate to prevent surface depression by the Anthony and Cline mechanism. Even given this condition, the narrow elastic deformation range of silicon may still preclude resolidification without cracking. In summary, a logical argument exists that would suggest that depth-localized melting in a small-area fast-scanned electron beam would not lead to resolidification cracking of a ductile metal. The applicability of this argument to the resolidification of silicon cannot be established at this time.

A second overall consideration is that while a significant degree of solid-phase structural ordering could be produced in the available fast-scan beam, the resulting film structure was far short of what is required for a practical thin-film solar cell. The arguments that a fast-scan of sufficient power density would give the required degree of structural organization are compelling; they are, however, not certain. It should also be pointed out that the power density obtainable from a continuous fast-scan beam can only approach the power density that can be obtained from a pulsed beam.

The utility of the preceding conclusions is a matter of cost effectiveness and the availability of other approaches. The technologies employed in this program, being based on machine operations, hold promise for low processing costs and are upward scalable. The energy utilization of electronic power supplies is high as compared to conventional processes. Further, the energy requirements for CVD deposition of silicon films are favorable as compared to techniques that require melting silicon metal. While all these factors suggest significant promise for the process that has been examined, this program cannot evaluate the ranking of this process with respect to other thin-film silicon technologies that are under development.

4.2 EFFORTS ON III-V COMPOUNDS

Because of the more diverse nature of the III-V work and because this effort represents an early stage in the development of the proposed processing, the conclusions that can be drawn from this program are both less sweeping and less secure. The following conclusions do, however, appear to be justified:

- a. Low energy ion implantation does appear to be a technically viable alternative to LPE or VPE for forming p-n junctions in III-V compounds.

- b. Capless pulsed electron beam annealing of ion-implanted III-V junctions does appear to be feasible.
- c. In situ formation of ternary III-V layers by high-dose ion implantation may be possible.

The ramifications of these conclusions must be considered with respect to some established economic frame. At the contractor's level, the potential for substituting an inexpensive process, ion implantation, for expensive processes, LPE and/or VPE, is significant. Its practical implementation rests, however, on the availability of high-quality III-V films. If the latter could only be obtained from LPE and/or VPE, there would be little incentive to incorporate a separate junction formation step. Conversely, a parallel with the development of silicon materials technology would seem to be predictable for III-V compounds. As a consequence, it could be anticipated that III-V films of the requisite bulk lifetime will become available in time. In this situation, the economic and energetic feasibility of ion implantation junction formation in III-V compounds would be expected to parallel that of silicon.

Given an ion-implanted junction, the capacity to perform capless annealing is an obvious economic advantage. Because pulsed electron beam annealing has been found to be superior to conventional thermal treatment for ion-implanted silicon, it can be presumed that application of this technique to III-V materials will ultimately produce parallel technical advantages as well.

The final facet of the III-V effort, ion beam epitaxy, or in situ ternary formation, is still in an embryonic stage. Its potential for solar cell fabrication is of significant technical import, subject only to a demonstration of actual ternary formation and, as noted previously, the availability of suitable starting films.

On an absolute basis, LPE and/or VPE do not appear to be compatible in the long term with the concept of low-cost, polycrystalline, thin-film, III-V solar cells. The three processes that have been examined in this program, by contrast, do appear to be compatible with these long-range goals.

REFERENCES

1. Spire Corporation, DOE/JPL Contract 954521, Interim Report No. 2 (March 1979).
2. M. Wolf and T.B.S. Chadda, in Conf. Rec. 10th IEEE Phot. Spec. Conf., p. 52 (Palo Alto, November 1973).
3. R.B. Hilborn, Jr., and J. Lin, in Proc. NSF National Workshop on Low Cost Silicon Solar Cells, p. 246 (Dallas, 1976).
4. J.H. Hovel, "Solar Cells", p. 103 ff. Semiconductors and Semimetals, v.11, R.K. Willardson and A.C. Beer, Eds., Academic Press, New York (1975).
5. S.I. Soclof and P.A. Iles, in Conf. Rec. 11th IEEE Phot. Spec. Conf., p. 56 (Scottsdale, May 1975).
6. T.I. Kamins, J. Manoliu, and R.N. Tucker, J. Appl. Phys. 43, 83 (1972).
7. G.C. Jain, B.K. Das, and S.P. Bhattacharjee, Appl. Phys. Lett. 33, 445 (1978).
8. C.D. Ouwers and H. Helijligers, Appl. Phys. Lett. 26, 569 (1975).
9. T.E. Everhart and P.H. Hoff, J. Appl. Phys. 42, 5837 (1971).
10. F.H. Brittain, RSIC Computer Code Collection, ORNL CCC-155; also Sandia Labs. SC-TM-68-713 (1968).
11. National Bureau of Standards, Energy Dissipation by Fast Electrons. L.V. Spencer, Government Printing Office, Washington (1959).
12. M. Lax, J. Appl. Phys. 48, 3919 (1977).
13. H.E. Cline and T.R. Anthony, J. Appl. Phys. 48, 3895 (1977).
14. T.I. Kamins and T.R. Cass, Thin Solid Films 16, 147 (1973).
15. J.C.C. Fan, H.J. Zeiger, and P.M. Zauracky, in Proc. NSF National Workshop on Low Cost Silicon Solar Cells, p. 89 (Dallas, 1976).
16. T.R. Anthony and H.E. Cline, J. Appl. Phys. 48, 3888 (1977).

APPENDIX A
ANALYTIC MODEL FOR DEPTH LOCALIZED HEATING

SECTION 1
ELECTRON ENERGY DEPOSITION IN SOLIDS

An energetic electron interacting with a solid absorber loses energy through radiative and ionizing collisions and, additionally, is scattered by elastic (no energy loss) collisions. As a consequence of scattering, the electron's path is tortuous. The total path length is an energy and material dependent multiple of the absorber thickness that is traversed (range). Range can be measured; path length can not. Energy loss to the absorber, since it is dependent upon the incident electron's actual collision history, is a function of path length, not range.

Electron energy loss per collision is a function of instantaneous electron energy; the instantaneous electron path with respect to nearby absorber atoms; and the concentration of bound electrons (proportional to atomic number, Z) in the absorber. As a consequence, each electron collision is an independent event. The relative importance of the various interaction mechanisms can be determined from an examination of the functional dependence of their probabilities, or as they are termed, collision cross sections.

Radiative interactions produce bremsstrahlung, a continuous x-ray spectrum that is due to inelastic collisions with the nuclei of absorber atoms. The cross section for radiative collisions is approximately^(A-1),

$$\sigma_{\text{rad}} = 1.6 Z^2/E \text{ barn/atom} \quad (1)$$

where E is the electron energy in keV. An estimate of the fraction of the electron's incident energy that is converted to bremsstrahlung, η_{rad} , is approximated by^(A-2),

$$\eta_{\text{rad}} = (7 \times 10^{-7}) ZE \text{ barn/atom} \quad (2)$$

For $E_{\text{max}} = 40 \text{ keV}$ and $Z = 14$ (silicon), $\eta_{\text{rad}} = 4 \times 10^{-4}$ and, hence, may be ignored.

