

LM-02K065  
August 12, 2002

---

## **Wafer-Bonded Internal Back-Surface Reflectors for Enhanced TPV Performance**

C.A. Wang, P.G. Murphy, P.W. O'Brien, D.A. Shiau,  
A.C. Anderson, Z.L. Liau, D.M. DePoy, G. Nichols

---

### **NOTICE**

This report was prepared as an account of work sponsored by the United States Government. Neither the United States, nor the United States Department of Energy, 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.

---

---

---

---

## Wafer-Bonded Internal Back-Surface Reflectors for Enhanced TPV Performance\*

C.A. Wang, P.G. Murphy, P.W. O'Brien, D.A. Shiao, A. C. Anderson, Z.L. Liau  
Lincoln Laboratory, Massachusetts Institute of Technology, Lexington, MA 02420-9108  
D.M. DePoy, G. Nichols  
Lockheed Martin Corporation, Schenectady, NY 12301

### ABSTRACT

This paper discusses recent efforts to realize GaInAsSb/GaSb TPV cells with an internal back-surface reflector (BSR). The cells are fabricated by wafer bonding the GaInAsSb/GaSb device layers to GaAs substrates with a dielectric/Au reflector, and subsequently removing the GaSb substrate. The internal BSR enhances optical absorption within the device while the dielectric layer provides electrical isolation. This approach is compatible with monolithic integration of series-connected TPV cells and can mitigate the requirements of filters used for front-surface spectral control.

### INTRODUCTION

High-efficiency thermophotovoltaic (TPV) systems require highly efficient TPV cells as well as excellent spectral control to recuperate below bandgap photons back to the radiator.<sup>1</sup> Various approaches for front-surface spectral control include dielectric stacks,<sup>2</sup> plasma filters,<sup>3</sup> or resonant arrays,<sup>4,5</sup> which are placed between the radiator and the front side of the TPV cell. Alternatively, spectral control can be achieved with a back-surface reflector (BSR)<sup>6</sup>, which is a highly reflecting mirror deposited on the backside of the cell. BSRs also have additional advantages related to improvements in TPV cell performance, since above bandgap photons that are not absorbed in the first pass are reflected back into the active layers for a second-pass absorption. Such BSRs have been incorporated into the design of InGaAs/InP TPV systems.<sup>7</sup> Recent efforts in GaSb-based TPV, however, have focused on front-surface spectral control since the effectiveness of the BSR is reduced by free-carrier absorption in the GaSb substrate.<sup>2,6</sup>

This paper describes a new approach for GaInAsSb/GaSb TPV cells with an internal BSR, which is formed by wafer-bonding and is located directly below the epitaxial device structure. After bonding the epitaxial TPV layers, the GaSb substrate is completely removed. This concept of wafer-bonding using metal as an adhesive layer is similar to that developed for integration of dissimilar materials<sup>8</sup> and for fabrication of internal mirrors for photovoltaic cells,<sup>9</sup> light emitting diodes,<sup>10</sup> and vertical-cavity surface-emitting lasers.<sup>11</sup> The resulting TPV device structure consists of a broad-band high-reflectivity dielectric/Au mirror sandwiched between the GaInAsSb/GaSb device layers and a GaAs handle substrate.

Wafer-bonded TPV cells with internal BSRs have the potential of improving TPV cell performance; providing spectral control; and allowing series connections of

\*This work was sponsored by the Department of Energy under AF Contract No. F19628-00-C-0002. The opinions, interpretations, conclusions and recommendations are those of the author and are not necessarily endorsed by the United States Government.

---

GaInAsSb/GaSb TPV devices. Specifically, the internal BSR enhances photon recycling effects, and as mentioned above, provides double-pass absorption so that the active layers can be thinner, which is advantageous for reducing dark current and increasing open circuit voltage. In addition, since the GaSb substrate is removed from the final device, reflection of below bandgap photons back to the radiator can be very high. Furthermore, since the epitaxial layers are electrically isolated from the handle substrate by a dielectric layer, TPV cells can be connected in series to fabricate monolithically integrated modules (MIMs).<sup>12</sup>

## EXPERIMENTAL PROCEDURES

TPV device structures were grown lattice matched to 5-cm-diam GaSb substrates by organometallic vapor phase epitaxy<sup>13</sup>. In order to obtain a p-on-n structure after wafer bonding, epitaxial layers were grown in a reverse sequence compared to conventional TPV structures, and in addition, included an InAsSb layer, which is used as an etch-stop layer. The as-grown inverted TPV structure shown in Figure 1a consists of the following layers grown on a (001) n-GaSb substrate miscut 6° toward (1-11)B: u-GaSb buffer layer, u-InAsSb etch-stop layer, p-GaSb contact layer, p-AlGaAsSb window layer, p-GaInAsSb emitter layer, n-GaInAsSb base layer, and n-GaSb lateral conduction layer. (In some structures, the p-AlGaAsSb window layer was omitted.) Although the InAsSb etch-stop layer is eventually removed during the fabrication of wafer-bonded epitaxial TPV structures, it is critical that this layer is also lattice-matched to GaSb since the GaInAsSb active layers are grown on top of the InAsSb etch-stop layer.

