

SANDIA REPORT

SAND97-0023 • UC-700

Unlimited Release

Printed January 1997

Use of High Index Substrates to Enable Dislocation Filtering in Large Mismatch Systems

John L. Reno, Robert M. Biefeld, Steve R. Kurtz, Kevin C. Baucom

Prepared by
Sandia National Laboratories
Albuquerque, New Mexico 87185 and Livermore, California 94550
for the United States Department of Energy
under Contract DE-AC04-94AL85000

Approved for public release; distribution is unlimited.

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

ph

MASTER

Issued by Sandia National Laboratories, operated for the United States Department of Energy by Sandia Corporation.

NOTICE: 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, nor any of their contractors, subcontractors, or 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, any agency thereof or any of their contractors or subcontractors. The views and opinions expressed herein do not necessarily state or reflect those of the United States Government, any agency thereof or any of their contractors.

Printed in the United States of America. This report has been reproduced directly from the best available copy.

Available to DOE and DOE contractors from
Office of Scientific and Technical Information
PO Box 62
Oak Ridge, TN 37831

Prices available from (615) 576-8401, FTS 626-8401

Available to the public from
National Technical Information Service
US Department of Commerce
5285 Port Royal Rd
Springfield, VA 22161

NTIS price codes
Printed copy: A03
Microfiche copy: A01

DISCLAIMER

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

Distribution
Category UC-700

SAND97-0023
Unlimited Release
Printed January 1997

**USE OF HIGH INDEX SUBSTRATES TO ENABLE DISLOCATION
FILTERING IN LARGE MISMATCH SYSTEMS**

John L. Reno, Robert M. Biefeld, Steve R. Kurtz,
and Kevin C. Baucom
Semiconductor Material and Device Sciences Department
Sandia National Laboratories
Albuquerque, NM 87185-0601

Abstract

We report results in three areas of research relevant to the fabrication of wide range of optoelectronic devices. (1) The development of a new x-ray diffraction technique that can be used to rapidly determine the optimal period of a strained layer superlattice to maximize the dislocation filtering. (2) The optimal MBE growth parameters for the growth of CdTe on GaAs(211). The determination of the relative efficiency of dislocation filtering in the (211) and (100) orientations. (3) The surface quality of InSb grown by MOCVD on InSb substrates is affected by the misorientation of the substrate.

Contents

Nomenclature	2
Introduction	3
New X-ray Diffraction Technique	4
MBE Growth of CdTe on GaAs(211)	5
Introduction	5
Substrate Pretreatment	5
Epitaxy and Control of Orientation	5
Strained Layer Superlattice Dislocation Reduction	6
InSb Growth by MOCVD	8
Conclusion	9
APPENDIX	10

Nomenclature

MBE	Molecular Beam Epitaxy, a crystal growth technique
MOCVD	Metal-Organic Chemical Vapor Deposition, a crystal growth technique
PLM	Photoluminescence Microscopy
TEM	Transmission Electron Microscopy
FWHM	Full Width at Half Maximum
SLS	Strained Layer Superlattice
GaAs	Gallium Arsenide
ZnTe	Zinc Telluride
CdTe	Cadmium Telluride
InSb	Indium Antimonide
InAsSb	Indium Arsenide Antimonide

Introduction

Strained-layer and lattice-mismatched structures have received a great deal of attention because of their intrinsic interest from the physics and materials science viewpoints and because of their possible applications in electronic devices. Many possible applications have been limited due to the need for substrates with an appropriate lattice parameter. If the device and the substrate on which it is fabricated are highly mismatched ($>2\%$), a large number of dislocations are created which are difficult, if not impossible, to keep out of the active part of the device. These dislocations can greatly deteriorate the performance of the device. This means that the majority of device structures must be placed on substrates with a small mismatch or lattice-matched substrates in order to be manufacturable. This constraint limits the choice of materials and parameters available for device design.

The use of strained-layer superlattices to filter threading dislocations has been demonstrated for systems with a small mismatch ($<2\%$), but has not been found to be effective for systems with a large mismatch ($>2\%$). Until recently all work has been performed on low index substrates such as (100), (110) or (111). Some work has also been done on substrates with slight amounts of miscut away from these low index planes. We believe, and have very preliminary experimental confirmation, that the use of substrates cut along higher index planes, such as (211), (311) or (221), will enable dislocation filtering to occur even for systems with a large lattice mismatch. This change in behavior is due to the decrease of the angle between the threading dislocation and the interfaces at which the filtering occurs.

The primary objective was to prove experimentally the validity of the concept by determining the decrease in the threading dislocation density with the insertion of a strained-layer superlattice. CdTe, InSb, and ZnTe samples were grown. GaAs(211) and misoriented substrates were used for all the materials systems. X-ray diffraction and photoluminescence microscopy were used to determine the dislocation density. Transmission electron microscopy was also performed.