Ionizing interactions with the bound electrons surrounding absorber atoms are the predominant energy transfer mechanism for keV range electrons. This type of inelastic

collision produces excitation and ionization of the absorber atoms. In the latter case, the ionized electron becomes an incident electron that also interacts with the absorber. The cross section for ionizing collisions is approximately^(A-1),

$$\sigma_{\text{ion}} = 1.3 \times 10^5 (Z/E^2) [\ln(E/I) + .35] \text{ barn/atom} \quad (3)$$

where I is the K-shell ionization potential, approximated by^(A-3),

$$I = (Z/11)^{2.243} \text{ keV} \quad (4)$$

The cross section ratio for $E_{\text{max}} = 40 \text{ keV}$ and $Z = 14$ is $\sigma_{\text{rad}}/\sigma_{\text{ion}} = 1.97 \times 10^{-3}$, confirming the earlier statement that ionizing collisions are the predominant energy loss mechanism.

While probabilities for occurrence of the two energy transfer interactions can be established, the actual energy lost in a given encounter cannot be determined, a priori. For ionizing interactions, the minimum energy transfer corresponds to the lowest excitation level of the absorber atoms and the maximum energy transfer is the full instantaneous energy of the electron. Similar limits apply to radiative interactions. That is, if it were possible to make energy measurements within the absorber, repetitions of an experiment that involve measuring the residual energy of an electron after a single inelastic encounter would give a distribution of energies. Other than that the probability for a large energy transfer encounter is small in comparison to the probability for a small energy transfer encounter, the details of the energy loss distribution are indeterminate. This phenomenon is known as energy straggling.

Elastic collisions between the incident (and secondary) electron and either the bound electrons or nuclei of the adsorber do not decrease the projected electron's energy but are responsible for the scattering that gives rise to range variation. The cross section of these two types of encounters is approximated by^(A-1),

$$\sigma_{\text{el}} = 1.3 \times 10^5 Z/E^2 \text{ barn/atom} \quad (5)$$

$$\sigma_{\text{nuc}} = 1.63 \times 10^4 Z^2/E^2 \text{ barn/atom} \quad (6)$$

where σ_{el} is evaluated for scattering up to $\pm 45^\circ$. For $Z = 14$ (silicon), $\sigma_{el}/\sigma_{nuc} = 0.57$. The significance of this ratio is that scattering from absorber nuclei can scatter electrons backwards while scattering from bound absorber electrons cannot. Since roughly 43 percent of the elastic collisions will be due to nuclear scattering, back scattering can occur, and the maximum of the energy deposition profile may not be at the absorber's surface. While relationships for the angular distribution of scattered electrons exist, their evaluation is quite another matter. A second aspect of the multiple scattering that accompanies electron absorption is that, because it is also a statistical process, an exact electron path length in the absorber cannot be calculated. The consequence of this phenomenon is that some electrons, those that are least scattered, penetrate deeper into the absorber than would be expected. As a consequence, the energy deposition curve would be expected to have a deep tail. This range straggle, due to elastic encounters, is superposed on the inelastic encounter energy straggle that was discussed previously.

The conversion of experimentally determined range-energy relations into energy deposition profiles can be realized through Monte Carlo computing techniques. A necessary preliminary simplification is that the statistical energy loss per event be replaced by the Bohr-Bethe, or continuous-slowng-down approximation^(A-4). This approximation replaces the actual electron path with a series of straight paths that connect high-angle scattering events. The Monte Carlo approach follows a single electron along this assumed path in the absorber, calculating energy loss and scattering angle at each event until the electron is thermalized. This calculation is repeated for a large number of electrons and the resultant energy loss in each strata is summed to give an energy deposition profile.

One of the better known complete programs for calculation of electron energy deposition profiles is ELTRAN^(A-3). An ELTRAN profile for the electron energy spectrum characteristic of Spire's pulsed electron beam systems, absorbed in silicon, is shown in Figure A-1. The validity of the Monte Carlo calculation approach has been confirmed by Everhart and Hoff^(A-5).

FIGURE A-1. ELECTRON BEAM ENERGY DEPOSITION PROFILE IN SILICON

Returning to the physics of electron absorption; since for a silicon absorber and $E_{\text{max}} = 40 \text{ keV}$ the energy loss to bremsstrahlung is negligible, and noting that the ultimate fate of electrons freed in ionizing encounters is excitation of some other atom, the absorption of electrons produces excited atoms that must decay to their ground state through radiationless transitions.

According to the quantum theory of solids, however, the energy levels of the absorber atoms are broadened into bands and the incident (and secondary) electrons interact with the absorber electrons in these bands. Further, these interactions are quantized such that one or more phonons is involved in each interaction. Since the emission of a phonon is formally equivalent to a change in lattice vibrational energy, classically identified as thermal energy, absorption of electrons corresponds to heating the absorber in the electron absorbing region. As a consequence, thermal conductivity considerations can be used to predict the magnitude and location of the temperature changes that are associated with electron absorption.

SECTION 2

THERMAL CHARACTERIZATION OF PULSED ENERGY ABSORPTION

As was just shown, the result of absorbing energetic electrons in a solid is localized heating. If this heating occurs within a period that is short in comparison to the time required for phonons to diffuse away from the heated region, i.e., the heating is adiabatic, the rapid thermal expansion of the heated region generates shock waves that are transmitted at sonic velocity through the (unheated) body of the absorber. If the transient pressure due to these shock waves is larger than the yield strength of the absorber, the latter will yield.

The first of the following subsections deals with calculation of temperatures in the absorber; the second subsection treats the necessary limitation on energy deposition due to shock wave generation. The figures referred to in this section are placed together in Section 3. (Note: Figure A-1, on p. A-4, is the exception.)

2.1 TEMPERATURE ANALYSIS

The temporal and spatial temperature variation of a solid absorber containing a localized thermal source can, in principle, be calculated from the defining heat transport relations^(A-6)

$$\nabla \cdot \bar{f} + \rho C_p (\partial T / \partial t) = \partial A / \partial t \quad (7a)$$

and

$$\bar{f} = -K \nabla T, \quad (7b)$$

where T is temperature; t is time; q is a spatial coordinate; ρ , C_p and K are, respectively, the absorber's density, (constant pressure) heat capacity and thermal conductivity, f is the heat flux; $A(q,t)$ is a time and position dependent source function; and $T(q,t)$ is a solution to the set of equations. The problem is to find a $T(q,t)$ that is a solution of (7a) and (7b) and satisfies the boundary conditions.

Consider the absorber to be a thick slab, normal to the z-axis of a rectangular coordinate system, that extends from the plane $z=0$ to the plane $z=L$, where the slab thickness, L , is sufficient that the slab appears to be infinitely thick within the time domain under consideration.