The inverted TPV structure on the GaSb substrate and a handle semi-insulating GaAs substrate were prepared for bonding with a dielectric/reflector. For demonstration of this new concept, experiments were performed using SiO<sub>x</sub> as the dielectric layer. Although an absorption peak at 7 μm was measured in BSRs using SiO<sub>x</sub>,<sup>14</sup> an in-house deposition process for SiO<sub>x</sub>/Au reflectors without surface defects had been previously established. It is essential to minimize surface defects for wafer-bonding.<sup>15</sup> First, both GaSb and GaAs surfaces were solvent cleaned and etched in HCl and NH<sub>4</sub>OH to remove native oxides. The GaSb epitaxial TPV structure was sputter-coated with a three-layer reflector consisting of SiO<sub>x</sub>/Ti/Au, while the GaAs was sputter-coated with Ti/Au. SiO<sub>x</sub> was used to increase the above band-gap reflection properties as well as to prevent alloying or diffusion of Au with GaSb, which would reduce the reflectivity. Although Ti decreases the reflectivity, it improves the adhesion of Au to both the SiO<sub>x</sub> and GaAs. To bond the wafers, the Au surfaces were contacted, and the wafers were heated under vacuum to a temperature of 250 °C and mechanical pressure of 250 psi. The low bonding temperature is compatible with subsequent wafer processing. In a separate set of experiments to study reflector properties, GaAs substrates were sputter-coated with SiO<sub>x</sub> of thickness varying from 500 to 3600 nm and a 0.5-μm-thick Au layer.

The 5-cm-diam bonded wafer was cut into four quarters for ease of handling and processing, and the GaSb substrate was spin-etched with H<sub>2</sub>O<sub>2</sub>:H<sub>2</sub>O:NaK tartrate tetrahydrate to remove the bulk of the substrate, then chemomechanically polished. The remaining GaSb substrate and GaSb buffer layer were selectively etched using

$\text{CrO}_3:\text{HF}:\text{H}_2\text{O}$  until the InAsSb layer was exposed. Finally, the InAsSb etch-stop layer was removed with  $\text{H}_2\text{O}_2$  saturated with citric acid. The resulting wafer-bonded epitaxy can then be processed into TPV devices using standard photolithographic processes and chemical etching to define the TPV mesas. Figure 1b illustrates the wafer-bonded GaInAsSb/GaSb TPV structure with the internal BSR.

The surface flatness of bonded wafers was measured with an interferometer. The bonded epitaxial structures as well as unbonded control structures were characterized by high-resolution x-ray diffraction (HRXRD) and photoluminescence (PL) measurements at room temperature. Reflectivity ( $R$ ) measurements were performed at near normal incidence over the spectral range from 1 to 20  $\mu\text{m}$ .

## RESULTS AND DISCUSSION

The  $R$  at normal incidence was modeled for GaAs coated with a  $\text{SiO}_x/\text{Au}$  reflector. Figure 2 shows  $R$  for various  $\text{SiO}_x$  thicknesses from 1 to 3  $\mu\text{m}$ . For simplicity, absorption in GaAs was not included.  $R$  increases with  $\text{SiO}_x$  thickness and is a maximum of 98.8% for a quarter-wave thickness of 360 nm. Measured  $R$  spectra for GaAs wafers that were coated with  $\text{SiO}_x/\text{Au}$  with  $\text{SiO}_x$  thickness of 50, 200, and 360 nm are shown in Figure 3. As expected,  $R$  increases with thickness, except in the wavelength range near 8 and 9.5  $\mu\text{m}$  because of  $\text{SiO}_x$  absorption, especially at 9.5  $\mu\text{m}$ . Lower  $R$  below 1.4  $\mu\text{m}$  is due to absorption in the GaAs substrate. High  $R$  below 2.5  $\mu\text{m}$  is important for enhancing TPV device performance, while above 2.5  $\mu\text{m}$  it is important for spectral control. The integrated  $R$  from 1.5 to 2.5  $\mu\text{m}$  (since GaAs is absorbing below 1.4  $\mu\text{m}$ ) is 0.962, 0.97, and 0.981 for  $\text{SiO}_x$  thickness of 50, 200, and 360 nm, respectively. For 2.5 to 15  $\mu\text{m}$ , the integrated  $R$  is 0.952, 0.943, and 0.936 for  $\text{SiO}_x$  thickness of 50, 200, and 360 nm, respectively. The high reflectivity over the wide wavelength range is extremely attractive for GaSb-based TPV, although, for  $\text{SiO}_x$ , there is a trade-off between above- and below-bandgap reflector performance. Further improvements in reflective properties of the internal BSR are expected by replacement of  $\text{SiO}_x$  with an alternative low index dielectric with low absorption below 2.5  $\mu\text{m}$ , such as  $\text{MgF}_2$ ,  $\text{AlF}_2$ , or other metal-fluorides. As a starting point in this study, the  $\text{SiO}_x$  thickness of the BSR layer used for wafer-bonded samples is 200 nm. In these structures, Ti was deposited on the  $\text{SiO}_x$  to improve Au adhesion, and  $R$  decreased by a few percent, depending on the Ti thickness.

