

SC5373.4FTR

SC5373.4FTR

Copy No. 10

PRODUCIBLE ALTERNATIVE TO CdTe FOR EPITAXY (PACE-2) OF LWIR HgCdTe

FINAL TECHNICAL REPORT FOR THE PERIOD
August 1, 1983 through July 31, 1984

AD-A150 678

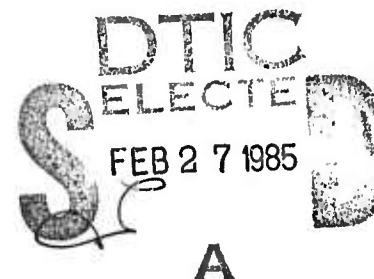
CONTRACT NO. MDA903-83-C-0379

Prepared for
Defense Advanced Research Projects Agency
1400 Wilson Boulevard
Arlington, VA 22209

E.R. Gertner
Principal Investigator

NOVEMBER 1984

Sponsored by
Defense Advanced Research Projects Agency (DoD)
DARPA Order No. 3704, Amd 7
Under Contract No. MDA903-83-C-0379 issued by
Department of Army, Defense Supply Service-Washington
Washington, DC 20310



DTIC FILE COPY

"The views and conclusions contained in this document are those of the authors and should not be interpreted as representing the official policies, either expressed or implied, of the Defense Advanced Research Projects Agency or the U.S. Government."



Rockwell International
Science Center

This document has been approved
for public release and sale; its
distribution is unlimited.

85 02 11 002

UNCLASSIFIED

SECURITY CLASSIFICATION OF THIS PAGE

REPORT DOCUMENTATION PAGE

1a. REPORT SECURITY CLASSIFICATION Unclassified		1b. RESTRICTIVE MARKINGS	
2a. SECURITY CLASSIFICATION AUTHORITY		3. DISTRIBUTION/AVAILABILITY OF REPORT Approved for public release; distribution unlimited.	
2b. DECLASSIFICATION/DOWNGRADING SCHEDULE			
4. PERFORMING ORGANIZATION REPORT NUMBER(S) SC5373.4FTR		5. MONITORING ORGANIZATION REPORT NUMBER(S)	
6a. NAME OF PERFORMING ORGANIZATION Rockwell International Science Center	6b. OFFICE SYMBOL (If applicable)	7a. NAME OF MONITORING ORGANIZATION	
6c. ADDRESS (City, State and ZIP Code) 1049 Camino Dos Rios Thousand Oaks, CA 91360		7b. ADDRESS (City, State and ZIP Code)	
8a. NAME OF FUNDING/SPONSORING ORGANIZATION Defense Advanced Research Projects Agency	8b. OFFICE SYMBOL (If applicable)	9. PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER Contract No. MDA903-83-C-0379	
8c. ADDRESS (City, State and ZIP Code) 1400 Wilson Boulevard Arlington, VA 22209		10. SOURCE OF FUNDING NOS.	
		PROGRAM ELEMENT NO. 62301E	PROJECT NO. DARPA NO. 3704, Amd 7
11. TITLE (Include Security Classification) PRODUCIBLE ALTERNATIVE TO CdTe FOR EPITAXY (PACE-2) OF LWIR HgCdTe (U)		TASK NO. PROGRAM CODE 3E20	WORK UNIT NO.
12. PERSONAL AUTHOR(S) Gertner, Edward R.			
13a. TYPE OF REPORT Final Technical Report	13b. TIME COVERED FROM 08/01/83 TO 07/31/84	14. DATE OF REPORT (Yr., Mo., Day) NOVEMBER 1984	15. PAGE COUNT 55
16. SUPPLEMENTARY NOTATION The views and conclusions contained in this document are those of the authors and should not be interpreted as representing the official policies, either expressed or implied, of the Defense Advanced Research Projects Agency or the United States Government.			
17. COSATI CODES		18. SUBJECT TERMS (Continue on reverse if necessary and identify by block number)	
FIELD	GROUP	SUB. GR.	
19. ABSTRACT (Continue on reverse if necessary and identify by block number) This is the final report of the first phase of a program whose objective is the development of a long wave infrared (LWIR) HgCdTe material technology based on heteroepitaxial growth on low cost substrates and to advance this technology to device processing and ultimately focal plane array demonstration. A matrix of five growth techniques and three base substrates (GaAs, Ge and Si) were used to identify the most promising approach. Three epitaxial vapor growth techniques, Laser Assisted Deposition and Annealing (LADA), Molecular Beam Epitaxy (MBE) and Organo-Metallic Vapor Phase Epitaxy (OMVPE) were used to grow epitaxial layers of CdTe on the base substrates. Single crystalline layers of CdTe with near-bulk qualities were obtained on all three base substrates (GaAs, Ge, Si) by all three CdTe vapor growth techniques (LADA, MBE, OM-VPE). OM-VPE growth CdTe on GaAs had the highest crystallinity as determined by x-ray double crystal diffraction. The growth of an additional CdTe layer by Liquid Phase Epitaxy (LPE) improved by the crystallinity of the vapor grown CdTe, but often resulted			
20. DISTRIBUTION/AVAILABILITY OF ABSTRACT UNCLASSIFIED/UNLIMITED ☐ SAME AS RPT. ☐ DTIC USERS ☐		21. ABSTRACT SECURITY CLASSIFICATION	
22a. NAME OF RESPONSIBLE INDIVIDUAL		22b. TELEPHONE NUMBER (Include Area Code)	22c. OFFICE SYMBOL

(Continued from Block 19)

in higher impurity levels of base substrate elements in the epitaxial CdTe layer due to slight chemical attack of the base substrate during the CdTe LPE cycle.

LPE and Isothermal VPE (ISO-VPE) were used for the epitaxial growth of the active HgCdTe layer. Isothermal VPE grown HgCdTe had the desired p-type conduction when grown on high quality PACE-2 substrates; i.e, those with high crystallinity and low impurity background. LPE growth of HgCdTe, in contrast to CdTe LPE, on PACE-2 substrates resulted in severe chemical attack of the base substrate yielding epitaxial HgCdTe layers of inferior quality. Based on these results, a baseline approach (plush back-up alternates) has been selected for the next phase. The baseline approach will be OM-VPE grown CdTe on GaAs followed by isothermal VPE of HgCdTe. This combination of substrate and growth techniques appears to be the best venue toward obtaining the desired HgCdTe qualities needed for high device performance.

Originator furnished keywords include:

52-104731 (Field 18)



SC5373.4FTR

TABLE OF CONTENTS

	<u>Page</u>
1.0 INTRODUCTION.....	1
2.0 BACKGROUND.....	3
3.0 OBJECTIVES.....	4
4.0 APPROACH.....	5
5.0 MATERIAL CHARACTERIZATION TECHNIQUES.....	20
6.0 RESULTS.....	21
6.1 Morphology.....	22
6.2 IR Spectroscopy.....	35
6.3 Double Crystal X-Ray Diffraction.....	37
6.4 Cathodoluminescence.....	40
6.5 SIMS Analysis and Results.....	43
6.6 Hall Effect Measurements.....	47
7.0 SUMMARY AND SELECTED BASELINE APPROACH.....	48
8.0 REFERENCES.....	50

Accession For	
NTIS GRA&I	☒
DTIC TAB	☐
Unannounced	☐
Justification	
In addition/	
Availability Codes	
and/or	
Special	
A-1	





LIST OF ILLUSTRATIONS

<u>Figure</u>		<u>Page</u>
1	The LADA apparatus.....	7
2	MBE apparatus.....	9
3	Schematic of the MBE apparatus.....	10
4	Simplified OM-VPE flow diagram schematic.....	11
5	Phase diagram for HgCdTe. Dotted lines are connecting lines between liquidus and solidus points, λ_c at 77K.....	13
6	Isothermal VPE growth apparatus.....	15
7	Composition of ISO-VPE $Hg_{1-x}Cd_xTe$ as a function of growth temperature.....	16
8	Relationship between HgCdTe composition and Te/Hg ratio of source in ISO-VPE at 500°C.....	17
9	Morphology and x-ray Laue diffraction of LADA CdTe/GaAs.....	23
10	MBE grown CdTe/GaAs. Surface morphology and cross-section.....	24
11	LPE CdTe on OM-VPE CdTe/Ge. 2 in. dia. wafer and surface morphology.....	25
12	Morphology OM-VPE CdTe on (a) Ge, (b) GaAs.....	25
13	ISO-VPE grown HgCdTe on LADA CdTe/GaAs. (a) Morphology and (b) cross-section.....	26
14	ISO-VPE HgCdTe on MBE CdTe/GaAs. (a) Morphology and (b) cross-section.....	27
15	Surface morphology of an ISO-VPE HgCdTe on a CdTe/Ge substrate.....	28
16	Surface morphology of a VPE HgCdTe on LADA CdTe/GaAs with defects.....	29
17	ISO-VPE HgCdTe grown on CdTe/Ge showing macro defects.....	30
18	Pin-hole defect in CdTe/Ge.....	30



LIST OF ILLUSTRATIONS

<u>Figure</u>		<u>Page</u>
19	X-ray diffraction spectrum of GeTe formed through pin holes in CdTe/Ge substrate.....	31
20	LPE grown HgCdTe on MBE CdTe/GaAs substrate.....	32
21	LPE HgCdTe on MBE CdTe/GaAs. Dissolved GaAs region.....	33
22	HgCdTe LPE growth on MBE CdTe/GaAs substrate. Morphology and cross-section.....	34
23	LPE HgCdTe on LADA CdTe/GaAs using super cooled solution.....	36
24	IR transmission of (a) CdTe/Ge and (b) CdTe/GaAs.....	37
25	IR transmission of ISO-VPE HgCdTe on (a) CdTe/GaAs and (b) CdTe/Ge.....	38
26	Cathodoluminescence of PACE-2 CdTe.....	41
27	Cathodoluminescence of PACE-2 CdTe and PACE-1 CdTe.....	42
28	SIMS impurity depth profile of LPE CdTe on OM-VPE CdTe/GaAs....	44
29	SIMS impurity depth profile of CdTe and HgCdTe on GaAs.....	45
30	SIMS impurity depth profile of CdTe and HgCdTe on Ge.....	46



LIST OF TABLES

<u>Table</u>		<u>Page</u>
1	Properties of Candidate Alternative Substrate Materials and CdTe.....	5
2	Growth Techniques.....	6
3	Goal for LWIR HgCdTe Material Characteristics.....	18
4	Division of Resources.....	19
5	Evaluation of PACE-2 CdTe and HgCdTe Material.....	20
6	Summary PACE-2.....	22
7	Morphology Evaluation.....	23
8	Double Crystal X-ray Diffraction of PACE-2 CdTe.....	40
9	Defect Density CdTe by Cathodoluminescence.....	41
10	SIMS Analysis of Base Substrate Elements in PACE-2 Material.....	44
11	Summary of p-Type Isothermal VPE HgCdTe on PACE-2 Substrates.....	47
12	Baseline Approach for Phase 2 of PACE-2.....	49



1.0 INTRODUCTION

This is the final report for the first phase of a program to develop a producible technology for high performance LWIR HgCdTe. A major bottleneck in the development of high quality epitaxial HgCdTe has been the inconsistent quality of bulk CdTe substrates. The limitations imposed by bulk CdTe substrates were successfully circumvented for SWIR and MWIR HgCdTe by using hybrid CdTe/sapphire substrates (PACE-1) suitable for backside illumination to approximately $5.5\ \mu\text{m}$ at which point sapphire becomes opaque to IR radiation. Thus, the objective of this first phase is the development of a high quality alternate CdTe substrate (PACE-2) for backside illuminated LWIR HgCdTe devices as the first step in the demonstration of device quality LWIR HgCdTe on alternate CdTe substrates.

A two-step approach was used. First was the heteroepitaxial growth of CdTe on low cost, high quality, commercially available base substrates followed by HgCdTe epitaxy. A matrix of three base substrates (GaAs, Ge and Si); three epitaxial growth techniques for CdTe (Laser Assisted Deposition and Annealing (LADA), Molecular Beam Epitaxy (MBE) and organo-metallic vapor phase epitaxy (OM-VPE)); and two epitaxial growth techniques for HgCdTe (liquid phase epitaxy (LPE), isothermal vapor phase epitaxy (ISO-VPE)) was used to identify the most promising combinations and to provide a comprehensive data base for the selection of a baseline approach for the second phase of this program. The following results were obtained.

Single crystalline layers of CdTe with near-bulk qualities were obtained on all three base substrates (GaAs, Ge, Si) by all three CdTe vapor growth techniques (LADA, MBE, OM-VPE). OM-VPE growth CdTe on GaAs had the highest crystallinity as determined by x-ray double crystal diffraction. The growth of an additional CdTe layer by LPE improved the crystallinity of the vapor grown CdTe, but often the result was higher impurity levels of base substrate elements in the epitaxial CdTe layer due to slight chemical attack of the base substrate during the CdTe LPE cycle.



SC5373.4FTR

Isothermal VPE grown HgCdTe had the desired p-type conduction when grown on high quality PACE-2 substrates; i.e., those with high crystallinity and low impurity background. LPE growth of HgCdTe, in contrast to CdTe LPE, on PACE-2 substrates resulted in severe chemical attack of the base substrate yielding epitaxial HgCdTe layers of inferior quality. Based on these results, a baseline approach (plus back-up alternates) has been selected for the next phase. The baseline approach will be OM-VPE grown CdTe on GaAs followed by isothermal VPE of HgCdTe. This combination of substrate and growth techniques appears to be the best venue toward obtaining the desired HgCdTe qualities needed for high device performance.



2.0 BACKGROUND

In recent years epitaxial HgCdTe has become the most important material for IR detection and imaging systems. In common with other epitaxial systems, the quality of the epitaxial HgCdTe depends critically on the quality of its natural substrate, bulk CdTe. A major impediment to the development of high quality epitaxial HgCdTe has been the inconsistent quality of bulk CdTe grown by the Bridgman method, currently the best of the known bulk CdTe growth techniques. The difficulties with bulk CdTe are rooted in its physical properties. First, a low thermal conductivity which makes it difficult to maintain a planar growth interface, second, a high vacancy concentration with high mobility at the melting point results in a large number of defects which, again because of high mobilities, interacts to form numerous extended dislocations, low angle grains and major grains which make it exceedingly difficult to synthesize large single crystals. In addition, typically single crystal grains are not uniform in their structural and chemical properties. Furthermore, the mechanical fragility of CdTe requires delicate handling to avoid breakage. To circumvent the limitations of bulk CdTe substrates, approaches based on "alternate" CdTe substrates were initiated. These approaches consisted typically of an epitaxial layer of CdTe on a high quality base substrate. A notable success of this approach is the development of CdTe/sapphire (called PACE-1 for the first Producible Alternative to CdTe for Epitaxy) which proved superior in many ways to bulk CdTe for MWIR HgCdTe epitaxy. Among the advantages found for PACE-1 HgCdTe are higher device yield, higher uniformity, higher overall device performance and, most importantly, reproducibility on a routine basis.¹⁻⁵

The purpose of this effort is to extend the advantages of the PACE-1 approach to the LWIR region (PACE-2) where another base substrate is required for backside illumination since sapphire becomes opaque to IR radiation beyond $\approx 5.5 \mu\text{m}$.



SC5373.4FTR

3.0 OBJECTIVES

The overall objective of this program is to demonstrate the feasibility of PACE-2 technology through fabrication and evaluation of multiplexed LWIR hybrid focal plane arrays fabricated in epitaxial HgCdTe layers grown on PACE-2 substrates.

The specific object of the initial first phase of this program was to grow and analyze LPE and VPE grown HgCdTe layers on CdTe/Si, CdTe/Ge and CdTe/GaAs substrates and to recommend a preferred approach (or preferred approaches) for the next phase of the program.



SC5373.4FTR

4.0 APPROACH

The primary goal of this effort is to develop a LWIR HgCdTe material technology based on heteroepitaxial growth on low cost, high quality, commercially available substrate. The base substrates were GaAs, Si and Ge. All have high transmissivity for LWIR radiation and have demonstrated size, availability, stability and excellent crystallinity at acceptable cost.

Table 1 summarizes some of the characteristics of the selected base substrates along with those of bulk CdTe and sapphire for comparison purposes.

Table 1
Properties of Candidate Alternative Substrate Materials and CdTe

Parameter	CdTe	Al ₂ O ₃	Si	Ge	GaAs
Size	15-20 cm ² (typical best)	20 cm ² routine	100 cm ² routine	20 cm ² routine	20 cm ² routine
Mechanical Strength	Fragile, breakage common, required high-skill handling	Very hard, no special handling	Hard, no special handling	Mod hard, no special handling	Mod hard, no special handling
Crystallinity	Often poor, twin and subgrains common	High	High	High	High
Stoichiometry	Often poor, Te inclusions, voids common	Excellent	Excellent	Excellent	Excellent
Purity	Usually many impurities	Good	Excellent	Excellent	Excellent
Availability	One reliable supplier, a few in-house efforts	Several suppliers	Many suppliers	Many suppliers	Many suppliers
Transparency	Poor-to-excellent, wide variation in undoped	Excellent (MMIR)	Excellent	Excellent	Excellent
Thermal Conductivity	Low 0.3-0.03 W/cm-K	15-200C CdTe	59-120X CdTe	15-25C CdTe	~ 10X CdTe
Thermal Expansion × 10 ⁻⁶ K ⁻¹ (300K/77K)	5.5/0.5	5.4/0.4	2.5/-0.5	5.5/1.1	5.8/0.9
Solubility in Melt	Soluble	Insoluble	Soluble	Soluble	Soluble
Lattice Mismatch	0.2%	36%	19%	15%	15%
Cost	\$125/cm ²	\$5/cm ²	< \$0.5/cm ²	\$1/cm ²	\$6/cm ²
Quality of HgCdTe Epitaxy	Poor-excellent	Good-excellent	Not demonstrated	Not demonstrated	Not demonstrated



SC5373.4FTR

A two-stage approach provided analytical convenience and the promise of higher material quality. First, an epitaxial layer of CdTe was grown on the selected base substrates, by one of three techniques: LADA (Laser-Assisted Deposition and Annealing), MBE (Molecular Beam Epitaxy) or OM-VPE (Organo-Metallic Vapor Phase Epitaxy) and second, epitaxial HgCdTe was grown on the composite alternate CdTe substrates by ISO-VPE (Isothermal Vapor Phase Epitaxy) or LPE (Liquid Phase Epitaxy). Table 2 lists the main characteristics of the growth techniques that were used in this effort. A brief description of each technique follows.