If the isotherms within the slab are planes that are parallel to the plane $z=0$, (7a) and (7b) can be reduced to their one-dimensional form

$$\partial(f_z)/\partial z + \rho C_p (\partial T/\partial t) = (\partial A/\partial t) \quad (8a)$$

and

$$f_z = -K(\partial T/\partial z). \quad (8b)$$

The conditions for this reduction are

$$\partial A(x,y,z,t)/\partial x = \partial A(x,y,z,t)/\partial y = 0, \quad (9)$$

i.e., that the source be uniformly distributed with respect to the x-y plane and

$$\partial \bar{f}/\partial x = \partial \bar{f}/\partial y \ll \partial f/\partial z, \quad 0 < t' \leq t, \quad (10)$$

i.e., the heat flux through the perimeter of the slab is small as compared to the heat flux through a $z=\text{constant}$ plane (in the slab) during the time domain being considered. Equation (9) is identically satisfied by the electron absorption process, if the incident beam is uniform. Except at the beam edges, this is essentially true. Equation (10) is satisfied if the depth of electron absorption (source thickness) is small as compared to the electron beam diameter and if, within the time domain of interest, the thermal conduction distance (proportional to $K/\rho C_p$) is also small as compared to the electron beam diameter. Since, as shown in Figure A-1, the electron absorption depth is of the order of 10^{-6} m while the beam diameter is of the order of 10^{-2} m, the first of these conditions is easily satisfied. That the second condition is also satisfied will be demonstrated later.

If the absorber's thermal conductivity, K , is

$$K \neq g(q, T), \quad (11)$$

i.e., it is isotropic and independent of temperature, (8a) and (8b) can be combined as

$$K(\partial^2 T / \partial z^2) - \rho C_p (\partial T / \partial t) = -\rho (\partial D / \partial t), \quad (12)$$

where $A(q, t)$ has been expressed in terms of the dose (energy/volume), $D(z, t)$, and the density term is due to the conventional dimensionality of D as energy/mass. The dose rate, $\partial D(z, t) / \partial t$, is defined from

$$\dot{F} \equiv \partial F(t) / \partial t = \rho \int_0^L [\partial D(z, t) / \partial t] dz, \quad (13)$$

where F is the fluence rate, or flux (energy/area-time), and the upper integration limit is for an absorber slab that behaves as though it were semi-infinite within the time domain of concern. Using the relation^(A-6)

$$\kappa = K / \rho C_p, \quad (14)$$

where κ is the thermal diffusivity, (12) can be written as

$$(\partial^2 T / \partial z^2) - (1/\kappa) (\partial T / \partial t) = (1/\kappa C_p) (\partial D / \partial t) \quad (15)$$

The applicable boundary condition on (15) is

$$\partial T(\zeta, \tau) / \partial \zeta = 0 \quad \zeta=0, \quad 0 \leq \tau \leq t \quad (16)$$

The implication of (16) is that radiative heat loss from the absorber's front surface is negligible as compared to (inward) conductive heat flow. This assumption will be justified later. For an initial ($t = t_0$) absorber temperature profile $T(\zeta, t_0)$, it can be shown that the temperature profile at any time, $t > t_0$, is given by^(A-7)

$$\begin{aligned}
T(z,t) = & [4\pi\kappa(t-t_o)]^{-\frac{1}{2}} \int_0^\infty \left\{ T(\zeta, t_o) \right. \\
& \times \left(\exp \left[-(z-\zeta)^2 / 4\kappa(t-t_o) \right] \right. \\
& \left. \left. + \exp \left[-(z+\zeta)^2 / 4\kappa(t-t_o) \right] \right) \right\} d\zeta.
\end{aligned} \tag{17}$$

If the initial ($t=t_o$) temperature profile is considered to result from the effects of an instantaneous (active from t_o to $t_o + \delta t_o$) plane source whose thermal strength is defined by

$$\Delta T(x, t_o) = (1/C_p) \left[\partial D(z, t_o) / \partial t \right] \delta t_o, \tag{18}$$

(17) can be written as

$$\begin{aligned}
\Delta T(z, t_o, t) = & (1/C_p) \left[4\pi\kappa(t-t_o) \right]^{-\frac{1}{2}} (\delta t_o) \\
& \times \int_0^\infty \left\{ \left[\partial D(\zeta, t_o) / \partial t \right] \left(\exp \left[-(z-\zeta)^2 / 4\kappa(t-t_o) \right] \right. \right. \\
& \left. \left. + \exp \left[-(z+\zeta)^2 / 4\kappa(t-t_o) \right] \right) \right\} d\zeta
\end{aligned} \tag{19}$$

Integrating (19) as the effects of a multiplicity of time dispersed plane sources that are active from $t=0$ to $t=t$ gives

$$\begin{aligned}
T(z,t) = (1/C_p) (1/4\pi\kappa)^{1/2} \int_0^t [1/(t-\tau)]^{1/2} \left\{ \int_0^\infty \right. \\
\left. \left[\partial D(\zeta, \tau) / \partial \tau \right] \left(\exp [-(z-\zeta)^2 / 4\kappa(t-\tau)] \right. \right. \\
\left. \left. + \exp [-(z+\zeta)^2 / 4\kappa(t-\tau)] \right) d\zeta \right\} d\tau.
\end{aligned} \tag{20}$$

Interchanging the order of integration (allowed because of the existence of the solution) and transforming the time basis of the source function from $D(\zeta, \tau)$ to $D(\zeta, t-\tau)$, (20) can be written as

$$\begin{aligned}
T(z,t) = (1/C_p) (1/4\pi\kappa)^{1/2} \int_0^\infty \left\{ \int_0^t (1/\tau)^{1/2} \left[\partial D(\zeta, t-\tau) / \partial (t-\tau) \right] \right. \\
\left. \times \left(\exp [-(z-\zeta)^2 / 4\kappa\tau] \right. \right. \\
\left. \left. + \exp [-(z+\zeta)^2 / 4\kappa\tau] \right) d\tau \right\} d\zeta.
\end{aligned} \tag{21}$$

For a time invariant dose rate (constant power) source

$$\partial D(z, t) / \partial t = G(z), \tag{22}$$

the source function can be removed from the time integral and (21) can be written as

$$\begin{aligned}
T(z,t) = (1/C_p) \int_0^\infty G(\zeta) \left\{ (1/\pi)^{1/2} \int_0^t (1/4\kappa\tau)^{1/2} \right. \\
\left. \times \left(\exp [-(z-\zeta)^2 / 4\kappa\tau] \right. \right. \\
\left. \left. + \exp [-(z+\zeta)^2 / 4\kappa\tau] \right) d\tau \right\} d\zeta \\
= (1/C_p) \int_0^\infty G(\zeta) H(\zeta) d\zeta,
\end{aligned} \tag{23}$$

where

$$H(\zeta) = (1/\pi)^{\frac{1}{2}} \int_0^t (1/4\kappa\tau)^{\frac{1}{2}} \left(\exp [-(z-\zeta)^2/4\kappa\tau] + \exp [-(z+\zeta)^2/4\kappa\tau] \right) d\tau. \quad (24)$$