New X-ray Diffraction Technique

One of the difficulties with this type of study is the determination of the optimal SLS to achieve filtering. A rapid technique that can be applied to many samples is required. TEM is the most accurate and quantitative technique but takes several days for the measurement of just one sample. A new x-ray diffraction technique has been developed which allows the experimental determination of the strained layer superlattice period required to optimize dislocation filtering. It does not give a value for the dislocation density. The technique measures the x-ray full width at half maximum (FWHM) of a cap layer that has been grown on top of the strained layer superlattice. When a plot of the x-ray FWHM vs the superlattice period is made, a minimum is found. This minimum is located at the optimal superlattice period. TEM of the sample at the minimum x-ray FWHM has been performed and confirms the filtering of dislocations and the high quality of the cap material. This one TEM also gives a value for the minimum dislocation density.

MBE Growth of CdTe on GaAs (211) Substrates

Introduction

The initial step necessary to carry out this research was to learn to grow on high index substrates. The system that was studied was CdTe on GaAs(211). We have been successful at growing this type of material. Because this is a high index plane there is a tendency for the surface to facet. Therefore a new procedure for growth on this high index substrate was developed different from that for growth on (100) substrates. The developed procedure consists of three steps: substrate pretreatment (both chemical etch and anneal), growth of a buffer and insertion of a superlattice.

Substrate Pretreatment

Prior to growth by MBE a wet chemical etch is carried out in order to remove surface contaminants and polishing damage. For GaAs(100) substrates a warm 5:1:1 solution of $H_2SO_4:H_2O_2:H_2O$ is typically used. For GaAs(211) substrates it is essential that the etch be allowed to cool to room temperature before use. If the etch is still warm the surface is roughened due to facetting.

After the sample is placed into the MBE system it is necessary to bake the substrate to remove the oxides that are present. For GaAs(100) this is normally done at about 600°C with an As flux. For GaAs(211) substrates the use of an As overpressure causes the surface to facet. We have found that baking without an As overpressure can lead to a flat, unfacetted surface if the temperature of the bake is not too high. Once the oxide is removed the temperature needs to be decreased immediately or facetting occurs.

Since the GaAs(211) face is a polar face, it was necessary to determine whether the A (Ga-terminated) or B (As-terminated) face was the best for epitaxial growth of CdTe. We have found that the B face is preferred.

Epitaxy and Control of Orientation

The epitaxial growth of CdTe on GaAs(211)B turns out to be quite interesting. This system has the capability of dual epitaxy. It is possible for both CdTe(211) and CdTe(331) to grow on GaAs(211)B substrates. In the case of CdTe(331) on GaAs(211)B the surface tends to be rough and faceted. Even though we have not yet been able to get a smooth surface for this epitaxial orientation, the crystal quality from

X-ray diffraction seems to be good. In the case of CdTe(211) on GaAs(211)B the surface can be smooth. X-ray diffraction shows the crystal quality to be good and that a tilt exists between the CdTe(211) planes and the GaAs(211) planes. The amount of tilt has not been carefully quantified but appears to be a few degrees.

It is possible to reproducibly control the orientation of the CdTe grown on GaAs(211)B with the correct pretreatment. CdTe(331) on GaAs(211)B occurs when either a high temperature anneal is used or when the anneal is done with an As flux present. As mentioned previously, both of these pretreatments lead to a rough faceted surface. We do not know at this time if it is possible to obtain CdTe(331) without this facetting. CdTe(211) on GaAs(211)B occurs when a low temperature anneal is used. The surface is rough in this case probably due to the incomplete removal of the oxide layer. If the growth of CdTe is begun and the substrate cooled as soon as it is determined by RHEED that the oxide has been removed, a smooth CdTe(211) layer is obtained. By far the easiest and most reproducible way to obtain smooth CdTe(211) on GaAs(211)B is to begin the growth with about 20 \AA or more of ZnTe. ZnTe does not exhibit dual epitaxy and always grows in the (211) orientation on GaAs(211)B.

Strained Layer Superlattice Dislocation Reduction

We have grown SLS to try to filter the dislocations present. By PLM we have found that it is possible to get a network of misfit dislocations in the interfaces of the SLS. This is an indication of dislocation filtering and dislocation density reduction.

Two series of samples were grown on (100) and (211) with a CdZnTe/CdTe strained layer superlattice inserted. The period of the strained layer superlattice was optimized using the x-ray technique described above. Both sets of samples exhibited a minimum in the plot of FWHM vs period. The existence of this minimum demonstrates a reduction in the dislocation density and dislocation filtering for both orientations. The value of the period at which the minimum x-ray FWHM was achieved was very different for the two orientations. For the (211) orientation the minimum occurred at approximately 100 \AA , while for the (100) orientation the minimum occurred at approximately 300 \AA . The smaller period needed for the (211) orientation indicates that less strain energy is needed to filter dislocations in this orientation. This is what we expected to find. These samples were then characterized by TEM to determine the dislocation density and to quantify the amount of reduction due to the superlattice.