Table 2
Growth Techniques

Technique	Key Feature	Ambient	Temperature Typical °C	Growth Rate μm/h	Sub Area Dia in	In-situ Analysis	Device Quality
LADA CdTe	Laser Evaporation	Medium Vacuum	300	1-12	1.0	Thickness Monitor Flux RGA Visual Sub-temp	Not Applicable
MBE CdTe	Thermal Evaporation	High Vacuum	300	1	1.0	Flux RGA Red AES Visual Sub-Temp	Not Applicable
OM-VPE CdTe	Thermal Pyrolysis	H ₂ - 1 atm	500	1-4	2.0	Flow Rates Visual Sub-Temp	Not Applicable
LPE HgCdTe	Solution	H ₂ Pressure	500	10	2.0	Visual Temperature	Routine on SWIR and MWIR PACE-1 and CdTe Subs
Isothermal VPE HgCdTe	Vapor Deposition and Exchange	H ₂ Pressure	550	4	2.0	Visual Temperature	Comparable to LPE Lower Yield



SC5373.4FTR

LADA, a novel thin film deposition technique, was developed at the Rockwell Science Center. In LADA, a high energy pulsed laser is used as an external power source to vaporize materials for deposition. This unique approach offers some advantages over the more conventional vacuum deposition methods for single crystal materials. The most important aspect is its ability to induce congruent vaporization even for very volatile and complex materials. This results in stoichiometric preservation in the transition from source material to the deposited layer. This feature is important in the vacuum deposition of CdTe which, while evaporating congruently, has different vapor pressures and diffusivities for Cd and Te₂. These different pressures and diffusivities can lead to nonstoichiometric growth conditions and/or deposits.

Figure 1 shows the schematic configuration of a LADA apparatus. The main chamber is a 12 in. I.D. all metal unit. It is pumped by a Hg diffusion pump stack with freon cooled baffle and liquid nitrogen trap. Its choice is based on the ease of operation and low impurity level since the pumping fluid, Hg, is already a constituent of HgCdTe system.

SC81-14639

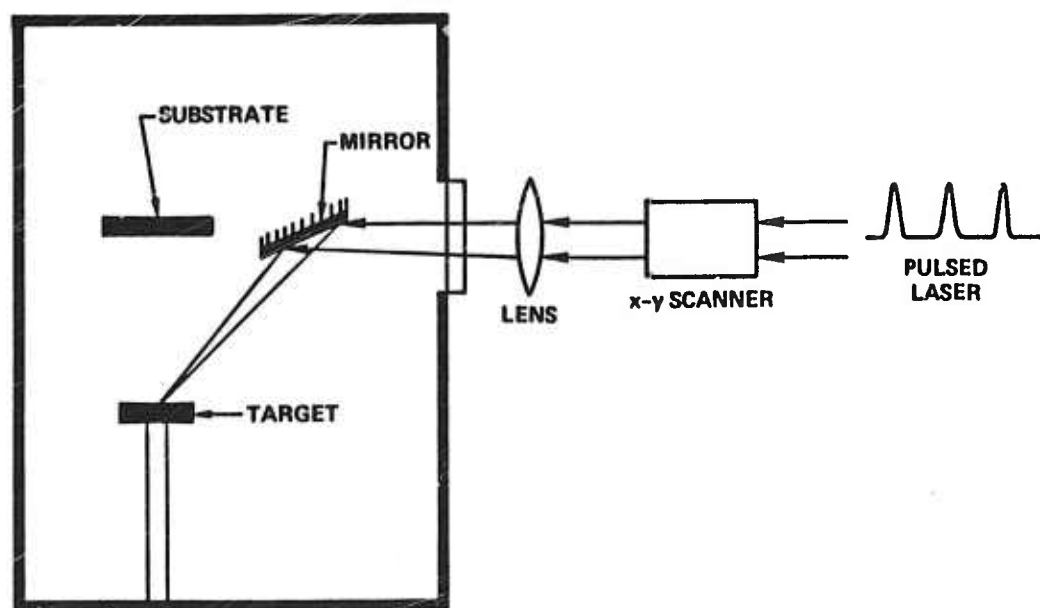


Fig. 1 The LADA apparatus.



SC5373.4FTR

The substrate holder is made of molybdenum. The temperature limit of about 800°C can be regulated to within $\pm 0.5^\circ\text{C}$. The holder area is 1.5 in. diameter. The source holder consists of two separate platforms mounted on a rotary feedthrough. This adds flexibility to the system by allowing multiple layers of different compositions to be grown. The source to substrate distance is 3 in.

The most vital part is the laser used in the congruent evaporation of the CdTe. It is a Nd:YAG unit at 1.06 μm with 100 W of maximum cw output. The laser is equipped with an acousto-optical Q-switch for pulsed operation. The beam can be scanned over the source by a pair of galvanometrically controlled mirrors. Laser power density is adjusted by focusing or defocusing the beam or by adjusting the pumping power.

The LADA technique was used to obtain the first reported growth of single crystalline CdTe on GaAs.⁶ It has also been used to grow epitaxial $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ layers on CdTe substrates and CdTe-HgTe superlattices.^{7,8}

Since its inception a decade ago, MBE has dominated the frontier of the material growth technology by enabling a great variety of novel epitaxial layer structures to be grown with exact control over composition, doping and thickness profiles.

The MBE is an in-house built apparatus as shown in Fig. 2, with a schematic of the apparatus shown in Fig. 3. The growth chamber is pumped by a 400 l/s ion pump and a cryopump, a substrate exchange mechanism is used to maintain the growth chamber at UHV ($< 5 \times 10^{-10}$ Torr). The sources are all arranged vertically and are cryoshrouded extensively, as is the growth volume. An Auger electron spectrometer and reflection electron diffraction system are included for surface chemical and structural analysis. A mass spectrometer is permanently installed to monitor the vacuum status and source purity. The individual source fluxes are measured as a partial pressure of each specie using a Bayard-Alpert gauge which can be rotated into the growth position.



SC5373.4FTR

SC83-20618

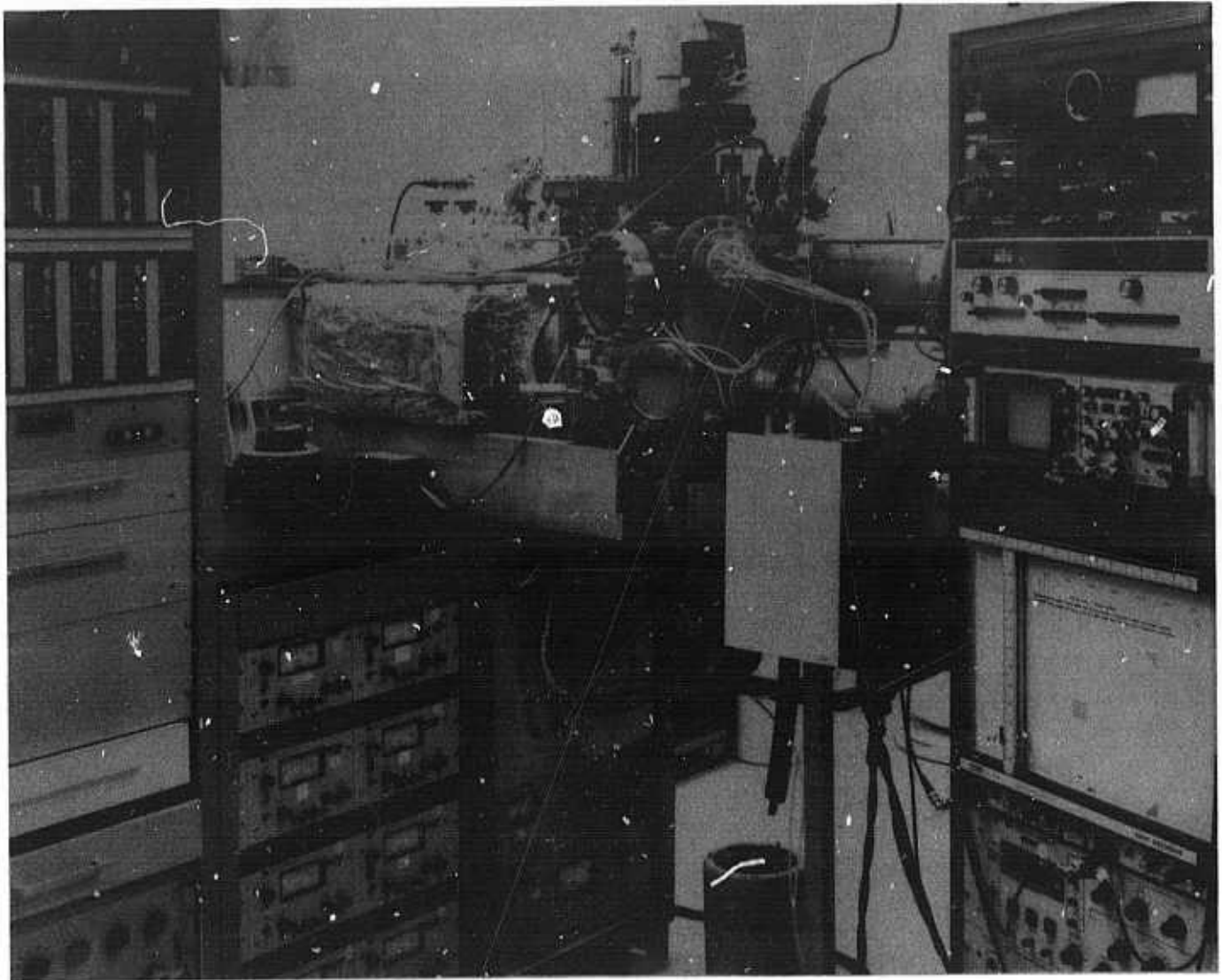


Fig. 2 MBE apparatus.

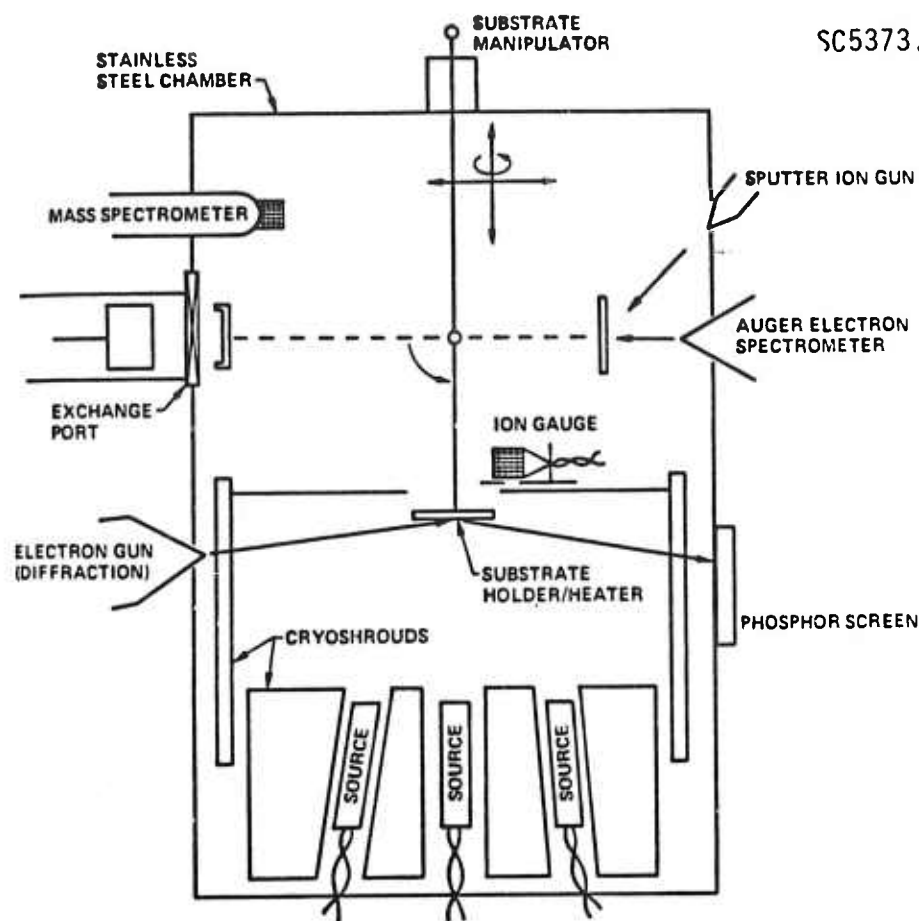


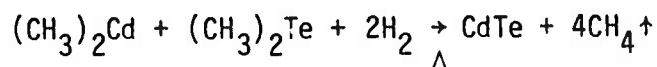
Fig. 3 Schematic of the MBE apparatus.

OM-VPE (or MO-CVD, metal-organic chemical vapor deposition) has been used successfully in the past decade in the synthesis of device quality III-V epitaxial layers. Concurrently at a much smaller level, the growth of the lower pressure II-VI compounds (i.e., CdTe, ZnSe, ZnTe) by OM-VPE resulted in epitaxial layers. In this growth process the layer constituents (Cd, Te) are transported to the reaction zone in the form of metal alkyls (dimethylcadmium and dimethyltellurium or diethyltellurium, DMCD, DMTE, DETE) via a carrier gas (typically high purity hydrogen). These metal alkyls are liquids at or near room temperature with appreciable vapor pressures. The simplicity of transporting gaseous reactants to the reaction zone forms the basic usefulness of OM-VPE as an epitaxial technology. The formation of CdTe occurs via pyrolysis of the organometallics and subsequent recombination of the atomic (Cd) or molecular



SC5373.4FTR

(Te₂) species at or near the substrate. For example, CdTe can be grown using DM Cd, (CH₃)Cd and DM Te, (CH₃)Te and the following reaction occurs:



The process can be controlled readily by using electronic mass flow controllers to fix the flow rates and thus the partial pressures of the reactants. The reaction requires that only the substrate be heated to ensure efficient deposition. Radiofrequency (RF) induction heating of a silicon carbide coated graphite susceptor was used in this particular application. Figure 4 shows a simple schematic drawing of the OM-VPE system illustrating the use electronic mass-flow controllers and remotely controlled valves for automated gas handling.

SC84-28537

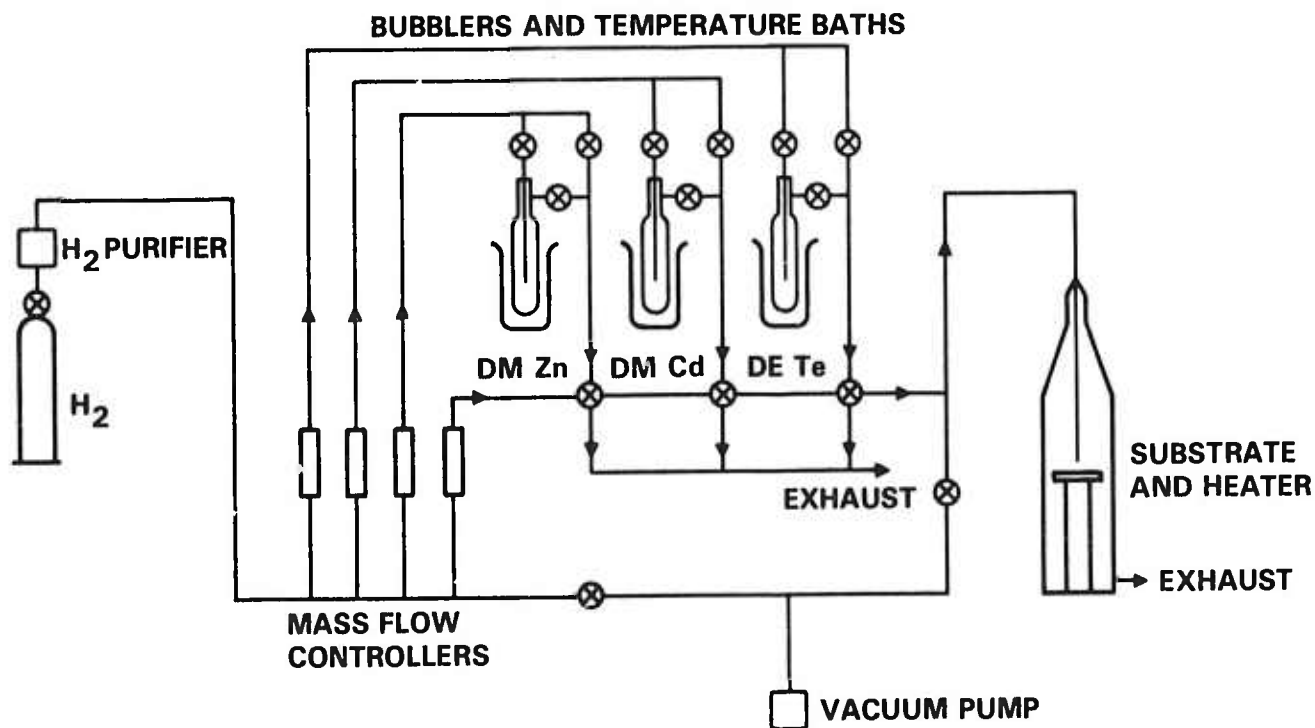


Fig. 4 Simplified OM-VPE flow diagram schematic.