Substituting

$$\beta_- = (z-\zeta), \quad \beta_+ = (z+\zeta) \quad (25a)$$

and

$$\phi = (1/4\kappa\tau)^{\frac{1}{2}} \quad (25b)$$

into (24) and making the corresponding change of integration limits gives

$$H(\zeta) = (1/\pi)^{\frac{1}{2}} (1/2\kappa) \int_{(1/4\kappa t)^{\frac{1}{2}}}^{\infty} (1/\phi^2) \times \left\{ \exp -[(\beta_-)\phi]^2 + \exp -[(\beta_+)\phi]^2 \right\} d\phi. \quad (26)$$

Integrating (26) by parts, and using the defining relations^(A-8)

$$\operatorname{erfc}(\eta) = (4/\pi)^{\frac{1}{2}} \int_{\eta}^{\infty} \exp(-\xi^2) d\xi = 1 - \operatorname{erf}(\eta) \quad (27a)$$

and

$$\operatorname{ierfc}(\eta) = (1/\pi)^{\frac{1}{2}} \exp(-\eta^2) - \eta \operatorname{erfc}(\eta) \quad (27b)$$

gives

$$H(\zeta) = (t/\kappa)^{\frac{1}{2}} \left\{ \operatorname{ierfc} [(|z-\zeta|)/(4\kappa t)^{\frac{1}{2}}] + \operatorname{ierfc} [(z+\zeta)/(4\kappa t)^{\frac{1}{2}}] \right\}, \quad (28)$$

where $\text{ierfc}(\eta)$, the first integral of the complementary error function^(A-9), is tabulated in the cited reference and the absolute value sign in the first term is imposed by the integration. Defining a characteristic distance, $\theta(t)$, by

$$\theta(t) = (4\kappa t)^{1/2} \quad (29)$$

$((\kappa t)^{1/2} = \text{length})$ allows (23) to be written as

$$\begin{aligned} T(z, t) = (\rho/2K) \theta(t) \int_0^\infty G(\zeta) \left\{ \text{ierfc} [(|z-\zeta|)/\theta(t)] \right. \\ \left. + \text{ierfc} [(z+\zeta)/\theta(t)] \right\} d\zeta. \end{aligned} \quad (30)$$

The absorbing slab's front ($z=0$) surface temperature, $T(0, t)$, from (30), is then

$$T(0, t) = (\rho/K) \theta(t) \int_0^\infty G(\zeta) \text{ierfc} [\zeta/\theta(t)] d\zeta. \quad (31)$$

For in-depth energy absorption, i.e., the incident energy is absorbed within a thickness, z , such that

$$0 \leq z \leq z_L, \quad (32)$$

where z_L is small compared to the slab thickness, (13) can be written as

$$\dot{F} = \rho \int_0^{z_L} G(\zeta) d\zeta. \quad (33)$$

For a time, t , sufficiently long that

$$\theta(t) \gg z_L, \quad (34)$$

or equivalently, in terms of a characteristic time, t_L (from (29))

$$t \gg t_L = (z_L)^2 / 4\kappa, \quad (35)$$

(31) can be written as

$$T(0, t)_D = (1/K) \theta(t) \dot{F} \int_0^{z_L} \text{ierfc}(\eta) d\zeta. \quad (36)$$

The value of $\text{ierfc}(\eta)$ at $\eta = 0$ is given by^(A-9)

$$\text{ierfc}(0) = 1/[2\Gamma(3/2)] = (1/\pi)^{1/2}. \quad (37)$$

Using (37) in (36) allows the late-time ($t \gg t_L$) surface ($z = 0$) temperature, for in-depth energy absorption to be expressible as

$$T(0, t)_D = (1/\pi)^{1/2} (1/K) \theta(t) \dot{F} \quad (t \gg t_L). \quad (38)$$

For surface energy absorption, defined as

$$G(\zeta) = (1/\rho) \dot{F} \delta(\zeta), \quad (39)$$

where $\delta(\zeta)$ is a delta function, the surface ($z = 0$) temperature, for all time, t , is, from (31), (37), and (39), given by

$$T(0, t)_S = (1/\pi)^{1/2} (1/K) \theta(t) \dot{F} \quad (40)$$

This result is identical to the late-time surface temperature, (38), that is produced by in-depth energy absorption. Consequently, the late-time ($t \gg t_L$) temperature that results from in-depth energy absorption can be approximated by the function (40) that gives the temperature for surface absorption. Thus

$$\begin{aligned} T(z, t) &= (1/K) \theta(t) \dot{F} \text{ierfc} [z/\theta(t)] \\ &= (\pi)^{1/2} T(0, t)_S \text{ierfc} [z/\theta(t)]. \end{aligned} \quad (41)$$

This result indicates that the late-time temperature, for in-depth energy absorption, is relatively insensitive to the exact shape of the electron energy deposition profile.

The absorber's late-time, $t \gg t_L$, surface-normalized, $T(z,t)/T(0,t)$, temperature, as a function of reduced depth, $z_R(t) = z/\theta(t)$, is plotted in Figure A-2. Note that by $z = \theta(t)$, one thermal diffusion length, $T(z)/T(0) \sim .1$, justifying the one-dimensional treatment of the problem. The reciprocal of the surface normalized temperature, a quantity that is more convenient for calculations, is shown in Figure A-3.

The temperature at any depth, z , at the end, $t = t_p$, of the electron-beam energy-deposition pulse is, from the first form of (41),

$$T(z, t_p) = (1/K) \theta(t_p) \dot{F} \text{ierfc} [z/\theta(t_p)] \quad (42)$$

Multiplying both sides of (42) by z and rearranging gives the dimensionless form

$$\begin{aligned} \dot{F} / (K [T(z, t_p) / z]) &= [z/\theta(t_p)] / \text{ierfc} [z/\theta(t_p)] \\ &= z_{Rp} / \text{ierfc} (z_{Rp}). \end{aligned} \quad (43)$$

Figure A-4 is a plot of the right side of (43) as a function of z_{Rp} .

At $t = t_p$, the ratio of the surface temperature $T(0, t_p)$ to the temperature at depth z , $T(z, t_p)$ is, using the second form of (41) and (37) for $T(0, t_p)$ and the first form of (41) for $T(z, t_p)$

$$T(0, t_p) / T(z, t_p) = T(0, t_p) / [(1/K) \theta(t_p) \dot{F} \text{ierfc} (z_{Rp})]. \quad (44)$$

The fluence, ΔF , necessary to produce this temperature distribution is

$$\Delta F = \dot{F} t_p \quad (45)$$

Substituting (45) in (44) and rearranging gives the dimensionless form

$$\Delta F / (k/\kappa) (z) T(z, t_p) = 1 / [4 z_{Rp} \text{ierfc} (z_{Rp})]. \quad (46)$$

Figure A-5 is a plot of the right side of (46) as a function of z_{Rp} .