TEM indicated that for both the (100) and (211) orientations the filtering was very effective only if the strain in the SLS was balanced. It also showed that the amount of filtering between the two orientations did not vary significantly. This disproved our initial hypothesis.

InSb Growth by MOCVD

InSb was grown by MOCVD on oriented and misoriented InSb and GaAs. On InSb substrates the surface morphology of the grown InSb was found to be very rough for growth temperatures $\leq 425^{\circ}\text{C}$. This surface roughness is associated with low temperature and excess Sb of high Sb to In ratio. Smoother surfaces were found when using the proper misoriented substrates. The details of the surface defects observed was dependent on the type of misorientation used and is related to the atomic structure of the surface steps. The smoothest surfaces were obtained for growth on InSb substrates misoriented 5° towards the $\langle 111 \rangle$ In planes. Similar experiments were carried out for the growth of InSb on misoriented GaAs substrates. Little or no improvement was found for material grown on GaAs. We believe that this is due to the small amount of misorientation used.

Conclusion

A new x-ray diffraction technique has been developed to rapidly optimize the SLS to provide the maximum dislocation filtering. This technique, along with TEM, has been used to demonstrate dislocation filtering in CdTe grown on GaAs in both the (100) and (211) orientations. The amount of filtering between the two orientations was found to not vary significantly.

InSb has been grown by MOCVD onto oriented and miscut InSb and GaAs. Significant improvement is found for the lattice matched InSb case. Little or no improvement was found for material grown on GaAs. We believe that this is due to the small amount of misorientation used.

APPENDIX

LDRD Data

Refereed Publications:

1. J. L. Reno, S. Chadda and K. Malloy, "Dislocation Reduction in CdZnTe on GaAs using Strained Layer Superlattices", *Applied Physics Letters* **63**, Sept. 27, 1993, pg. 1827.
2. R. M. Biefeld and K. C. Baucom, "Substrate Orientation and Surface Morphology Improvements for InSb Grown by MOCVD", *Journal of Crystal Growth* **135**, Feb. 1994, pg. 401.
3. R. M. Biefeld, "The Growth of InSb using Alternative Organometallic Sb Sources", *Journal of Crystal Growth* **128**, Feb. 1993, pg. 511.
4. S. Chadda, K. Malloy, and J. L. Reno, "Defect Reduction in CdTe Epilayers on GaAs", *Mat. Res. Soc. Proc.* Vol. 299, 1994, pg. 191.
5. R. M. Biefeld and K. C. Baucom, "Effects of Growth Conditions and Substrate Orientation on the Properties of InSb", *Mat. Res. Soc. Proc.* Vol. 312, 1994, pg. 179.

Oral Presentation:

1. J. L. Reno, S. Chadda and K. Malloy, "The Use of CdZnTe/CdTe Strained Layer Superlattices for Defect Reduction in CdZnTe Epilayers on GaAs", The 1993 March Meeting of the American Physical Society, Seattle, WA, March 22-26, 1993.
2. S. Chadda, K. Malloy, and J. L. Reno, "Defect Reduction in CdTe Epilayers on GaAs", The Spring Meeting of the Materials Research Society, San Francisco, CA, April 12-16, 1993.
3. R. M. Biefeld and K. C. Baucom, "Effects of Growth Conditions and Substrate Orientation on the Properties of InSb", The Spring Meeting of the Materials Research Society, San Francisco, CA, April 12-16, 1993.

PhD Thesis

1. Saket Chadda, *Structural Evaluation of Novel Semiconductor Radiation Detectors*, University of New Mexico, December 1993.

Patent Disclosures: 1

Patent Applications: 1

Patents: 0

Copyrights: 0

Students: 0

Post Docs: 0

Permanent Staff Hired: 0

Awards: 0

Follow-on work: None

DISTRIBUTION

1 MS9018 Central Technical Files, 8940-2
5 MS0899 Technical Library, 4414
2 MS0619 Review & Approval Desk, 12630
for DOE/OSTI

1 MS1436 LDRD Office, 4523
1 MS1427 S. T. Picraux, 1100
1 MS0601 J. S. Nelson, 1113
5 MS0601 J. L. Reno, 1113
1 MS0601 R. M. Biefeld, 1113
1 MS0601 K. C. Baucom, 1126
1 MS0601 J. Y. Tsao, 1126
1 MS0603 S. R. Kurtz, 1312
1 MS0603 A. Owyoung, 1312