SC5373.4FTR

The reason for selecting only vapor phase growth techniques for the growth of CdTe on the base substrates is twofold. First, the equilibrium growth techniques such as LPE typically result in poor nucleation and subsequent poor growth when used for chemically dissimilar and lattice-mismatched substrate/ epilayer systems such as considered here. Second, dissolution of the base substrates (GaAs, Si, Ge) could occur in the Te-rich liquids typically used for CdTe LPE. Once a CdTe layer has been grown by a vapor phase technique, however, in theory LPE techniques can be used since the melt and substrate are in equilibrium.

The variety of techniques used permitted exploration of a wide range of CdTe nucleation and growth conditions. Both the LADA and MBE techniques require a high to medium vacuum ambient which limits growth temperatures to approximately 300°C due to the high vapor pressure of Cd. OM-VPE supplements these two techniques by allowing growth at higher temperature (up to approximately 600°C) since growth is carried out in a H₂ ambient at atmospheric pressure. The qualities desired for vapor grown epitaxial CdTe layer on the base substrate are: crystallinity comparable to the best bulk CdTe, low impurity concentration, high IR transmissivity and overall uniformity.

LPE⁹ and isothermal VPE¹⁰ were used to grow the active HgCdTe layers on the alternative CdTe substrates. Both techniques have a proven capability in producing device quality HgCdTe material. In simple terms, LPE is a solution growth technique and involves controlled precipitation onto a single crystal substrate of a solute dissolved in a solvent. As carried out at Rockwell's Science Center, Te is used as the solvent with Hg and Cd added in predetermined amounts to obtain specific x values for the Hg_{1-x}Cd_xTe epitaxial layers. The empirically determined phase diagram is shown in Fig. 5. Growth is carried out in a horizontal graphite boat with no moving parts held in a quartz tube sealed by removable stainless steel flanges. After saturation at the desired temperature (i.e., complete dissolution of all melt components), growth is initiated by rolling the melt onto the substrate using a tipping motion and terminating the growth in a similar manner. Hg loss from the melt



SC5373.4FTR

(due to the high Hg vapor pressure at elevated temperatures) is controlled by using high background H_2 pressure that acts as a diffusion barrier for the evaporated Hg and that reduces to negligible the loss of Hg during the growth cycle. LPE growth carried out in this manner has resulted in high performance device quality SWIR, MWIR and LWIR HgCdTe with large (up to 25 cm^2) compositionally uniform HgCdTe on a reproducible basis.

SC84-29511

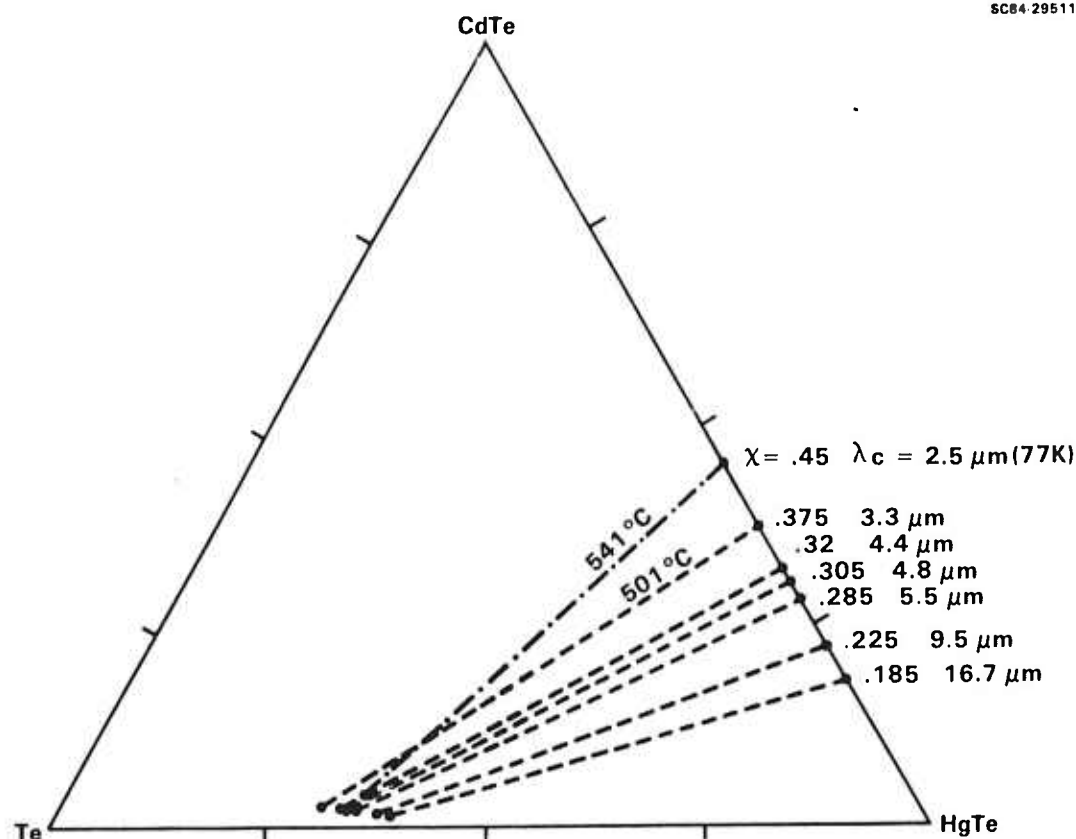


Fig. 5 Phase diagram for HgCdTe. Dotted lines are connecting lines between liquidus and solidus points, λ_c at 77K.

With the use of alternate hybrid CdTe substrates special precautions must be taken with the LPE technique. While near equilibrium between CdTe and Hg-CdTe melts can be readily established, no such relationship exists between



SC5373.4FTR

Ge, Si or GaAs - all of them readily dissolve in Hg-Cd-Te melts at the LPE growth temperatures used (450-550°C). Care needs to be taken that the melt contact only the CdTe surface of the hybrid CdTe substrate. Melt contact with the base substrate would result in partial dissolution of that substrate with subsequent layer, i.e., high dopant levels and/or poor epitaxy due to changes in the chemical composition of the melt. To reduce this risk the LPE boat was modified with special inserts intended to confine contact of the Hg-Cd-Te melt to the CdTe surface only, and not the edges and backside of the base substrate.

Isothermal vapor growth of HgCdTe (also called "close-space" vapor transport) involves the transport of Hg and Te₂ from an appropriate source to a single crystalline CdTe substrate surface. Hg is the dominant species because of its high vapor pressure compared to Te₂ and Cd. Hg and Te₂ react on the CdTe surface to form HgTe and subsequently Hg_{1-x}Cd_xTe by an interdiffusion/exchange mechanism with the CdTe substrate. This growth mechanism leads to a compositionally graded layer (x varies as a function of layer thickness). A major innovation to the growth technology was contributed by Rockwell in developing an "open tube" approach for isothermal VPE growth of HgCdTe. Traditionally carried out in closed ampules to control the Hg partial vapor pressure, the technique had limited appeal for volume production applications due to the necessity of loading and sealing off individual ampules.

At Rockwell, the isothermal VPE growth is carried out in an open tube reactor derived from, and very similar to, the LPE reactor. SWIR and MWIR device quality HgCdTe layers have been grown by this technique¹⁰ with $R_0A > 10^7 \Omega\text{-cm}^2$ for $\lambda_c = 4.0 \mu\text{m}$ at 77K and $R_0A > 2 \times 10^6 \Omega\text{-cm}^2$ for $\lambda_c = 4.65 \mu\text{m}$ at 77K on both CdTe and CdTe/sapphire substrates respectively.

The VPE growth system is shown in Fig. 6 and is basically a modified vertical LPE growth system. A background gas (H₂) is kept at high pressure to reduce Hg loss to a reasonable level during the growth cycle. The apparatus consists of two concentric quartz tubes, an outer heavy wall and inner thin wall, supported and sealed by stainless steel flanges that ensure a leak-free environment. The loading flange has provisions for substrate positioning as



SC5373.4FTR

SC85-22899

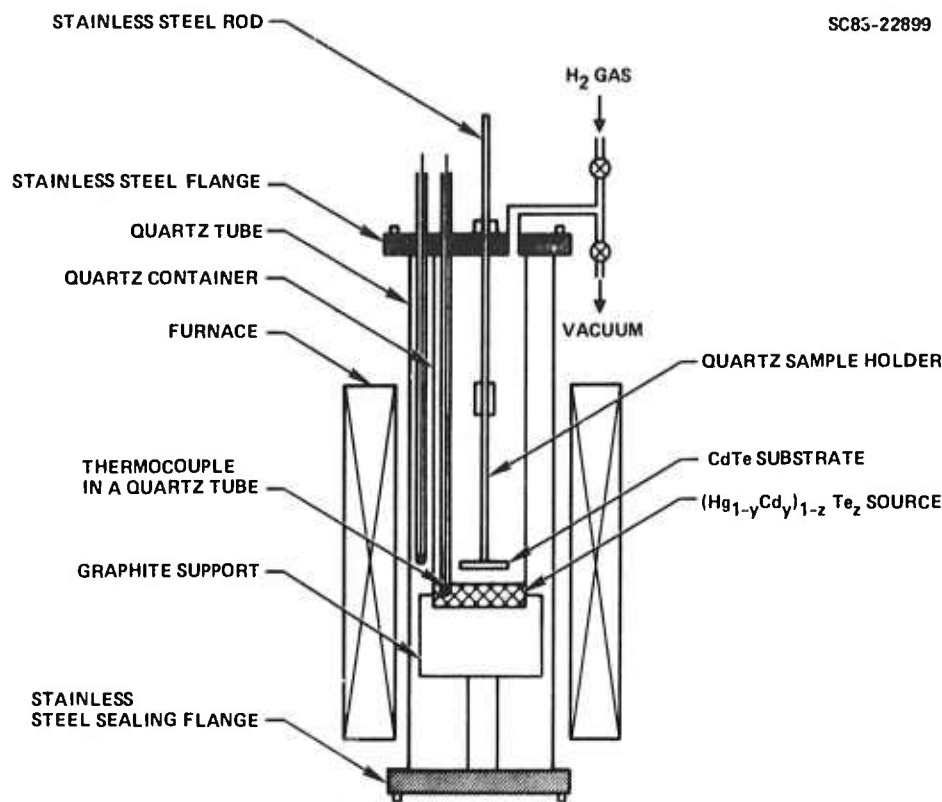


Fig. 6 Isothermal VPE growth apparatus.

well as connections to either vacuum or H_2 gas ambients. Two thermocouples are positioned in the growth apparatus. One, between the quartz tubes, provides feedback to a high resolution temperature controller; while the other, positioned as close as possible to the source charge, monitors the actual growth temperature. A thin gold layer is used as the infrared reflector, so the furnace itself is transparent. Thus, visual observation of the source and substrate during the growth cycle is allowed.

A typical growth run consists of the following. A properly prepared substrate and a source consisting of elemental Hg, Cd, and Te are placed in the growth chamber. The chamber is sealed, evacuated, backfilled and pressurized with H_2 . After the elements of the source are reacted and homogenized for an hour, the temperature is lowered to the growth temperature. The substrate, kept in a cold zone during the reaction cycle, is brought to a spe-



SC5373.4FTR

cific distance above the source where a small temperature difference causes growth to occur. Growth rates are approximately 4 $\mu\text{m/h}$. After the desired epitaxial layer thickness is reached, the substrate is withdrawn to the upper cold zone and the power is turned off. After the temperature of the furnace reaches ambient, the substrate is removed. Compositional control of the x valve is achieved by varying the composition of the source and/or the temperature. Figures 7 and 8 show the empirically established relationships between source composition, layer composition and growth rate. The major advantage of the isothermal VPE technique for this application is that physical contact between source and substrate is not required; growth proceeds by vapor transport and a diffusion exchange mechanism.

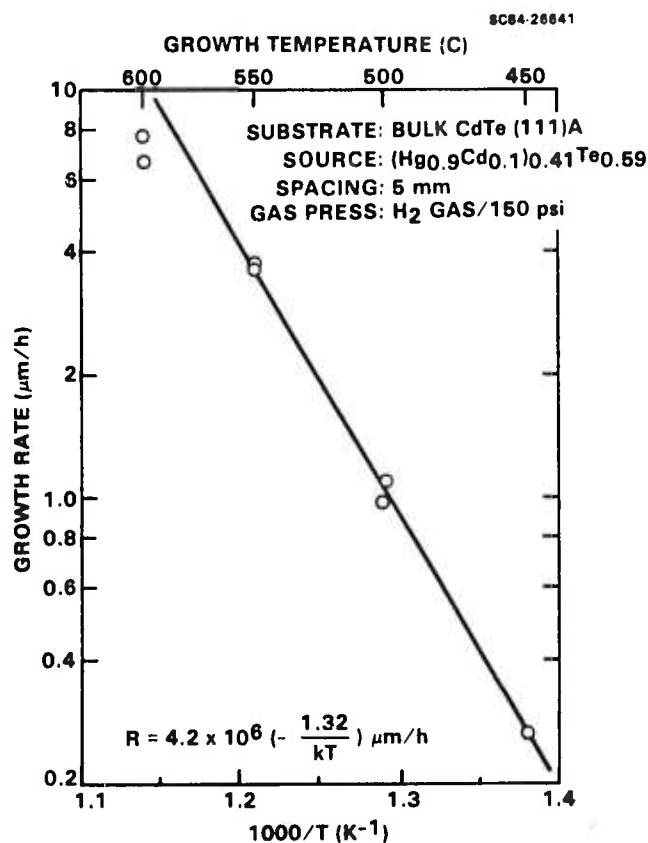


Fig. 7 Composition of ISO-VPE $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ as a function of growth temperature.



SC5373.4FTR

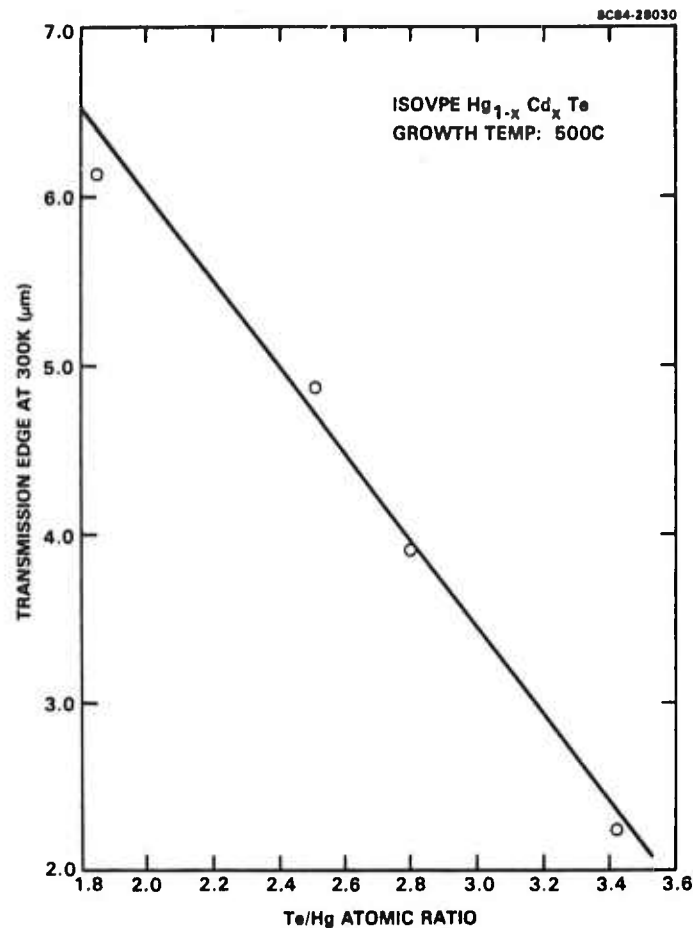


Fig. 8 Relationship between HgCdTe composition and Te/Hg of source in ISO-VPE at 500°C.

From previous experience with epitaxial LWIR HgCdTe, the following goals have been established to obtain device quality material. They are summarized in Table 3.