The quantity of heat, Q , contained in a layer of thickness z that is at a temperature $T(z, t_p)$ is given by

$$dQ = \rho C_p dT dV = A \rho C_p T(z, t_p) dz, \quad (47)$$

where V is volume and A is area. The fraction, λ , of the incident energy that is effectively utilized in heating this thickness of absorber is obtained from integrating (47) with the first form of (41) for $T(z, t_p)$. The result is

$$\lambda(z, t_p) = 1 - 4 i^2 \text{erfc}(z_{Rp}) \quad (48)$$

Figure A-6 is a plot of the right side of (48) as a function of z_{Rp} .

The thermal radiation loss, H_R , from the absorber's front face is given by

$$H_R = \epsilon \sigma T^4, \quad (49a)$$

where ϵ is the emissivity and σ is the Stefan-Boltzmann constant. Since maximum radiation loss will occur when the front surface is at melt temperature, a worst case value for H_R is

$$\begin{aligned} H_R &= (0.5)(5.67 \times 10^{-12})(1685)^4 \\ &\approx 23 \text{ W/cm}^2 \end{aligned} \quad (49b)$$

A typical electron-beam fluence for this work is $\sim 1 \text{ J/cm}^2$. This energy is delivered in $\sim 1 \times 10^{-5}$ s. The incident power, H_T , is then

$$H_T \approx (1) / 1 \times 10^{-5} = 10^5 \text{ W/cm}^2. \quad (50)$$

Since the conduction loss, H_c is

$$H_c = H_T - H_R \approx H_c, \quad (51)$$

ignoring radiation losses is fully justified.

2.2 PRESSURE PULSE CONSIDERATIONS

When energy is deposited in a media so rapidly that pressure relaxation, via thermal expansion, is negligible within the time domain of interest, the absorption occurs at constant volume. The amplitude of the pressure pulse that is generated by the energy absorption is obtained from the Gruneisen constant, γ . The latter is given by^(A-10)

$$\gamma = V(\partial p / \partial U)_V = (\partial p / \partial u)_V, \quad (52)$$

where p is pressure, V is volume, U is internal energy and u is internal energy/unit volume. Equating the deposited dose, D , to the internal energy change, and transforming (52) to differential form gives

$$\Delta p|_V = \gamma \Delta u|_V = \rho \gamma \Delta D, \quad (53a)$$

where the density factor is again due to the conventional dimensionality of D as energy/mass. The spatial dependence of the energy absorption produces the same spatial dependence of the pressure pulse. Thus (53a) can be written as

$$\Delta p(z) = \rho \gamma \Delta D(z). \quad (53b)$$

For one-dimensional energy deposition, two equal pressure pulses, of amplitude $\Delta p(z)/2$, depart in opposite directions, from their plane of production, at the acoustic velocity of the absorber. If the energy deposition occurs near the absorber's front surface, the acoustic wave approaching the front of the absorber is reflected, with amplitude reversal. Ultimately then, a bipolar pressure pulse moves through the absorber with velocity v_0 . From (53b), this pressure is

$$\begin{aligned} \Delta p(z, t) &= \Delta p(z - v_0 t)/2 - \Delta p(v_0 t - z)/2 \\ &= (\Delta p_0) [\phi(z - v_0 t)]/2, \end{aligned} \quad (54)$$

where Δp_0 is the peak value of $\Delta p(z)$ and $\phi(z - v_0 t)$ is the peak normalized pressure wave shape.

The fluence, ΔF , that is associated with the energy deposition, $\Delta D(z)$, is

$$\begin{aligned}
 \Delta F &= \int_0^{\infty} \rho \Delta D(z) \, dz \\
 &= \rho \Delta D_0 \int_0^{\infty} \left([\Delta D(z)] / (\Delta D_0) \right) dz \\
 &= \rho \Delta D_0 z_D,
 \end{aligned} \tag{55}$$

where ΔD_0 is the peak value of $\Delta D(z)$ and z_D is the effective width of the dose profile. Substituting from (54) and (55) into (53a) gives

$$\begin{aligned}
 \Delta p_0 / 2 &= \rho \gamma \Delta D_0 / 2 \\
 &= \gamma \Delta F / 2 z_D
 \end{aligned} \tag{56}$$

for the relation between fluence and peak pressure.

For an energy deposition that is extended in time, the resulting pressure pulse is derived from a sum of instantaneous energy depositions

$$\Delta D(z) = [\partial D(z, t) / \partial t] \Delta t = \dot{D}(z, t) \Delta t \tag{57}$$

such that, from (56)

$$\begin{aligned}
 \Delta p_0(\tau) &= \rho \gamma \Delta D_0(\tau) / 2 \\
 &= [\gamma \dot{F}(\tau) / 2 z_D] \Delta t
 \end{aligned} \tag{58}$$

and, from (54)

$$p(z,t) = (\gamma/2z_D) \int \dot{F}(\tau) \phi[z-v_o(t-\tau)] d\tau. \quad (59)$$

For a time invariant dose rate (constant power),

$$\dot{F} \neq g(t) \quad (60)$$

and (59) can be written as

$$p(z,t) = (\gamma\dot{F}/2z_D) \int \phi[z-v_o(t-\tau)] d\tau. \quad (61)$$

The maximum of $p(z,t)$ occurs when only one of the lobes of the bipolar pressure pulse is within the time domain of the integration.

A Gaussian energy deposition profile is both analytically trackable and a reasonable representation of actual electron energy deposition profiles. For the Gaussian dose

$$\Delta D(z) = \Delta D_o \exp[-z^2/a^2], \quad (62)$$

the corresponding fluence is, from (55),

$$\Delta F = (\pi/4)^{1/2} a \rho \Delta D_o, \quad (63)$$

where z_D can be formally identified as

$$z_D = (\pi/4)^{1/2} a. \quad (64)$$

The instantaneous temperature profile is then, by definition,

$$\begin{aligned} \Delta T(z) &= (1/C_p) \Delta D(z) \\ &= (4/\pi)^{1/2} (1/a\rho C_p) \Delta F \exp(-z^2/a^2) \\ &= \Delta T_o \exp(-z^2/a^2) \end{aligned} \quad (65)$$

With this initial temperature, the solution to the one-dimensional heat flow equation, (15) with $\dot{D} = 0$, is

$$\Delta T(z, t) = \left[1/(1 + t/t_0)\right]^{1/2} \Delta T_0 \times \exp \left[-(z^2/a^2)/(1 + t/t_0)\right], \quad (66)$$

where ΔT_0 is from (65) and

$$t_0 = a^2/4\kappa. \quad (67)$$

The absorber's surface ($z = 0$) temperature is, from (66),

$$\Delta T(0, t) = \left[1/(1 + t/t_0)\right]^{1/2} \Delta T_0. \quad (68)$$

If the fluence pulse is extended in time, the resulting temperature profile is produced by the sum of the instantaneous energy depositions, in analogy with (57),

$$\Delta D(z, t) = \Delta D_0(t) \exp(-z^2/a^2), \quad (69)$$

where, from (63),

$$\Delta D_0(t) = \dot{D}_0(t) \Delta t = (4/\pi)^{1/2} (1/a\rho) \dot{F} \Delta t. \quad (70)$$