The key technical issues with this heteroepitaxial approach for an alternative substrate lie in three areas. First, lattice mismatch between CdTe and the base substrate results in a high defect density in the CdTe near the mismatched interface. To obtain high quality CdTe this defect density must be reduced in the bulk of the epilayer. Second, potential doping of the epilayer by base substrate elements. Ga is a fast diffusing n type dopant in CdTe and HgCdTe; As is p-type; Si and Ge may be amphoteric, i.e., behaving



SC5373.4FTR

Table 3
Goal for LWIR HgCdTe Material Characteristics

Wafer Size	> 2 in. diameter
Morphology	Minimal terracing, suitable for device processing as-grown
Composition, x	≈ 0.2
Thickness	$\approx 20 \mu\text{m}$
Defect Density	Lower than LPE on bulk CdTe
Conductivity Type	p-type, suitable for junction-formation via ion-implantation
Carrier Concentration	$< 1 \times 10^{16} \text{ cm}^{-3}$

either n- or p-type, depending on growth conditions and other factors. Third, the orderly nucleation of a polar compound (CdTe) on a nonpolar element (Si, Ge) poses special problems because of the necessity to ensure proper site selection during the initial phase of the growth. Failure to do so results in numerous stacking faults and anti-phase domains which consequently degrade the crystalline quality of the epitaxial layer.

To summarize the approach: two distinct efforts were pursued in order to achieve the objective of this program. First, the synthesis of a suitable alternate CdTe substrate and second, the growth of the active LWIR HgCdTe on that substrate. The key technical issues concerned the achievement of a high quality alternate CdTe substrate since no major obstacles were anticipated in obtaining high quality HgCdTe by LPE on ISO-VPE given a quality substrate. As indicated in Table 4, experimental results obtained early in the program led to a division of resources for the various growth technique/substrate combinations. The broad approach was also intended as an aid in selecting a baseline (and alternate) approach for the subsequent phases of this program by quickly identifying the most promising growth technique/substrate combination.



SC5373.4FTR

Table 4
Division of Resources

Technique	Base Substrate		
	GaAs	Si	Ge
LADA CdTe	X		
MBE CdTe		X	
OM-VPE CdTe	X		X
LPE HgCdTe	X		
Isothermal VPE HgCdTe	X	X	X

X = Concentrated Effort

Before presenting results, the analytical methods used in characterizing the growth material will be discussed.



5.0 MATERIAL CHARACTERIZATION TECHNIQUES

The primary characterization techniques used in the evaluation of material quality of the epitaxial CdTe and HgCdTe were the following. Optical microscopy was used to assess surface morphology, to document macroscopic defects, and to determine layer thicknesses from cleaved cross-sections. IR spectroscopy was used to determine the IR properties of epitaxial CdTe layers as well as to determine their thickness nondestructively and the composition of HgCdTe layers from the room temperature absorption edge. Scanning electron cathodoluminescence was used to determine the defect structure of the CdTe layers as well as its spatial distribution. Double crystal x-ray rocking curves were used to determine the crystallinity of the epitaxial CdTe layers. Strain, subgrains and defects cause broadening of the x-ray diffraction curve, thus the width of the x-ray diffraction curve is a direct measure of crystallinity. Secondary ion mass spectroscopy (SIMS) was used to determine the absolute level of selected impurities in the CdTe and HgCdTe layers along with their depth profiles. Hall effect was used to determine carrier type, concentration and mobility for the HgCdTe epitaxial layers. Table 5 summarizes the characterization methods used and indicates their primary functions.

Table 5
Evaluation of PACE-2 CdTe and HgCdTe Material

Technique	Function
Optical	Morphology, Thickness
IR Spectroscopy	Composition, Thickness
Cathodoluminescence	Defect Structure
X-ray Diffraction	Crystallinity
SIMS	Impurity Level and Distribution
Hall Effect	Carrier Type, Concentration and Mobility



SC5373.4FTR

6.0 RESULTS

The results have been summarized and condensed into tabular form in each of the characterization categories described above. The progress highlights can be summarized in four main points.

- Single crystal layers of CdTe were obtained on GaAs, Ge on Si by all three vapor growth techniques, i.e., by LADA, MBE and OM-VPE.
- LPE grown CdTe on a vapor nucleated CdTe improved the crystallinity and reduced the defect density.
- Isothermal VPE grown HgCdTe exhibited p-type conduction when grown on high quality PACE-2 substrates.
- The LPE growth of HgCdTe on PACE-2 substrates typically resulted in chemical attack of the base substrates.

Each of the above main points will be discussed in the following sections. Table 6 summarizes the results obtained during this phase of the program. Shown are the three base substrates versus the three CdTe vapor growth techniques with the results of isothermal VPE growth of HgCdTe shown in a subsection for each CdTe vapor growth technique/base substrate combination. Results for LPE growth of HgCdTe are not listed, since chemical attack occurred for all three base substrates. As a reference and for comparison purposes, the values for defect density, determined by cathodoluminescence, and the value for $\Delta\theta$, the width at half maximum of the x-ray diffraction rocking curve, have been listed for PACE-1 CdTe and bulk CdTe.



SC5373.4FTR

Table 6
Summary PACE-2

Technique	Base Substrate		
	GaAs	Si	Ge
LADA	Smooth Morphology $\Delta\theta = 4.8$ Defects: $1E7$ SIMS: 10^{16} - 10^{18} Ga	Semi-Crystalline	No Attempts
	HCT: n- and p-Type SIMS: $7E15$ Ga	HCT: n-Type SIMS: $5E14$ Si	
MBE	Smooth Morphology $\Delta\theta$: 2.3, 1.9 (LPE) Defects: $2E7$, $6E7$ (LPE) SIMS: $3E17$ Ga	Nonuniform Morphology $\Delta\theta$: 3.3, 1.9 (LPE) Defects: $4E7$ SIMS: $1E14$ Si	No Attempts
	HCT: n-Type SIMS: $2E16$ Ga	HCT: No Attempts	
OM-VPE	Smooth Morphology $\Delta\theta$: 2.1, 1.5 (LPE) Defects: $2E7$ SIMS: $8E15$ Ga, $2E18$ Ga (LPE)	Polycrystalline direct Single Crystal with Ge Buffer Layer $\Delta\theta = 5$ (LPE)	Smooth Morphology $\Delta\theta$: 4.7, 1.8 (LPE) Defects: $4E7$ SIMS: $5E15$ Ge, $1E18$ Ge (LPE)
	HCT: No Attempts		HCT: n- and p-type SIMS: $3E16$ Ge

$\Delta\theta$ (min)
Defects cm^{-2}
SIMS cm^{-3}

- HgCdTe results are for isothermal VPE growth
 - LPE HgCdTe results in chemical attack of base substrate
 - Reference PACE-1
Bulk CdTe
- $\Delta\theta = 1.5$ min
 $\Delta\theta = 1$ to 2 min
- Defects = $5E6 \text{ cm}^{-2}$
Defects = $2E6 \text{ cm}^{-2}$

6.1 Morphology

Smooth surface morphologies are desirable if not necessary for successful device processing especially for large area, high density, planar device architectures where repeated masking and processing steps are required.

Table 7 lists the results of the optical morphology evaluation for CdTe and HgCdTe, starting with the smoothest combination at the top. Not surprisingly, the smoothest CdTe epilayers were grown by LADA or MBE on GaAs (Figs. 9 and 10); CdTe layers were virtually featureless with well-defined, flat interfaces. All LPE grown CdTe layers displayed a slight wavy morphology where waviness increased with misorientation from the nominal axis ((100) for

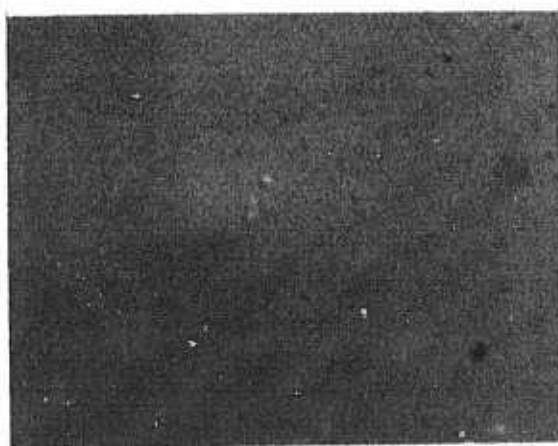


Table 7
Morphology Evaluation

CdTe	Morphology
Growth Technique	
MBE or LADA CdTe/GaAs	Specular, Mirror Smooth
LPE/OM CdTe/GaAs or CdTe/Ge	Minor Terracing
OM CdTe/GaAs or CdTe/Ge	Faceted
HgCdTe	
Growth Techniques	
ISO-VPE on LADA or MBE CdTe/GaAs	Specular
ISO-VPE on LPE/OM CdTe/GaAs or CdTe/Ge	Smooth, better than LPE on PACE-1
LPE, all substrates	Rough, worse than LPE on PACE-1

SC82-19350

10 μ m



SURFACE MORPHOLOGY



X-RAY LAUE PATTERN

Fig. 9 Morphology and X-ray Laue diffraction of LADA CdTe/GaAs layer.



SC83-24417

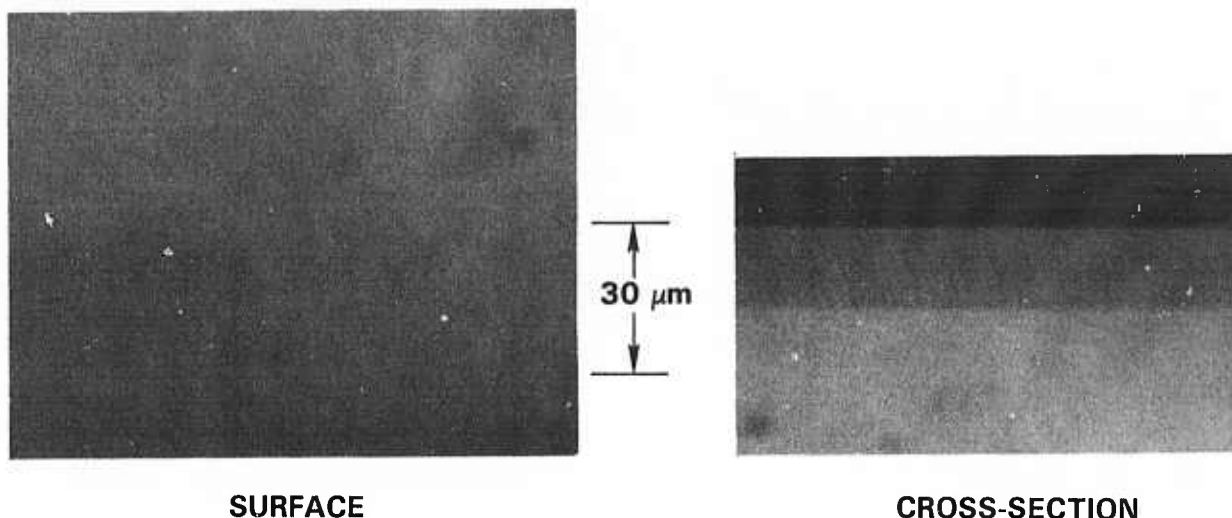


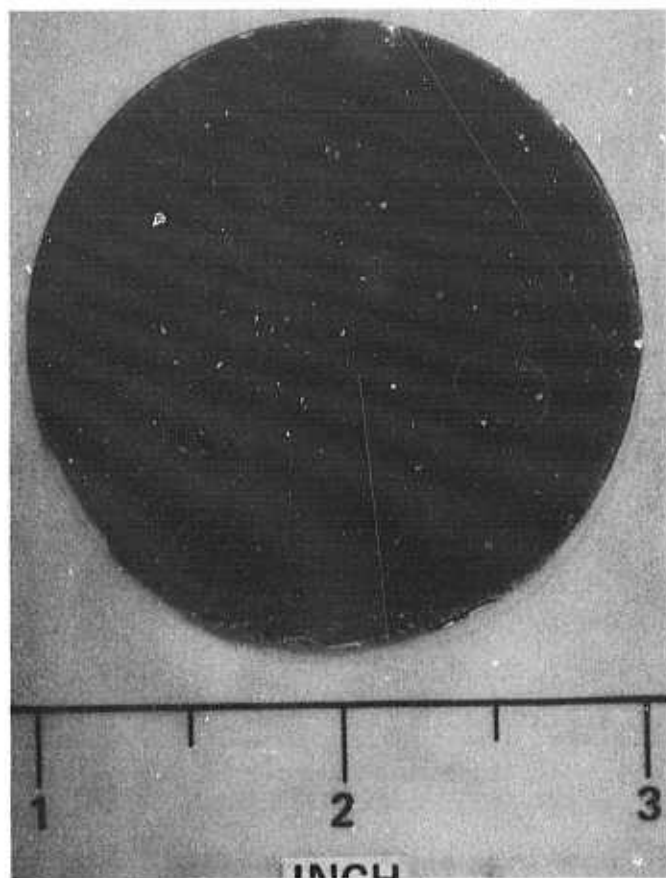
Fig. 10 MBE Grown CdTe/GaAs. Surface morphology and cross-section.

GaAs, (111) for Ge and Si)). Figure 11 shows a 2 in. diameter wafer of CdTe on Ge. The detailed surface morphology shown is that of the LPE grown CdTe on the OM-VPE nucleated CdTe layer. Figure 12 shows the morphologies of OM-VPE grown CdTe on Ge and GaAs. In contrast to the LADA or MBE grown CdTe, the OM-VPE grown CdTe morphology is strongly faceted, which is partly due to the high growth temperature of the OM-VPE technique.

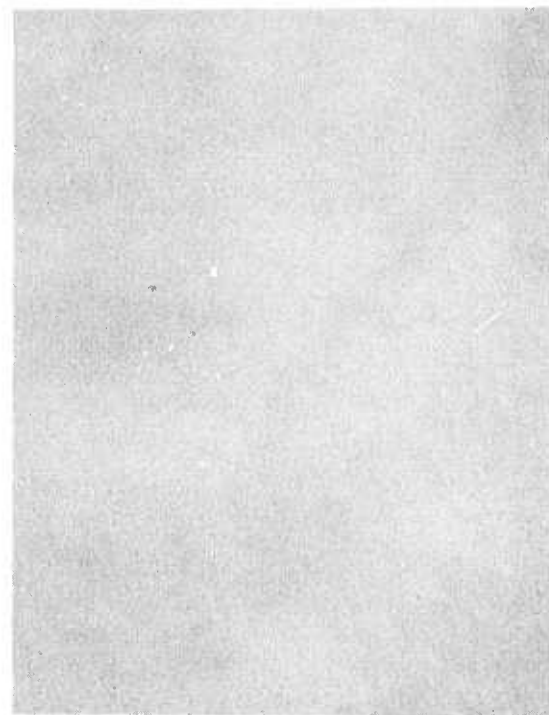
The smoothest HgCdTe morphology was achieved for HgCdTe epitaxial layers grown by isothermal VPE on LADA CdTe/GaAs substrates (Fig. 13). ISO-VPE HgCdTe on MBE CdTe/GaAs showed some surface structure and was also quite smooth (Fig. 14). Isothermal VPE growth of HgCdTe on CdTe/Ge substrates resulted in smooth epitaxial layers often with less surface structure than the original structure. Figure 15 shows the surface morphology of an isothermal VPE grown HgCdTe layer on a CdTe/Ge substrate.



SC84-26036



WAFER

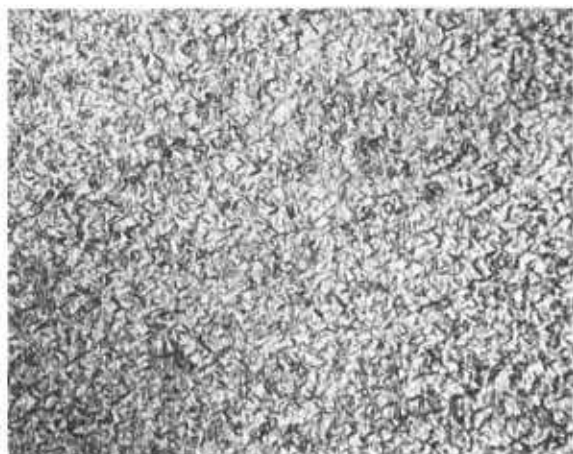


SURFACE MORPHOLOGY

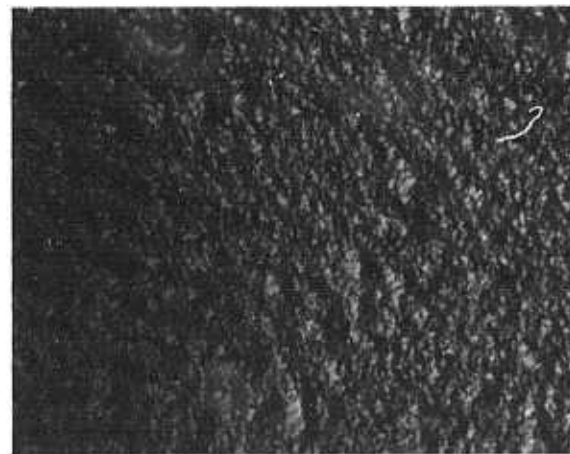
300 μm

Fig. 11 LPE CdTe on OM-VPE CdTe/Ge. 2 in. dia. wafer and surface morphology.

SC85-29798



(a)



(b)

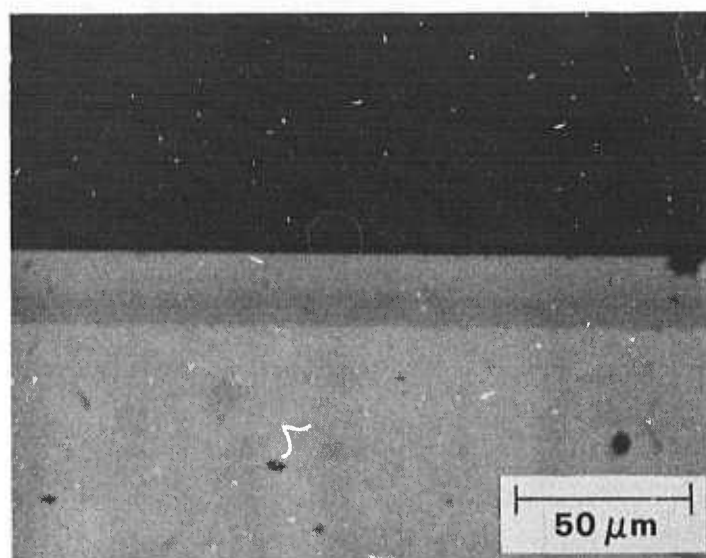
30 μm

Fig. 12 Morphology OM-VPE CdTe on (a) Ge, (b) GaAs.



SC5373.4FTR

SC83-24168

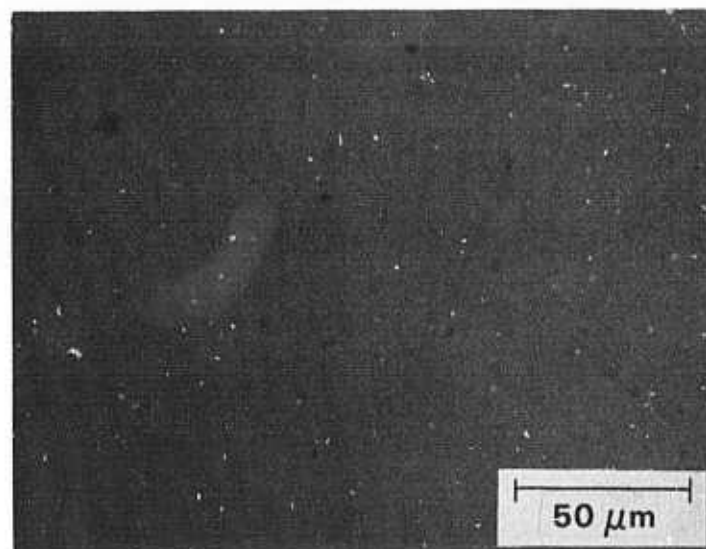


(a)

HgCdTe (100)

CdTe (100)

GaAs (100)

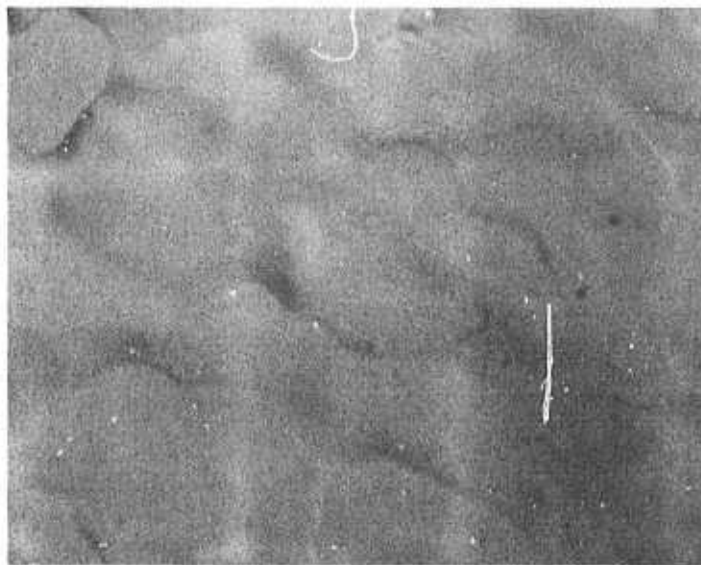


(b)

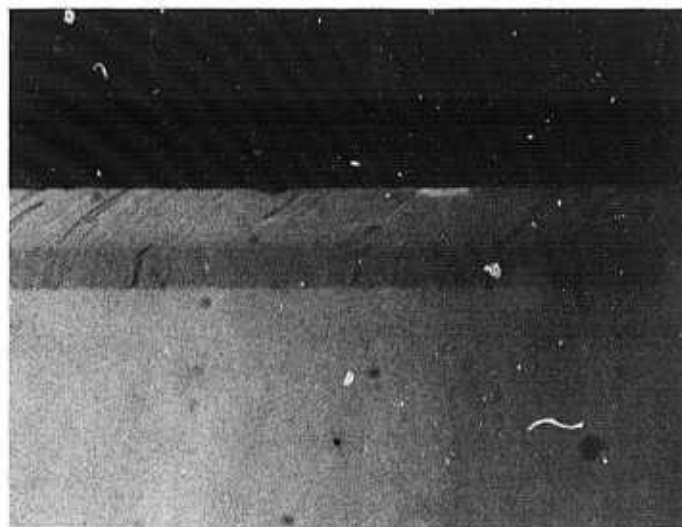
Fig. 13 ISO-VPE grown HgCdTe on LADA CdTe/GaAs. (a) Morphology and (b) cross-section.



SC85-29797



└50 μm ┘



← HgCdTe

← CdTe

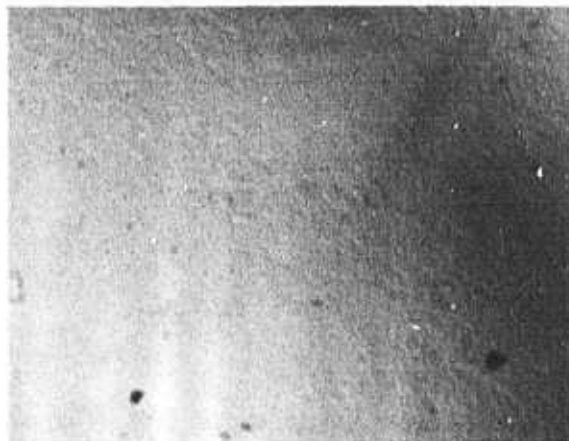
← GaAs

└30 μm ┘

Fig. 14 ISO-VPE HgCdTe on MBE CdTe/GaAs. (a) Morphology and (b) cross-section.



SC84-26020



100 μm
(a)



25 μm
(b)

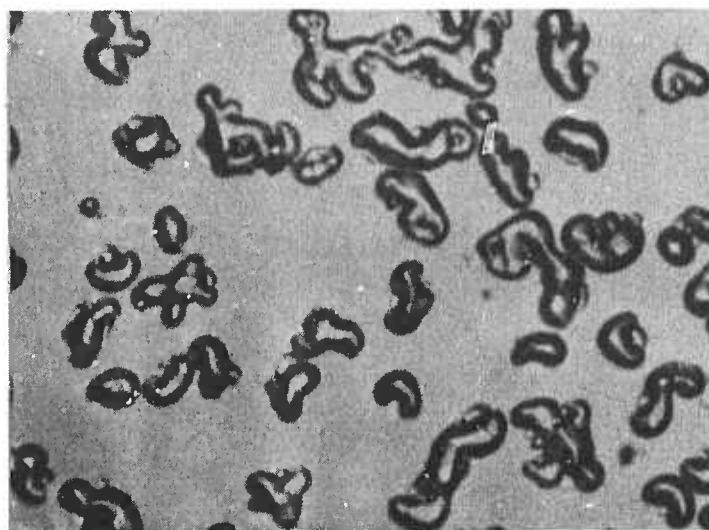
Fig. 15 Surface morphology of an ISO-VPE HgCdTe on a CdTe/Ge substrate.

Isothermal VPE of HgCdTe on substrates with structural defects resulted in rougher morphologies and surface defects such as shown in Figs. 16 and 17. Figure 16 shows the surface morphology of an isothermal VPE HgCdTe on a LADA CdTe/GaAs substrate with localized defects that caused poor HgCdTe growth. Figure 17 shows large local defects in an isothermal VPE HgCdTe on OM-VPE CdTe/Ge substrates. These defects were caused by pinholes in the CdTe layer (Fig. 18) and allowed the interaction between the Ge and Te vapor to occur in the isothermal HgCdTe growth cycle. The reaction results in the formation of GeTe, established by x-ray powder diffraction, which marred the otherwise smooth growth surface (see Fig. 11).



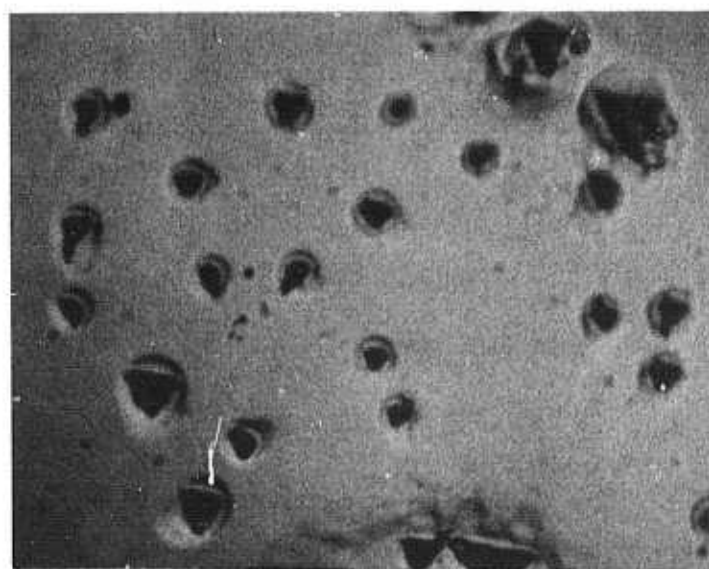
SC5373.4FTR

SC84-26033



50 μm

(a) AS-GROWN SURFACE



50 μm

(b) STAINED SURFACE

Fig. 16 Surface morphology of a VPE HgCdTe on LADA CdTe/GaAs with defects.



SC84-26029

SC5373.4FTR

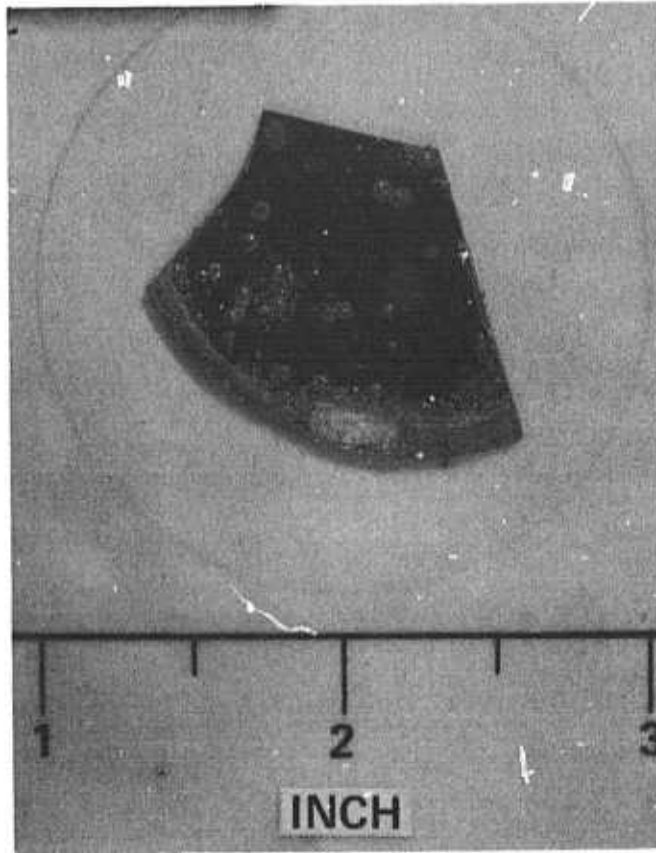


Fig. 17 ISO-VPE HgCdTe grown on CdTe/Ge showing macro defects.

SC84-26037

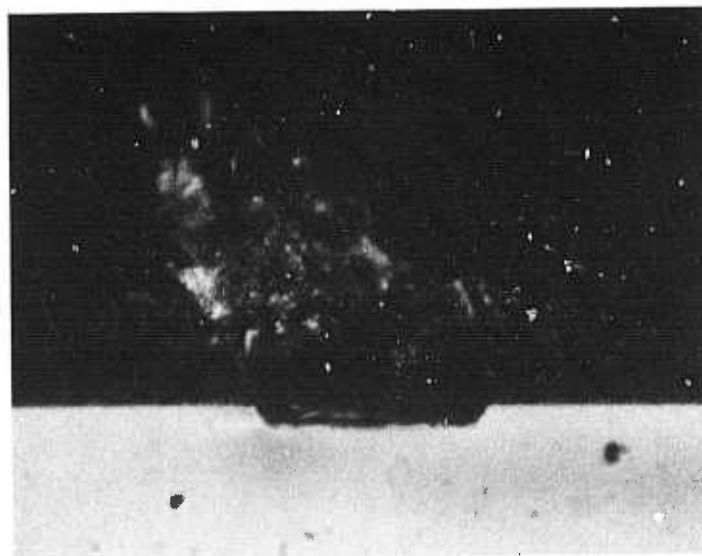


Fig. 18 Pin-hole defect in CdTe/Ge.



SC5373.4FTR

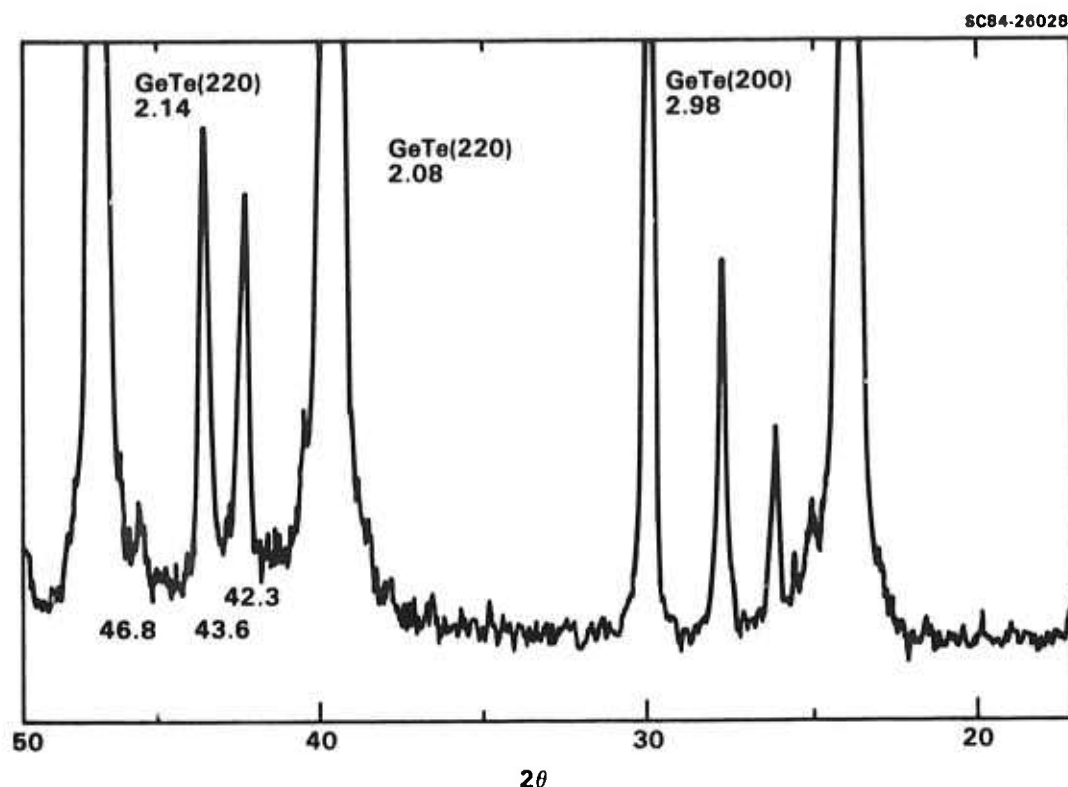
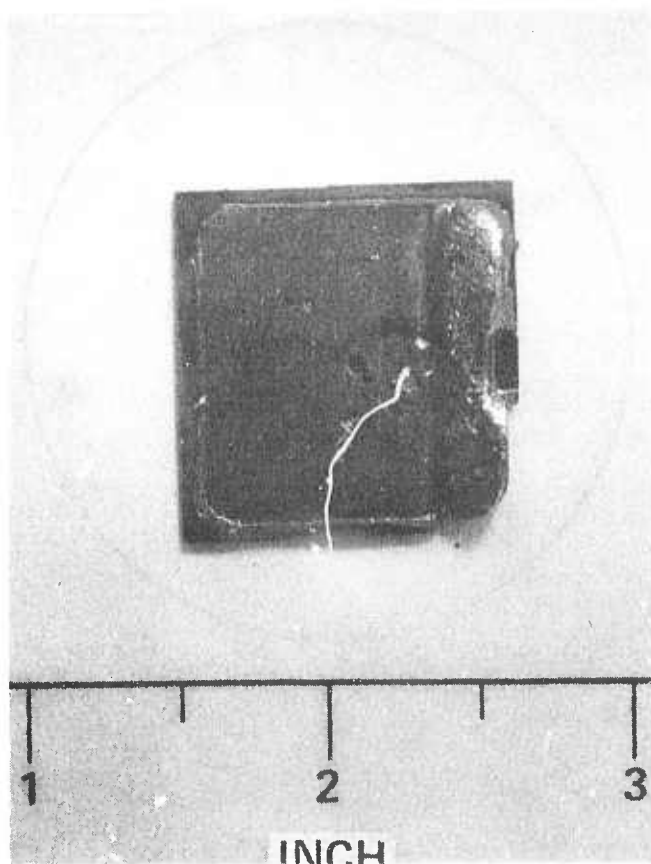


Fig. 19 X-ray diffraction spectrum of GeTe formed through pin holes in CdTe/Ge substrate.