Using (70) in (68) and integrating gives

$$T(0, t) = (4/\pi)^{1/2} (1/a\rho C_p) \int_0^t \left\{1/[1 + (t-\tau)/t_0]\right\}^{1/2} \dot{F}(\tau) d\tau. \quad (71)$$

If $F \neq g(t)$, the maximum surface temperature for an energy deposition pulse of length t_p is, from (71),

$$\begin{aligned}\Delta T_{\max} &= T(0, t_p) \\ &= (1/\pi)^{1/2} (4/a\rho C_p) [(1 + t_p/t_o)^{1/2} - 1] t_o \dot{F}.\end{aligned}\tag{72}$$

The fluence, ΔF , required to reach this temperature is

$$\begin{aligned}\Delta F &= \dot{F} t_p \\ &= (\pi)^{1/2} (a\rho C_p/4) \Delta T_{\max} \\ &\quad \times \left\{ (t_p/t_o) / [(1 + t_p/t_o)^{1/2} - 1] \right\}.\end{aligned}\tag{73}$$

In terms of the assumed Gaussian energy deposition profile, the peak pressure, developed only if $t_p \gg z_D/v_o$, is, from (61) and (55)

$$\begin{aligned}\Delta p_{\max} &= (\gamma \dot{F}/2z_D) \int_0^\infty \phi(v_o \tau) d\tau \\ &= \gamma \dot{F}/2v_o\end{aligned}\tag{74a}$$

$$= \gamma F/2v_o t_p.\tag{74b}$$

The ratio of $\Delta p_{\max}$ to $\Delta T_{\max}$ is, from (72) and (74b),

$$\begin{aligned}\Delta p_{\max}/\Delta T_{\max} &= (\pi/64)^{1/2} (a\gamma\rho C_p/v_o t_o) \\ &\quad \times \left\{ 1/[1 + t_p/t_o]^{1/2} - 1 \right\}.\end{aligned}\tag{75}$$

Note that this ratio is independent of fluence.

Figure A-7 shows the comparison between a (peak-normalized) Monte Carlo calculation by Spencer^(A-11) of a monoenergetic ($25 \leq E_{\text{keV}} \leq 200$) electron energy-deposition profile in Al and a (peak-normalized) Gaussian profile of equal area. The ordinate of Figure A-7 is also normalized as

$$y = r/r_o = \rho z/z_o, \quad (76a)$$

where for Al, and quite closely for Si,

$$r_o \approx (E_{\text{kev}}^{1.73})/155 \text{ mg/cm}^2 \quad (76b)$$

Since

$$\exp(-\pi y^2) = \exp(-\pi \rho^2 z^2 / r_o^2) = \exp(-z^2/a^2), \quad (77a)$$

then

$$\rho a = r_o/(\pi)^{1/2} \approx (E_{\text{kev}}^{1.73})/275 \text{ mg/cm}^2. \quad (77b)$$

The characteristic thermal time, t_o , from (67) and (77b) is

$$\begin{aligned} t_o &= a/4\kappa = (\rho a)^2/4\rho^2\kappa \\ &= C_p/4\rho K \left[(E_{\text{kev}}^{1.73})/275 \right]^2. \end{aligned}$$

Figure A-8 is a plot of t_o as a function of E for temperature range-average values of C_p and K :

$$\bar{C}_p = .92 \text{ J/g-K}^\circ$$

$$K = .48 \text{ W/cm-K}^\circ.$$

The approximate velocity of sound and the Gruneisen constant for Si are:

$$v_o \approx 1.3 \times 10^4 \text{ m/s}$$

$$\gamma \approx 1.9.$$

Figure A-9 is a graph of peak pressure as a function of pulse width from (74). Figure A-10, a plot of (75), shows the ratio of peak pressure to peak temperature as a function of electron energy with pulse width as a parameter. Figure A-11 is a plot of the fluence per degree increase in surface temperature, $\Delta F/\Delta T_{\max}$, as a function of electron beam energy with pulse width as a parameter. This relation is plotted from (73)/(74).

SECTION 3

MODEL APPLICATION

In order to make the results developed in Section 2 readily available, these results, in the form of graphs, are included in this section along with an explanation of their interpretation. The section concludes with two examples of the use of these results.

3.1 GRAPHICAL RESULTS

Figures A-2 - A-6 and A8 - A11 present the numeric results of the model that has been developed. Figure A-7 is an energy deposition profile. The results have been calculated in normalized form so as to be universally applicable. Since these results are the solution to the differential equations of heat conductivity, they are applicable to materials other than silicon by scaling of the material's diffusivity.

3.1.1 Temperature Profile (Figure A-2)

Figure A-2 is the temperature profile in the absorber at a time after the pulse that is long compared to the length of the pulse. It is plotted with the ratio of the temperature at any depth to the surface temperature as ordinate and the ratio of the depth to the characteristic thermal distance as abscissa. This reduced depth is used as the abscissa in Figures A-2 - A-6. For fixed depth, the reduced depth is proportional to the reciprocal of the square root of time and to the reciprocal of the square root of the material's thermal diffusivity. While Figure A-2 can be used to calculate the temperature at any depth, for a given surface temperature and time, this calculation is more conveniently done from Figure A-3. The principal attribute of Figure A-2 is to illustrate the very rapid decrease in temperature with depth that is characteristic of pulse heating.

3.1.2 Reciprocal Temperature Profile (Figure A-3)

Figure A-3 is a graph of the same information that was displayed in Figure A-2 except that the reciprocal of the surface normalized temperature is used as ordinate. Lower curvature allows more accurate interpolation. The principal use of this curve is determining the temperature at a given depth for a known surface temperature and time. This allows a calculation of, for example, the thickness of the film that can be

brought to melt temperature, T_m , for a heating pulse that produces a given surface temperature, or, conversely, the surface temperature that would result from an arbitrary heating pulse that raised some given depth to T_m .

3.1.3 Temperature at Depth/Unit Flux (Figure A-4)

The ordinate in Figure A-4 is in reality the reciprocal of the temperature, at any depth, for unit heating flux. This curve is used either to determine the temperature at a given depth for known incident flux or to establish the flux that is required to bring a given depth to a given temperature. Note that the abscissa is now normalized to the characteristic distance associated with a given pulse width since the ordinate is pulse width dependent.

3.1.4 Temperature at Depth/Unit Fluence (Figure A-5)

The ordinate in Figure A-5 is the reciprocal of the temperature, at any depth, for unit heating fluence. Since this quantity is also pulse width dependent, the abscissa is again normalized to the characteristic distance associated with a given pulse width. This curve is used to establish the temperature at a given depth for known fluence or to estimate the fluence required to bring a given depth to a given temperature.

3.1.5 Energy Efficiency (Figure A-6)

The abscissa in Figure A-6 is the fraction of the total deposited heat that is utilized in heating a given thickness of absorber. For given reduced absorber thickness, again referred to the characteristic distance associated with a given pulse width, heat not deposited in that thickness will be absorbed in material located behind the layer of interest. Since this curve is dependent only on pulse width, for a given material, it is used to insure that the selected heating pulse, in terms of energy utilization, is a reasonable one.