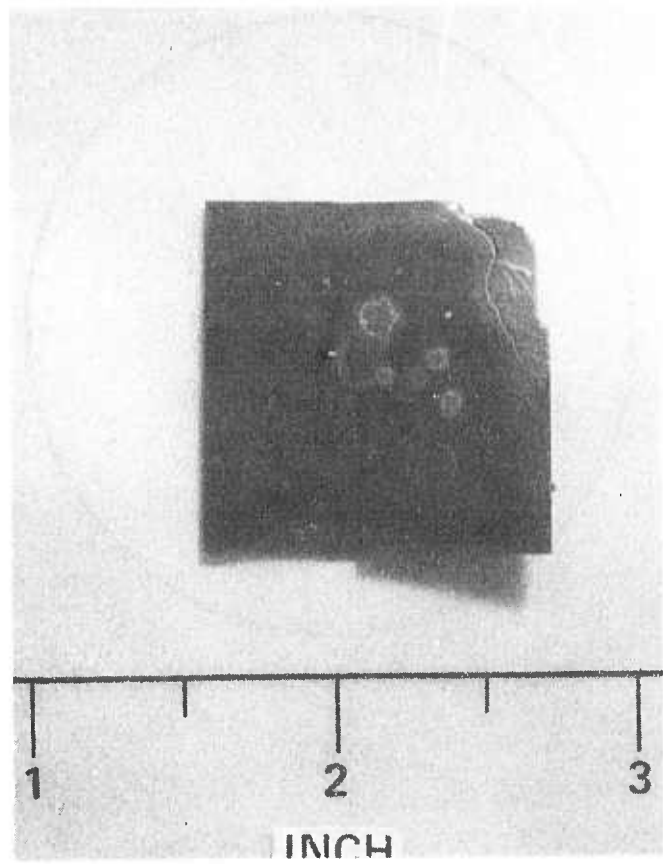
Poor morphologies were obtained for LPE HgCdTe growth attempts on all alternate CdTe substrates. Precaution was taken to confine the HgCdTe melt to the central portion of the substrate and away from the edges where chemical attack on the base substrates could occur. Despite these precautions, partial dissolution of the base substrates occurred due to chemical attack by the LPE melt. Figure 20 shows the front or epi-side, as well as the backside of an LPE HgCdTe growth attempt on a MBE grown CdTe/GaAs substrate. Chemical attack



SC83-24936



EPI SIDE



BACK SIDE

Fig. 20 LPE grown HgCdTe on MBE CdTe/GaAs substrate.

of the GaAs substrate occurred in two modes. In one mode, the melt attacked the substrate at one edge, as can be seen in the upper right-hand corner of the backside photo. The other modes of chemical attack occurred through the CdTe layer itself via regions of poor crystallinity that allowed the melt to communicate with the GaAs substrate, leading to chemical dissolution that is visible as spots on the backside of the GaAs wafer.

Figure 21 is a cleave through one of these spots clearly showing a hole in the GaAs wafer where the HgCdTe melt had locally dissolved the GaAs. Figure 22 shows the resulted surface morphology which is quite rough and structured partly due to the chemical contamination of the melt. A cross-section of the layers showing the GaAs substrate and the CdTe and HgCdTe



Rockwell International

Science Center

SC5373.4FTR

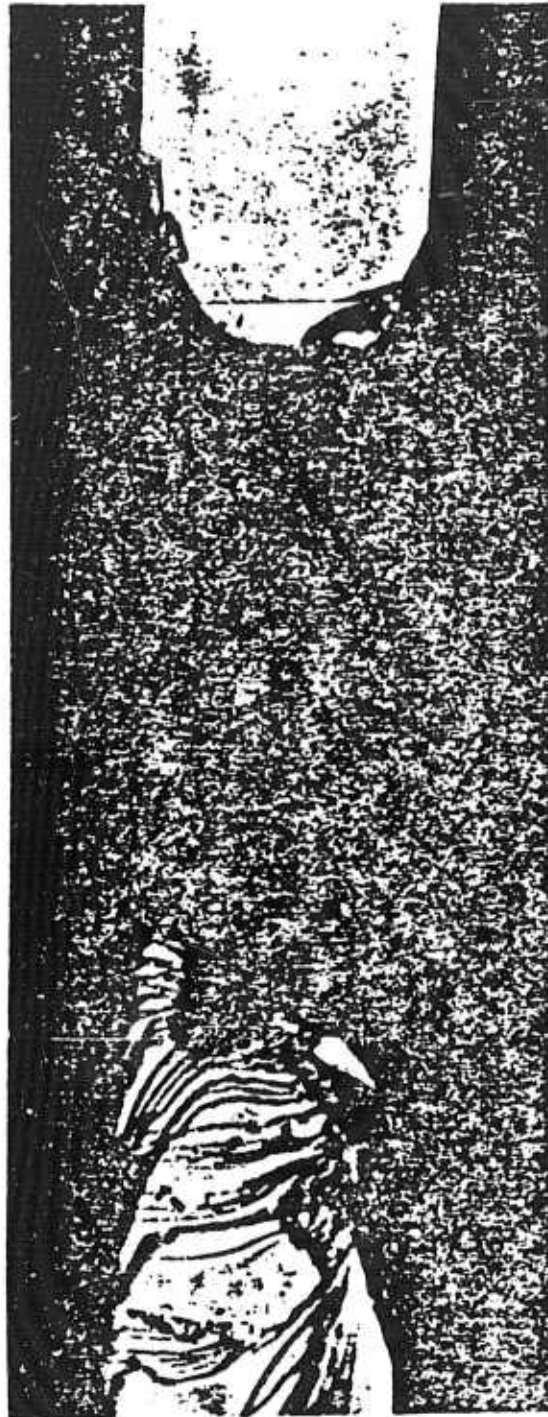
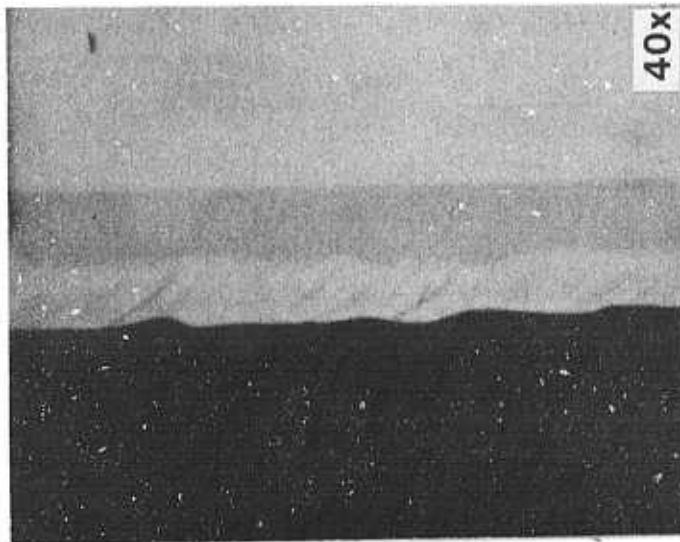


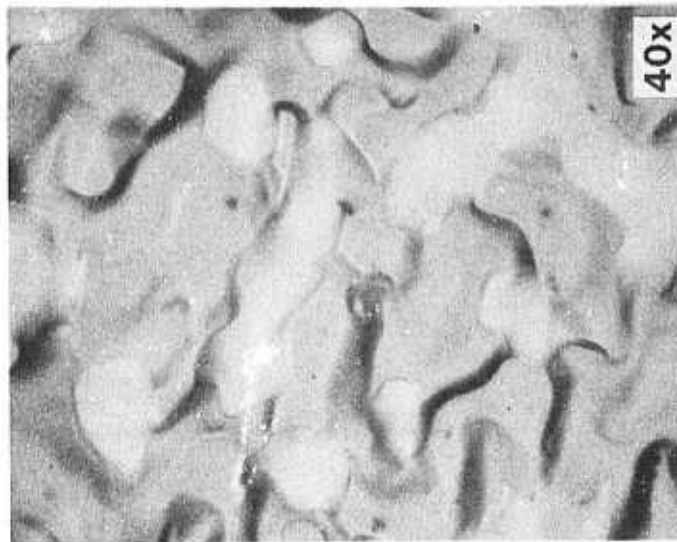
Fig. 21 LPE HgCdTe on MBE CdTe/GaAs. Dissolved GaAs region.



SC83-24935



CROSS-SECTION



SURFACE MORPHOLOGY

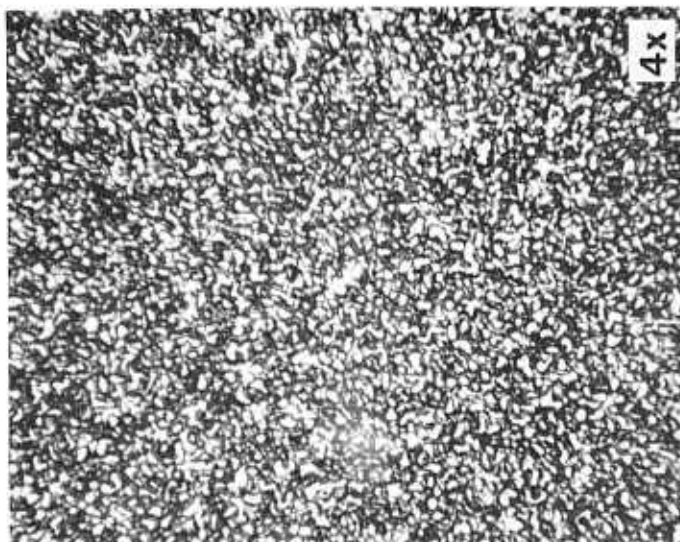


Fig. 22 HgCdTe LPE growth on MBE CdTe/GaAs substrate.
Morphology and cross-section.



SC5373.4FTR

layers is also shown in Fig. 22. Similar results were obtained for CdTe/Ge and CdTe/Si substrates although the magnitude of the chemical attack on the Si substrate was considerably less than for GaAs and Ge base substrates.

Attempts to use supercooled melts (used successfully in the LPE growth of CdTe on alternate substrates) to prevent chemical attack during the LPE of HgCdTe proved only partially successful. The use of a super cooled melt results in very high initial growth rates that quickly isolate the base substrate from the growth solution. Chemical attack of the base substrate was considerably reduced or often eliminated. However, rough morphologies typically were obtained, because, unlike the CdTe case, the HgCdTe solid is heavier than the liquid. Thus, excess solid formed in the solution during the rapid initial growth from supersaturation sinks into the growing epilayer surface and causes melt retention at the end of the growth. Figure 23 shows the typical result of an attempt to use a supercooled melt during HgCdTe LPE on a LADA CdTe/GaAs substrate. The wafer has numerous melt spots that are caused by excess solid precipitating out of the melt during the initial rapid growth of the first part of the growth cycle, and a rough morphology with numerous local defects. The cross-section shows flat and well defined interfaces as expected for this type of growth.

Because of the difficulties associated with the use of LPE techniques from Te rich melts on the base substrates, emphasis was placed on the isothermal VPE HgCdTe growth technique where substrate and source are physically separated.

6.2 IR Spectroscopy

IR transmission and absorption were used routinely for optical characterization of both CdTe and HgCdTe layers. Figure 24 shows the IR transmission of LPE grown CdTe on OM-VPE CdTe/GaAs and CdTe/Ge substrates. Transmissivity without AR coating is close to the theoretical limit for CdTe/GaAs (58%) and CdTe/Ge (55%). Interference fringes were well defined, indicating flat, planar interfaces, and allowed nondestructive layer thickness determination. IR absorption spectra are shown in Fig. 25 for isothermal VPE-grown



SC5373.4FTR

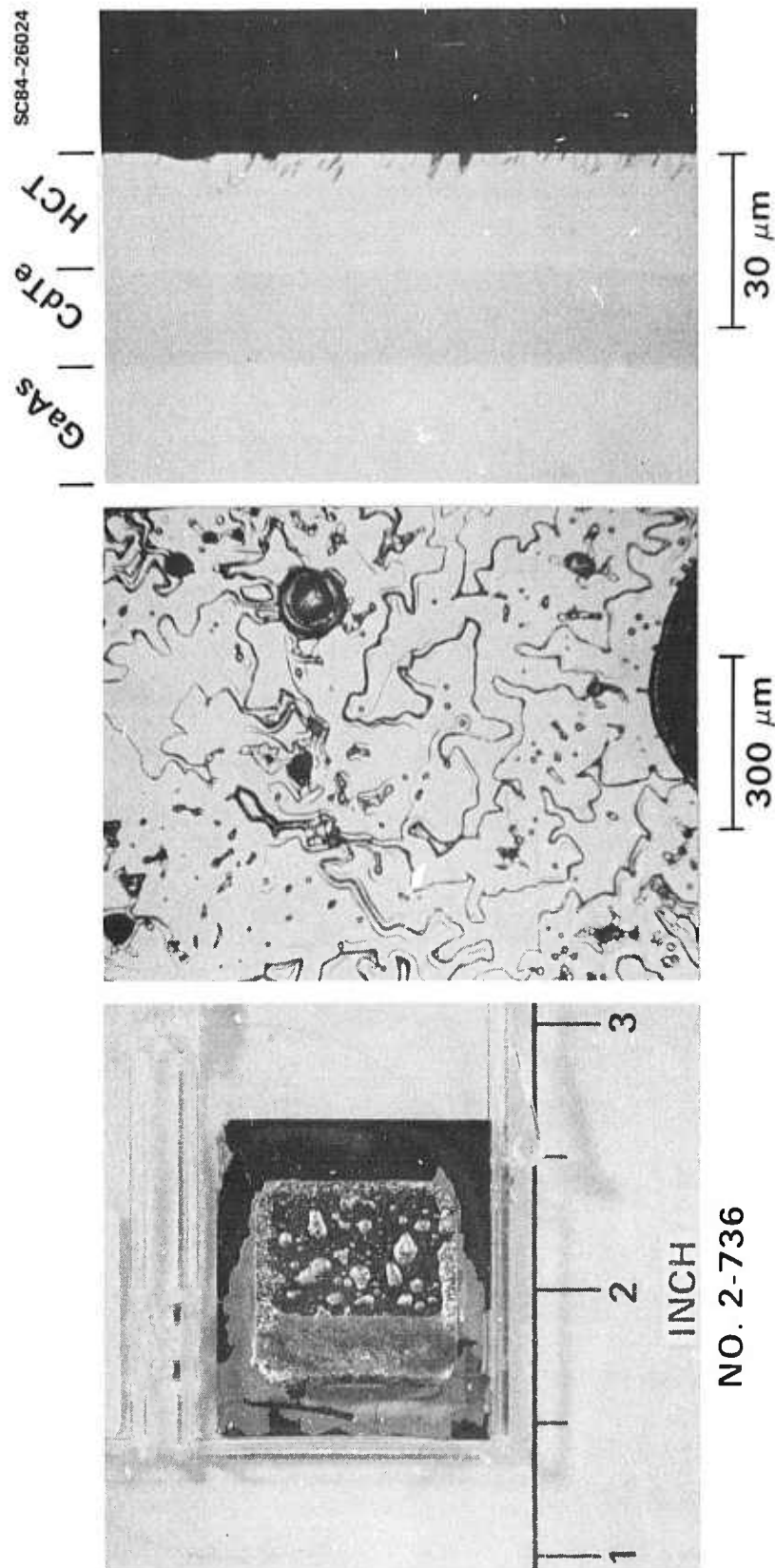


Fig. 23 LPE HgCdTe on LADA CdTe/GaAs using super cooled solution.

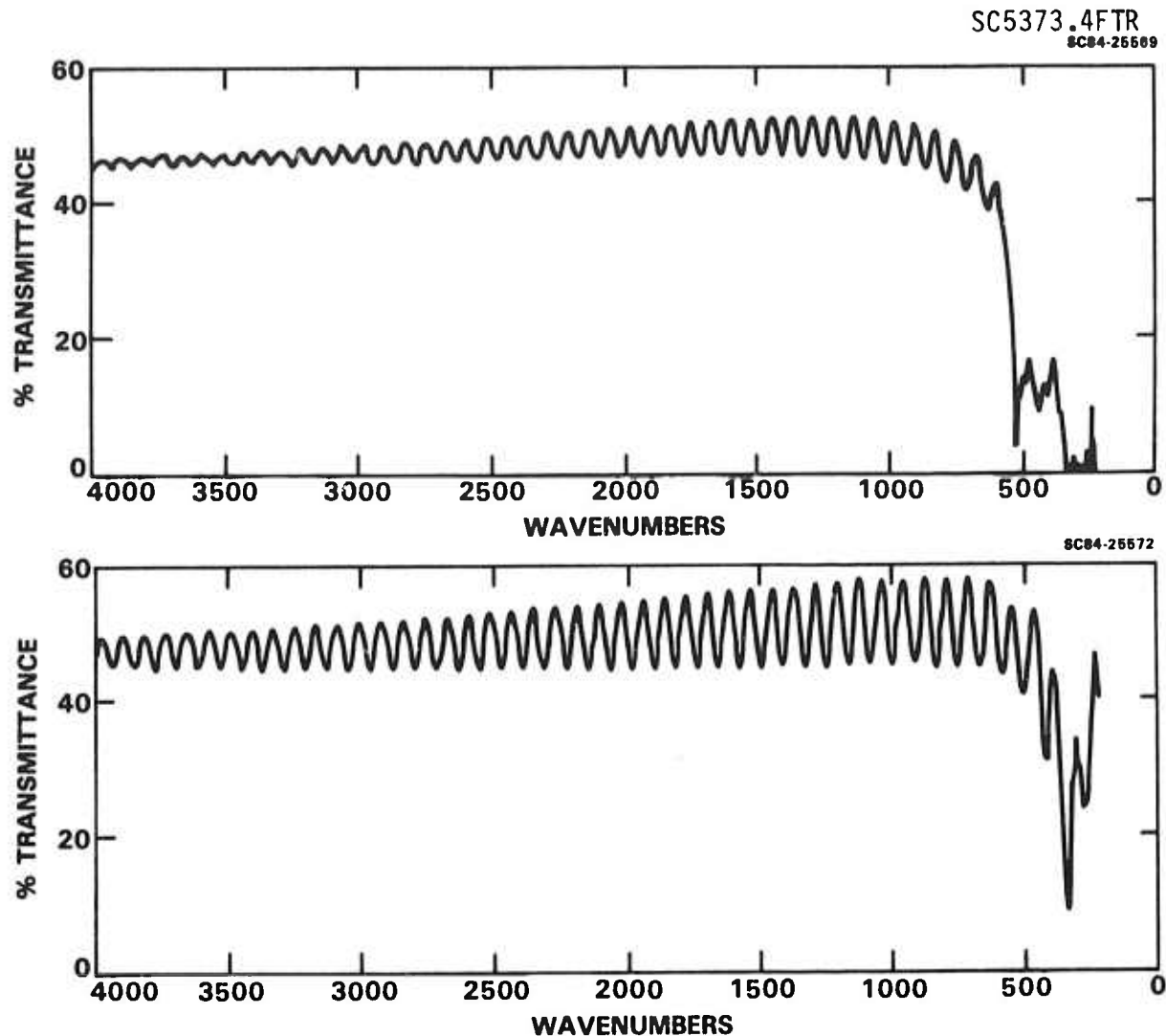


Fig. 24 IR transmission of (a) CdTe/Ge and (b) CdTe/GaAs.