3.1.6 Gaussian Energy Deposition (Figure A-7)

Figure A-7 is a normalized Gaussian energy deposition profile. This figure also displays a calculated electron energy deposition profile for comparison. Figure A-7 is used for determining the characteristics of the energy deposition process.

3.1.7 Gaussian Characteristic Time (Figure A-8)

Figures A-9 - A-11 are based on the Gaussian energy deposition profile shown in Figure A-7. The ordinate in Figure A-8 is incident electron energy and the abscissa is the characteristic thermal time, a function of material parameters, associated with the Gaussian deposition profile. For given incident electron energy, this curve gives the characteristic thermal time. The pulse width of the heating pulse must be short as compared to this time for the model to be applicable.

3.1.8 Maximum Pressure (Figure A-9)

Figure A-9 has the maximum pressure for unit fluence as ordinate and the characteristic time for a given pulse width as abscissa. For a given fluence and pulse width, the curve gives the maximum pressure developed.

3.1.9 Pressure/Temperature Ratio (Figure A-10)

The ordinate in Figure A-10 is peak pressure divided by peak temperature. The abscissa is incident electron beam energy. Pulse width is the parameter. This curve is used to determine the peak pressure for a given process temperature, pulse width and electron beam energy.

3.1.10 Fluence Requirement (Figure A-11)

The ordinate in Figure A-11 is, in reality, the fluence necessary to raise the absorber to the required process temperature. The abscissa is incident electron energy and the parameter is pulse width. Note that pulse width is only important at lower electron energies. This curve gives the fluence necessary for the heating task at hand.

3.2 SAMPLE CALCULATIONS

3.2.1 Maximum Film Thickness for Existing Equipment

The presently used pulsed electron beam system is characterized by:

$$\Delta F_{\max} \approx 8.4 \times 10^3 \text{ J/m}^2,$$
$$t_p \approx 1 \times 10^{-7} \text{ s.}$$

The object is to determine the maximum thickness of silicon film that can be heated to melt temperature, T_m , with this equipment.

The system characteristics give:

$$\dot{F}_{\max} = \Delta F_{\max} / t_p \approx 8.4 \times 10^{10} \text{ W/m}^2,$$

$$\theta(t_p) = (4\kappa t_p)^{1/2} \approx 3 \times 10^{-6} \text{ m}.$$

The next step is to calculate the temperature at some large depth, 1×10^{-6} m, say. Entering Figure A-5 for $z/\theta(t_p) = 1/3$,

$$\Delta F / (K/\kappa) (1 \times 10^{-6}) T(1 \times 10^{-6}, 1 \times 10^{-7}) \approx 2.5.$$

Using temperature range average approximations to the values of K and κ gives

$$T(1 \times 10^{-6}, 1 \times 10^{-7}) = 1560^\circ\text{K},$$

which is below silicon's melting temperature ($T_m = 1690^\circ\text{K}$).

Consequently, a beam of these characteristics will not produce melting temperature at a depth of 1×10^{-6} m.

Next examine the temperature at a depth of $.3 \times 10^{-6}$ m. Entering Figure A-5 for $z/\theta(t_p) = .1$,

$$\Delta F / (K/\kappa) (.3 \times 10^{-6}) T(.3 \times 10^{-6}, 1 \times 10^{-7}) \approx 5.3,$$

and hence

$$T(.3 \times 10^{-6}, 1 \times 10^{-7}) \approx 2450^\circ\text{K},$$

which is above T_m . Consequently, an electron beam with the given characteristics will produce a temperature above the melting point of silicon at a depth of $.3 \times 10^{-6}$ m.

If the beam has sufficient total energy to supply the heat of fusion as well as produce the desired temperature rise, the $.3 \times 10^{-6}$ m layer will melt. Using

$$H_E = \rho C_p (T_{.3} - T_m)$$

for an estimate of the energy supplied in excess of that required to heat the $.3 \times 10^{-6}$ m thick layer to T_m gives $H_E \approx 392$ cal/g. This, within the accuracy of the calculation, is nearly equal to the heat of fusion, $H_f = 430$ cal/g. It may therefore be concluded that an electron beam of the given characteristics will melt a silicon film approximately $.3 \times 10^{-6}$ thick.

3.2.2 Equipment Parameters for Melting a 50×10^{-6} m Film

This calculation begins with an estimate of the minimum energy necessary to heat a 50×10^{-6} m thick silicon film to T_m and to supply the heat of fusion, H_f . This is

$$H_T = H_f + \rho \bar{C}_p \Delta T \approx 3.6 \times 10^5 \text{ j/m}^2.$$

The energy required to heat this layer to T_m , alone, is

$$H_m = \rho C_p \Delta T \approx 1.5 \times 10^5 \text{ j/m}^2.$$

The ratio of $H_m/H_T \approx .41$. Entering Figure A-7 (Gaussian) at $D(y)/D_{\max} = .41$ gives $y \approx .53$. For $y = r/r_o$ and $r = 50 \times 10^{-6}$ m,

$$r_o = 94 \times 10^{-6} \text{ m}$$

and from

$$r_o \approx (E^{1.73})/155,$$

$E = 110$ keV.

Entering Figure A-8 at 110 keV gives $t_o \approx 30 \times 10^{-6}$ s. Consequently, a 110 keV electron pulse with a pulse width of 1×10^{-6} s should melt a 50×10^{-6} m thick film with little heating of the substrate.

The fluence required to melt the film surface (and its full 50×10^{-6} m depth) is obtained from the peak surface temperature, T_o , and

$$\Delta T_o = 2 \Delta F / (\pi)^{1/2} a \rho C_p.$$

Taking ΔT_o as

$$\Delta T_o = T_m + H_m / C_p \approx 3375^\circ \text{C}$$

gives

$$\Delta F \approx 6 \times 10^5 \text{ J/m}^2.$$

The maximum pressure is obtained by entering Figure A-9 for $t_p = 1 \times 10^{-6}$ s and obtaining

$$\Delta p_{\max} / \Delta F \approx 7.2 \times 10^{-4} \text{ bar.}$$

Multiplying by the calculated F gives

$$\Delta p_{\max} \approx 430 \text{ bar.}$$

Since this value is less than the $\sim 1 \times 10^3$ bar yield strength, the film will not fracture.