HgCdTe on CdTe/GaAs and CdTe/Ge substrates. The sharp absorption edge indicates homogeneous HgCdTe material, and interference fringes indicate planar interfaces.

6.3 Double Crystal X-Ray Diffraction

Double crystal x-ray rocking curves were used to determine the crystalline perfection of the epitaxial CdTe layers. Strain and defects in the lattice cause scattering of the x-ray beam and thus widen the diffraction curve. To obtain monochromatic radiation, a GaAs first crystal was used with



SC5373.4FTR

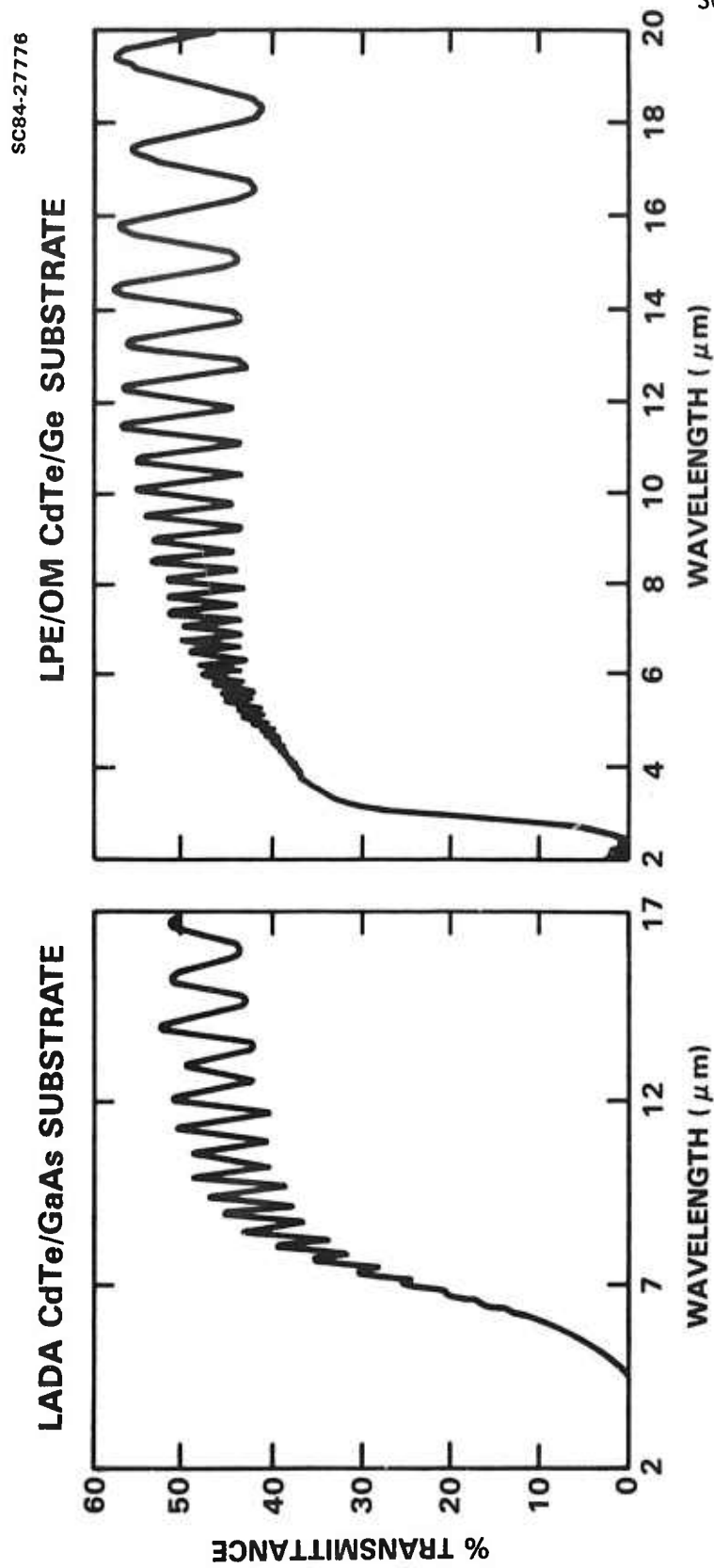


Fig. 25 IR transmission of ISO-VPE HgCdTe on (a) CdTe/GaAs and (b) CdTe/Ge.



SC5373.4FTR

the (400) reflection. The Cu $K_{\alpha 1}$ radiation was then diffracted by the sample to be analyzed using the (111) and (400) reflection respectively for (111) and (100) oriented samples. The spot size was approximately 1×2 mm with a resolution of better than 20 arc-s determined by using the same GaAs wafer as both the first and second crystals. Analysis concentrated on the epitaxial CdTe layers since their crystallinity determined the subsequent HgCdTe layer crystallinity. The results are tabulated in Table 8. As a reference, the values of PACE-1 LPE CdTe and the range for bulk CdTe have been included. Crystallinity comparable to bulk was found for several cases. In all cases LPE growth of CdTe improved in crystallinity over the vapor nucleated CdTe. For example, lines 1 and 2, LPE/OM CdTe/GaAs with a $\Delta\theta$ of 1.3 min compared with 1.7 min for the initial OM CdTe/GaAs layer. Similarly, a comparison of lines 4 and 6 shows that LPE growth of CdTe on MBE grown CdTe/GaAs reduced the $\Delta\theta$ from 2.3 to 1.9 min. Other examples can be found by comparing lines 5 and 7, and lines 3 and 8. In each case improved crystallinity was observed for the LPE CdTe layer. Another interesting observation can be made by comparing lines 2 and 8, i.e., OM-VPE growth of CdTe on GaAs and Ge respectively. Both have the same lattice mismatch with CdTe (15%), yet the crystallinity of the CdTe/GaAs is much higher. The reason lies in the difficulty in nucleating a polar compound, CdTe, on a nonpolar element Ge. In the initial nucleation of CdTe on Ge both Ge-Te and Ge-Cd bonds can form. This leads to the formation of stacking faults and antiphase domains which broaden the x-ray diffraction curve.

In the case of CdTe on GaAs, a polar on polar case, the natural preference for one bond to occur dominates the nucleation process. Thus, on the GaAs (111)As faces, CdTe with the (111)Te face was obtained; while on (111)Ga GaAs, the (111)Cd face of CdTe was obtained.

To summarize, the x-ray diffraction data bulk values were obtained for CdTe on GaAs while near bulk values were obtained for CdTe on Ge and Si substrates. In all cases, LPE growth improved the crystallinity, of vapor grown CdTe. Of the three vapor growth techniques used, OM-VPE grown CdTe on GaAs had the narrowest diffraction curves and the highest crystallinity, possibly due to the higher growth temperature of OM-VPE compared to LADA or MBE.



SC5373.4FTR

Table 8
Double Crystal X-ray Diffraction of
PACE-2 CdTe

Substrate	$\Delta\theta$ (min)
1. LPE/OM CdTe/GaAs	1.3
2. OM CdTe/GaAs	1.7
3. LPE/OM CdTe/Ge	1.8
4. LPE/MBE CdTe/GaAs	1.9
5. LPE/MBE CdTe/Si	1.9
6. MBE CdTe/GaAs	2.3
7. MBE CdTe/Si	3.3
8. OM CdTe/Ge	4.7
References: LPE PACE-1 CdTe	1.5 min
Bulk CdTe	1 to 2 min

6.4 Cathodoluminescence

Cathodoluminescence reveals nonradiative defect centers in semiconductor material and can be used effectively to determine the defect density and its spatial distribution. Scanning electron microscope cathodoluminescence was used to determine the defect distribution and density on a variety of PACE-2 substrates. The results are tabulated in Table 9. As a reference, values for bulk CdTe and PACE-1 have been included. Higher defect densities were observed for PACE-2 CdTe than for PACE-1 and bulk CdTe. The defect density of CdTe on GaAs by various techniques was up to five times lower than on Ge or Si substrates. This again illustrates the above mentioned difficulty in nucleating a polar compound on a nonpolar element. Figures 26 and 27 are examples of CL images of various PACE-2 CdTe, with PACE-1 CdTe included for comparison purposes.

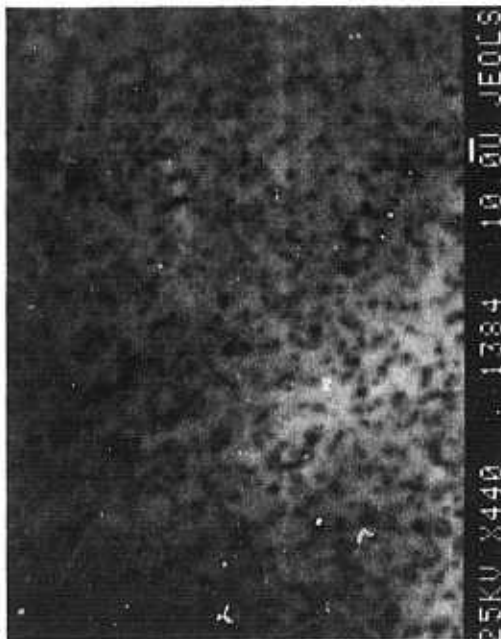


Table 9

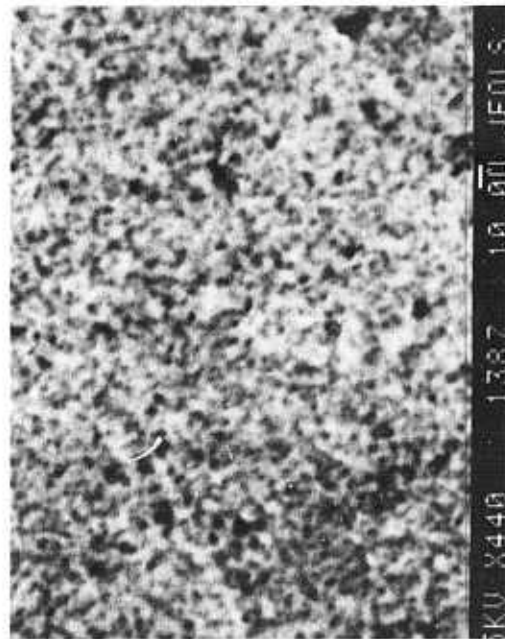
Defect Density of PACE-2 CdTe by Cathodoluminescence

LPE/MBE CdTe/GaAs	$8 \times 10^6 \text{ cm}^{-2}$
LADA CdTe/GaAs	$1 \times 10^7 \text{ cm}^{-2}$
MBE CdTe/GaAs	$2 \times 10^7 \text{ cm}^{-2}$
LPE/OM CdTe/GaAs	$2 \times 10^7 \text{ cm}^{-2}$
LPE/OM CdTe/Ge	$\approx 4 \times 10^7 \text{ cm}^{-2}$ (clustering)
LPE/MBE CdTe/Si	$4 \times 10^7 \text{ cm}^{-2}$
Reference: PACE-1	$5 \times 10^6 \text{ cm}^{-2}$
Bulk CdTe	$2 \times 10^{-6} \text{ cm}^{-2}$ (excluding grain boundaries)

SC84-27821



LPE/MBE CdTe/GaAs

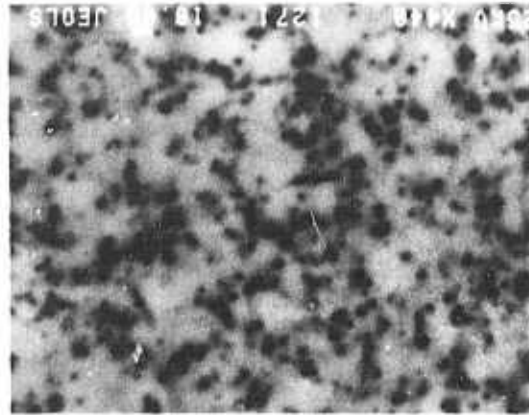


LADA CdTe/GaAs

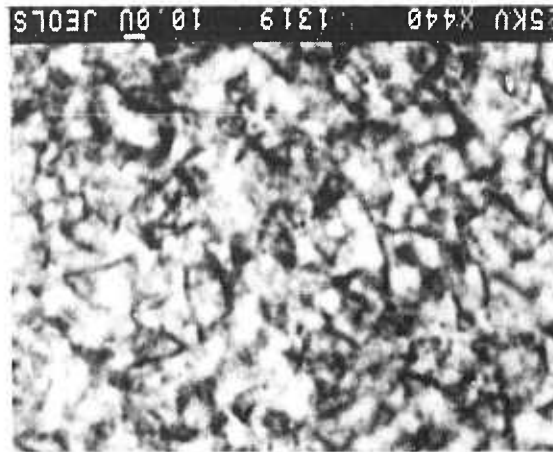
Fig. 26 Cathodoluminescence of PACE-2 CdTe.



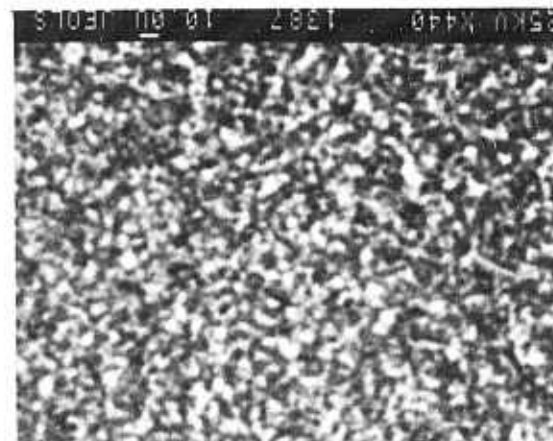
SC84-27822



PACE-1



LPE/OM CdTe/Ge



LPE/MBE CdTe/Si

Fig. 27 Cathodoluminescence of PACE-2 CdTe and PACE-1 CdTe.



SC5373.4FTR

6.5 SIMS Analysis and Results

SIMS (Secondary Ion Mass Spectroscopy) analysis was carried out to determine the level and distribution of background impurities as well as that of base substrate elements in the CdTe and HgCdTe epitaxial layers. The technique is capable of both compositional and impurity concentration analysis. Sensitivity varies but can be as high as 10^{13} atom/cm³. The instrument forms a mass-resolved, real image of the secondary ions and diaphragms are used to isolate selected areas for ion counting. Either O_2^+ or C_s^+ primary ions can be used to generate positive or negative secondary ions. Sputtering capability allows compositional and impurity depth profiling. The results of the SIMS analysis are tabulated in Table 10 for the base substrate elements. Background impurities were found at similar levels as for PACE-1 and bulk CdTe except for Li which is consistently lower in PACE-2 (and similarly for PACE-1 CdTe) compared to bulk CdTe. Lowest levels of base substrate elements were found in CdTe grown on Si and Ge substrates. Ga was found at higher levels in the range from 2×10^{16} to 2×10^{18} cm⁻². For HgCdTe similar results were obtained, although typically lower levels of base substrate elements were found relative to the CdTe layer. Typical SIMS profiles were quite complicated, with impurity pile-up at interfaces and areas of poor crystallinity. In general it can be said that higher crystallinity resulted in lower outdiffusion of base substrate elements and thus lower levels in the epilayers. Also it was found that in the LPE CdTe cycle, often some slight dissolution of the base substrate must have occurred despite the use of supercooled melts and high growth rates. Often higher concentrations of base substrate elements were found in LPE grown CdTe compared to vapor grown CdTe, despite the known higher crystallinity of LPE grown CdTe. Figure 28 is an example where the level of Ga is higher in the LPE layer than the initial OM-VPE CdTe layer on GaAs, because of slight chemical attack of the GaAs by the growth liquid and subsequent incorporation in the growing CdTe layer. Figures 29 and 30 are typical SIMS profiles for CdTe and HgCdTe grown by various techniques on GaAs and Ge base substrates. The distinct impurity spikes seen in the isothermally grown HgCdTe on the LADA CdTe/GaAs and the LPE/OM CdTe/Ge substrates is due to



Table 10
SIMS Analysis of Base Substrate Elements in PACE-2 Material CdTe and HgCdTe

CdTe		ISO-VPE HgCdTe	
LPE/MBE CdTe/Si	$\cong 1 \times 10^{14} \text{ cm}^{-3}, \text{ Si}$	LADA CdTe/Si	$\cong 5 \times 10^{14} \text{ cm}^{-3}, \text{ Si}$
OM CdTe/Ge	$< 5 \times 10^{15} \text{ cm}^{-3}, \text{ Ge}$	LADA CdTe/GaAs	$7 \times 10^{15} \text{ cm}^{-3}, \text{ Ga}$
LPE/OM CdTe/Ge	$< 5 \times 10^{15} \text{ cm}^{-3}, \text{ Ge}$	LPE/OM CdTe/Ge	$3 \times 10^{16} \text{ cm}^{-3}, \text{ Ge}$
OM CdTe/GaAs	$2 \times 10^{16} \text{ cm}^{-3}, \text{ Ga}$		
MBE CdTe/GaAs	$3 \times 10^{17} \text{ cm}^{-3}, \text{ Ga}$	MBE CdTe/GaAs	$2 \times 10^{16} \text{ cm}^{-3}, \text{ Ga}$
LPE/OM CdTe/GaAs	$2 \times 10^{18} \text{ cm}^{-3}, \text{ Ga}$		

Level of background impurities similar to that found for PACE-1 and bulk except Li which is consistently lower.

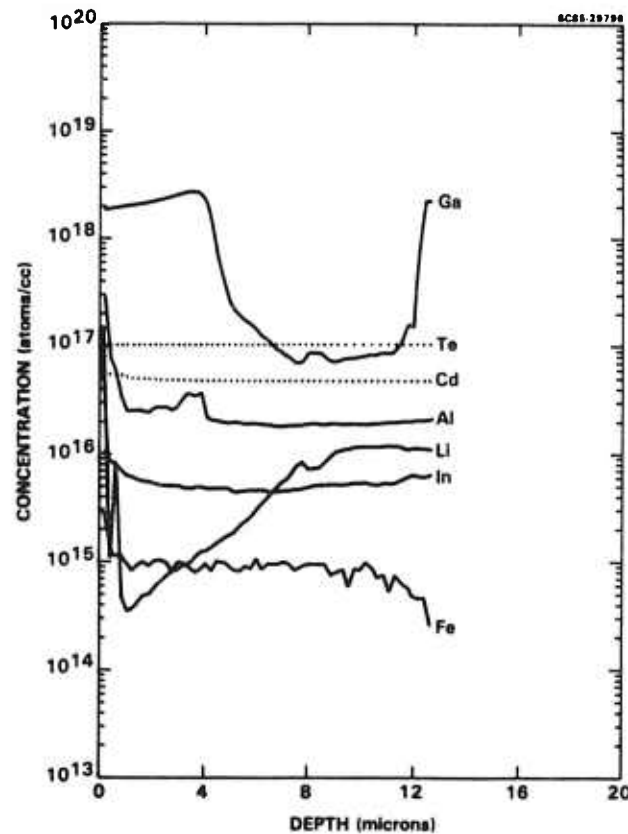


Fig. 28 SIMS impurity depth profile of LPE CdTe on OM-VPE CdTe/GaAs.



SC5373.4FTR

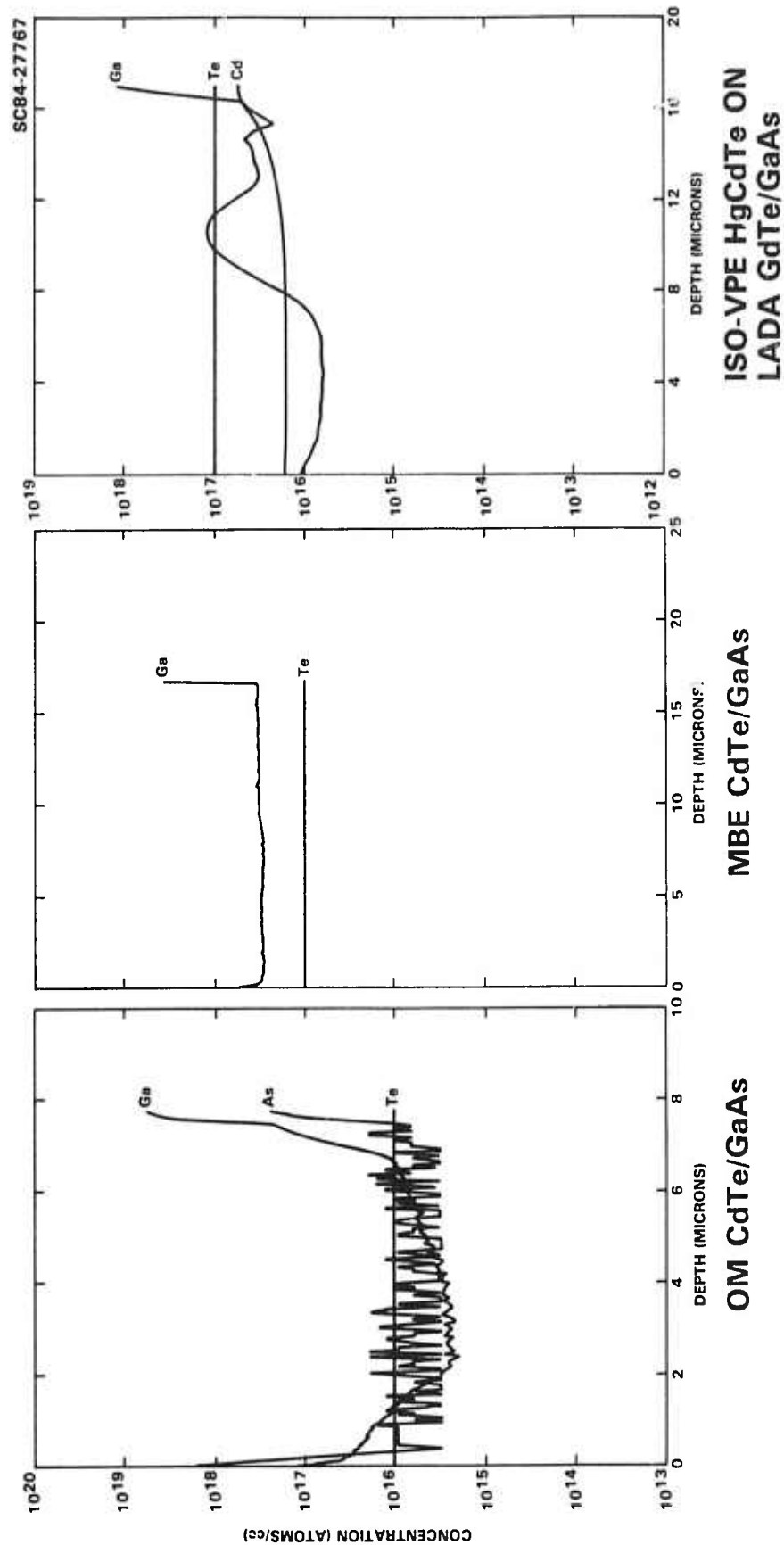


Fig. 29 SIMS depth profile of CdTe and HgCdTe on GaAs.

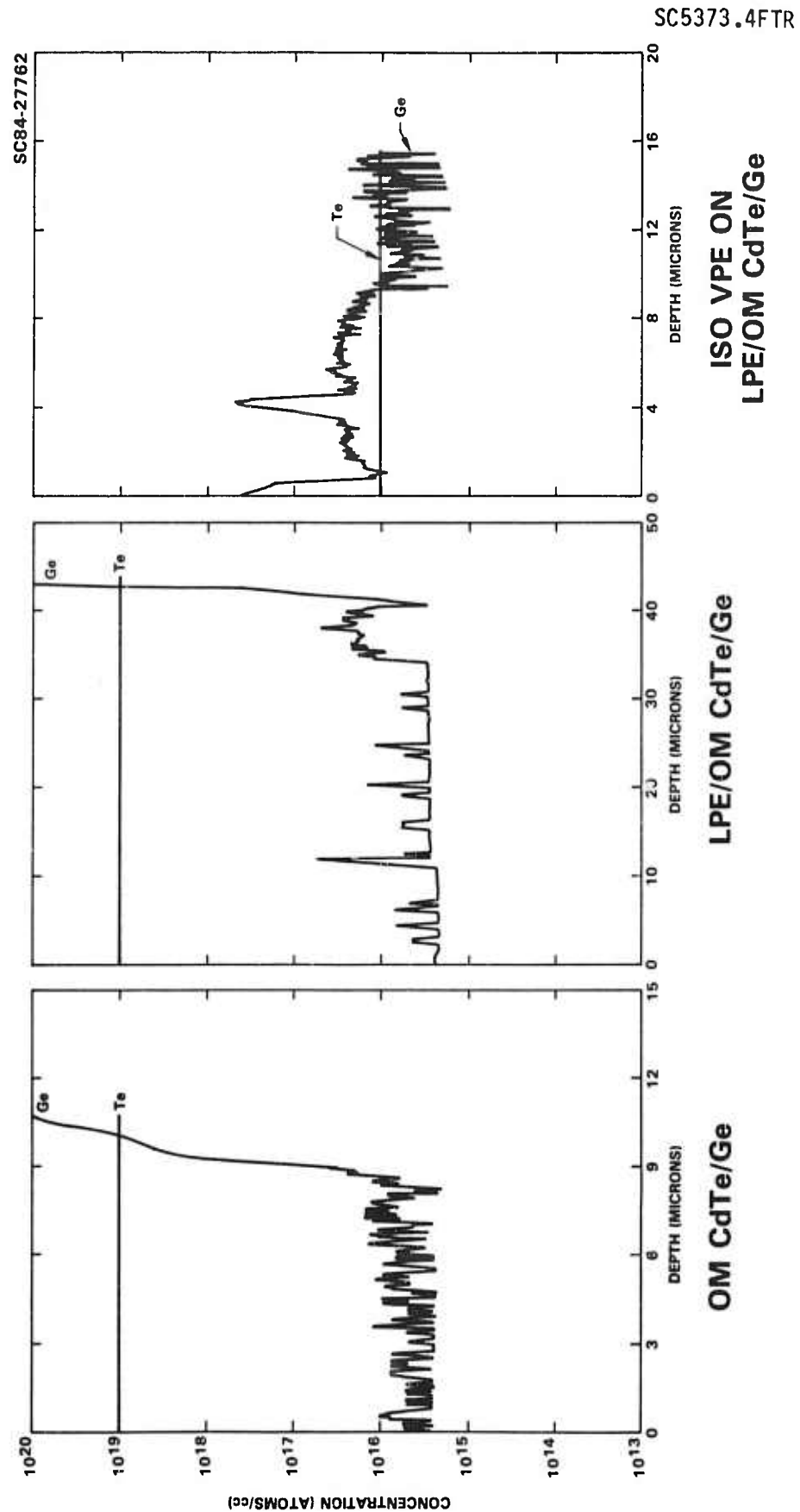


Fig. 30 SIMS impurity depth profile of CdTe and HgCdTe on Ge.



impurity pileup at the original CdTe interface. A possible cause is degraded surface crystallinity that occurs during the heatup and stabilization of the HgCdTe growth system.

6.6 Hall Effect Measurements

The carrier type, concentration and mobility were determined by Hall effect measurements using the Van der Pauw geometry. Epitaxial layers of CdTe were not analyzed due to difficulties in making ohmic contacts. HgCdTe layers were analyzed on a routine basis. The goal for the HgCdTe was an as-grown p-type conduction in order to be suitable for junction formation by ion implantation. The majority of the as-grown PACE-2 HgCdTe layers, however, were n-type and could be converted to p-type conduction only occasionally. The characteristics of the p-type layers obtained, as-grown and annealed, are shown in Table 11. The HgCdTe were all grown by isothermal VPE on various PACE-2 substrates. In all cases, the carrier mobility is lower than expected for the corresponding carrier concentration and composition indicated by λ_a (300K). The reason for this behavior, as well as for the n-type conduction, appears to be enhanced base substrate outdiffusion which caused either the HgCdTe layer to be n-type or highly compensated.

Table 11
Summary p-Type Isothermal VPE HgCdTe on PACE-2 Substrates

Substrate	Thickness (μm)	λ_a (300K) (μm)	HgCdTe Carrier Concentration (cm^{-3} 77K)	Carrier Mobility ($\text{cm}^2/\text{v-s}$ 77K)	
LADA CdTe/GaAs	16	6.0	1.7E17	169	Annealed
LADA CdTe/GaAs	6	4.5	2.4E16	155	Annealed
VPE/OM CdTe/Ge	10	2.7	4.8E15	165	Annealed
OM/LPE/OM CdTe/Ge	17	3.3	2.5E16	-	As Grown
VPE/OM CdTe/Ge	9	3.1	1.1E17	121	As Grown



7.0 SUMMARY AND SELECTED BASELINE APPROACH

A variety of vapor growth techniques were used to grow CdTe on epitaxial layers of CdTe on three base substrates -- GaAs, Ge, and Si. Single crystal layers of CdTe were obtained on all three base substrates. Of the three CdTe vapor growth techniques used OM-VPE growth of CdTe on GaAs resulted in the highest crystallinity with a $\Delta\theta = 1.7$ min, as determined by double crystal x-ray diffraction. As witnessed by decreasing $\Delta\theta$ values in all cases, LPE growth of CdTe on a vapor nucleated CdTe increased the crystallinity and reduced the nonradiative defect density as determined by scanning electron microscope cathodoluminescence. SIMS analysis, however, showed higher levels of base substrate elements in LPE grown CdTe due to slight chemical attack of the base substrate during the LPE cycle. This resulted in contamination of the melt by base substrate elements and their subsequent incorporation into the growing CdTe layer. SIMS also revealed generally lower levels of Si and Ge in CdTe grown on those substrates relative to Ga in CdTe on GaAs.

Two techniques were used to grow the active HgCdTe layer on the PACE-2 substrates, LPE and isothermal VPE. With LPE, severe base substrate chemical attack occurred which precluded its further use, so that efforts were concentrated on the isothermal VPE growth of HgCdTe. The desired p-type conduction for isothermally grown HgCdTe was achieved, provided the PACE-2 substrate were of sufficient quality; i.e., high crystallinity and low impurity background.

On the basis of the data obtained, the following baseline approach has been selected for the next phase of this program and is shown in Table 12 along with alternate back-up approaches. Isothermal VPE of HgCdTe will be used to grow the active HgCdTe layer in view of the difficulties with LPE growth on alternate base substrates. The primary substrate for the isothermal will be OM-VPE grown CdTe on GaAs. This combination had the best crystallinity ($\Delta\theta = 1.7$) and lowest Ga level ($2 \times 10^{16} \text{ cm}^{-3}$) of the vapor grown epitaxial CdTe layers. The lower Ga level is a direct result of the higher crystallinity observed for OM-VPE grown CdTe despite the higher growth temperatures of that technique ($\sim 500^\circ\text{C}$) compared with LADA or MBE ($\sim 300^\circ\text{C}$). Furthermore, with greater emphasis placed on the OM-VPE growth of CdTe on GaAs



Table 12
Baseline Approach for Phase 2 of PACE-2

Technique	Structure	
1. OM-VPE	CdTe/GaAs	Baseline
2. OM-VPE	CdTe/Ge	
3. MBE	CdTe/Si	Alternatives
4. MBE	CdTe/Ge	

(secondary to CdTe on Ge during the initial phase, see Table 4) we expect further improvements in crystallinity and reduction of impurities via growth parameter refinements leading to the routine synthesis of p-type HgCdTe layers suitable for device processing and evaluation.



SC5373.4FTR

8.0 REFERENCES

1. E.R. Gertner, R.A. Reidel, N.H. Sheng, D.D. Edwall, L.E. Wood, J.D. Blackwell, L.O. Bubulac, J. Bajaj, J.G. Pasko, D.T. Cheung and W.E. Tennant, Proceedings of IRIS, National 1983.
2. E.R. Gertner, D.D. Edwall, L.O. Bubulac, L.E. Wood, J. Bajaj, S.H. Shin and W.E. Tennant, Proceedings of IRIS, Detector Specialty Group, 1983.
3. N.H. Sheng, J.d. Blackwell, E.R. Gertner, L.E. Wood, D.D. Edwall, W.E. Tennant and J.P. Rode, Proceedings of IRIS, Detector Specialty Group, 1983.
4. W.E. Tennant, IDEM Technical Digest, 704, (1983).
5. J.P. Rode, Proceedings of SPIE 443, 120 (1983).
6. J.T. Cheung and T. Magee, J. Vac. Sci. Technol. A1, 1604 (1983).
7. J.T. Cheung and D.T. Cheung, J. Vac. Sci. Technol. 21, 182 (1983).
8. J.T. Cheung, Appl. Phys. Lett. 43, 255 (1983).
9. D.D. Edwall, E.R. Gertner and W.E. Tennant, J. Appl. Phys. 55, 1453 (1984).
10. S.H. Shin and J.G. Pasko, Appl. Phys. Lett. 14, 423 (1984).