In summary then, a 110 keV beam with a pulse width of 1×10^{-6} s and a fluence of $6 \times 10^5 \text{ J/m}^2$ would be required to melt a 50×10^{-6} m thick silicon film.

$$\frac{T(z,t)}{T(0,t)}$$

FIGURE A-2. SURFACE NORMALIZED TEMPERATURE AS A FUNCTION OF REDUCED DEPTH FOR $t \gg t_L$

FIGURE A-3. RECIPROCAL OF SURFACE NORMALIZED TEMPERATURE AS A FUNCTION OF REDUCED DEPTH FOR $t \gg t_L$

FIGURE A-4. DIMENSIONLESS TEMPERATURE AT ANY DEPTH AS A FUNCTION OF REDUCED DEPTH AT THE END OF THE ENERGY DEPOSITION PULSE

FIGURE A-5. FLUENCE REQUIRED TO PRODUCE SPECIFIED SURFACE AND SUBSURFACE TEMPERATURE AT THE END OF THE ENERGY DEPOSITION PULSE

FIGURE A-6. HEAT UTILIZATION EFFICIENCY

FIGURE A-7. GAUSSIAN AND SPENCER ELECTRON ENERGY DEPOSITION PROFILES IN ALUMINUM

A-35

E
(keV)

FIGURE A-8. CHARACTERISTIC THERMAL TIME, t_0 , FOR A GAUSSIAN ELECTRON ENERGY ABSORPTION PROFILE AS A FUNCTION OF ELECTRON ENERGY

FIGURE A-9. MAXIMUM PRESSURE FOR A GIVEN FLUENCE AS A FUNCTION OF PULSE WIDTH

FIGURE A-10. RATIO OF PEAK PRESSURE TO PEAK TEMPERATURE AS A FUNCTION OF ELECTRON ENERGY

FIGURE A-11. FLUENCE PER DEGREE INCREASE IN SURFACE TEMPERATURE AS A FUNCTION OF ELECTRON ENERGY

REFERENCES

- A-1. R. D. Evans, The Atomic Nucleus, p. 607. McGraw-Hill, New York (1955).
- A-2. Ibid., p. 617.
- A-3. F. H. Brittain, RSIC Computer Code Collection, ORNL CCC-155; also Sandia Labs. SC-TM-68-713 (1968).
- A-4. M. J. Berger and S. M. Seltzer, Nat. Acad. Sci. - Nat. Res. Council Publ. No. 1133, p. 205 (1964).
- A-5. T. E. Everhart and P. H. Hoff, J. Appl. Phys. 42, 5837 (1971).
- A-6. H. S. Carslaw and J. C. Jaeger, Conduction of Heat in Solids, pp. 1.5 and 1.6. Oxford, London (1959).
- A-7. Ibid., pp. 10.8 and 10.10.
- A-8. Ibid., Appendix II.
- A-9. National Bureau of Standards, Handbook of Mathematical Functions, pp. 7.2.7 and 6.1.9. M. Abramowitz and I. A. Stegun, Eds., Government Printing Office, Washington (1975).
- A-10. C. Kittel, Introduction to Solid State Physics, p. 154. Wiley, New York (1956).
- A-11. National Bureau of Standards, Energy Dissipation by Fast Electrons. L. V. Spencer, Government Printing Office, Washington (1959).

APPENDIX B

CLINE AND ANTHONY HEATING ANALYSIS

For shallow absorption of electron beam deposited energy (compared to the characteristic distance for thermal diffusion), the steady state solution to the heating of a medium by a scanning beam is given by Cline and Anthony^(B-1). Using their notation,

X = direction of scan
 Z = depth of material
 Y = perpendicular to scanning direction
 V = scan velocity
 D = material diffusivity (formerly K, constant)
 C = specific heat per unit volume (constant)
 P = total beam power (absorbed)
 T = temperature

All dimensions are relative to the current location of the center of the Gaussian profile beam spot, FWHM radius R. (Note that the Gaussian radial profile of beam power is not the same as the deposition profile discussed in Appendix A.)

$$T = fP/CDR \quad (1)$$

where the function f is given by

$$f = \int_0^{\infty} \exp(-H) / \left[(2\pi^3)^{1/2} (1+\mu^2) \right] d\mu \quad (2)$$

and H is defined as

$$H = \left[(X/R + \rho\mu^2/2)^2 + (Y/R)^2 \right] / \left[(1+\mu^2) + (Z/R)^2 / 2\mu^2 \right] \quad (3)$$

$$\mu^2 \equiv 2Dt' / R^2$$

$$\rho \equiv RV/D$$

Here t' is the real integration variable as Equation (2) sums the contribution to the temperature T from all earlier times that the beam was scanning before reaching the point $X/R = Y/R = 0$. The solution for f , the normalized temperature, is given by Figures 3, 4, 5 and 6 of Reference (B-1) and Figure B-1, computed for $Z/R = 0$ and $RV/D = 1$. The last assumption is for a slow scanning beam where the maximum electron range is small compared to R . For a fast scanning beam, $RV/D \geq 20$ and the maximum temperature will be confined to the region of direct deposition (i.e., where electrons are absorbed) that is ignored here.

For calculations, assume $D = 0.224 \text{ cm}^2/\text{s}$ (crystal silicon) and $C = 2.14 \text{ J/cm}^3\text{-}^\circ\text{C}$. To melt the material we can use an equivalent temperature, $T = T_m + H_m/C \cong 3375^\circ\text{C}$, noting that the theory does not really account for a change in phase. With $RV/D=1$, the maximum normalized temperature f is 0.14, so that from Equation (1):

$$RV = 0.224 \text{ cm}^2/\text{s}$$

$$P/R = 4.8 \text{ kW/cm to reach } T_m$$

$$P/R = 11.6 \text{ kW/cm to melt the surface}$$

This assumed a shallow-deposition-profile, low-electron-energy beam. The error introduced can be computed from Appendix A results. For a thin profile

$$T_o = \dot{F} (4t_p/\pi K\rho C)^{1/2} \quad (4)$$

(see Equation (40) in Appendix A and for a Gaussian deposition profile

$$T_o = \dot{F} (4t_p/\pi K\rho C)^{1/2} \times \left\{ \left[(t_o/t_p) + 1 \right]^{1/2} - (t_o/t_p)^{1/2} \right\} \quad (5)$$

from Equation (73) in Appendix A). Here T_o is the surface temperature, t_p is the pulse width, and t_o is the characteristic thermal diffusion time for the electron beam depth dose profile (see Appendix A). The fractional difference is plotted as a function of t_o/t_p in Figure B-2. For long pulse widths, or slowly scanning beams, the correction factor approaches unity.

FIGURE B-1. SELECTED SURFACE ($Z/R=0$) VALUES OF f ON THE X-Y HALF-PLANE FOR $RV/D=1$

FIGURE B-2. CORRECTION TO THIN SURFACE DEPOSITION ASSUMPTION AS A FUNCTION OF PULSE WIDTH

As an example, consider a 10-keV electron beam. The maximum range in silicon is about $1.5\mu\text{m}$, giving $t_o = 7.9\text{ ns}$ for a characteristic thermal diffusion time. For a realistic beam focus:

$$R = 0.005\text{ cm} = 50\text{ }\mu\text{m} \text{ (4 mils)}$$

$$V = 45\text{ cm/s}$$

$$I = 6\text{ mA}$$

to melt the surface of the sample. The correction (see Figure B-2) is negligible as $t_p \cong 2V/R = 0.22\text{ ms}$ and t_o/t_p is less than 4×10^{-5} .

REFERENCES

- B-1. H.E. Cline and T. R. Anthony, J. Appl. Phys. 48, 3895 (1977).