Interferograms of the GaInAsSb/GaSb and GaAs bonded wafers are shown in Figure 4. The GaSb wafer is concave and exhibits an average wafer bow of 22  $\mu\text{m}$ , while the GaAs is convex with bow of 24  $\mu\text{m}$ . The circular fringes and nearly symmetrical wafer bow is indicative that wafer bonding of the TPV device layer and GaAs substrate was achieved over the entire 5-cm-diameter. The bow is due to residual stress in the bonded wafers, and results from different thermal expansion coefficients of the  $\text{SiO}_x$ , Au, GaSb and GaAs alloys. If this residual stress exceeds the mechanical bond strength of the sputtered and bonded layers, debonding can occur. Furthermore, adhesion of the sputtered layers and the bonded interface must be able to withstand substrate removal and multiple processes during TPV fabrication. In numerous tests, the integrity of the Au-bonded epitaxial layers was maintained throughout all processing steps.

The HRXRD rocking curves for the control and wafer-bonded GaInAsSb/GaSb TPV device layers after removal of the GaSb substrate and InAsSb etch-stop layer are shown in Figures 5a and 5b, respectively. The diffraction intensity is lower for the wafer-bonded TPV device structure since the GaSb substrate has been removed and only the epitaxial layers that were grown lattice-matched to GaSb are remaining. The slightly broadened peak of the wafer-bonded structure is due to the residual stress and wafer bow.

Figure 6 shows R of the wafer-bonded GaInAsSb/GaSb TPV device layers. The reflectivity oscillates due to interference between reflections from the air/GaSb ( $R \sim 34\%$ ) and GaSb/SiO<sub>x</sub>/Ti/Au interfaces. Such effects introduce resonant absorption losses and reduce the efficiency of the internal BSR.<sup>16</sup> There are, however, approaches that could minimize this affect. One is to utilize a thinner TPV device layer structure, which increases the resonant fringe spacing, combined with the deposition of an anti-reflection coating on the front surface of the TPV cell to minimize resonant absorption of above-bandgap photons. Alternatively, epitaxial transfer of the GaInAsSb/GaSb TPV device layers can be achieved by direct fusion to the GaAs substrate, as shown in Figure 7, and the BSR deposited on the back side of the GaAs substrate.

Figure 8 shows 300 K PL spectra for the control and wafer-bonded GaInAsSb/GaSb TPV device layers. Multiple peaks in the PL spectrum of the wafer-bonded sample are observed and are related to resonant cavity effects. The PL peak intensity of the wafer-bonded epitaxy is over two times greater than that of the control TPV structure. These results suggest that there is minimal material degradation after wafer bonding and substrate removal, and in addition, the optical efficiency is enhanced as a result of the internal BSR.

## CONCLUSIONS

In conclusion, wafer bonding of epitaxial GaInAsSb/GaSb TPV device layers to GaAs substrates with a high-reflectivity broad-band mirror has been achieved, and TPV device structures with an internal BSR have been demonstrated. The reflective properties of the BSR should improve TPV cell performance as well as aid in spectral control of below bandgap radiation. In addition, since the BSR provides electrical isolation of the TPV device layers, GaInAsSb MIM devices can be fabricated. The structural and optical properties of the wafer-bonded TPV device layers were maintained after fabrication. This wafer bonding process is not limited to GaAs substrates, and alternative handle substrates can also be considered.

## ACKNOWLEDGMENTS

The authors gratefully acknowledge D.R. Calawa, J. Caissie, J.W. Chludzinski, P. Foti, S. Hoyt, J.M. Porter, and P.M. Nitishin of MIT Lincoln Laboratory for technical assistance and P. Dutta and I. Bhat for guidance in selective etching. This work was sponsored by the Department of Energy under AF Contract No. F19628-00-C-0002. The opinions, interpretations, conclusions, and recommendations are those of the author and are not necessarily endorsed by the U.S. Air Force.

---

## REFERENCES

1. P.F. Baldasaro, J.E. Raynolds, G.W. Charache, D.M. DePoy, C.T. Ballinger, T. Donovan, J.M. Borrego, 'Thermodynamic analysis of thermophotovoltaic efficiency and power density tradeoffs,' *J. Appl. Phys.* 89, 3319-3327 (2001).
2. G.W. Charache, J.L. Egley, D.M. DePoy, L.R. Danielson, M.J. Freeman, R.J. Dziendziel, J.F. Moynihan, P.F. Baldasaro, B.C. Campbell, C.A. Wang, H.K. Choi, G.W. Turner, S.J. Wojtczuk, P. Colter, P. Sharps, M. Timmons, R.E. Fahey, K. Zhang, 'Infrared Materials for Thermophotovoltaic Applications,' *J. Electron. Mater.* 27, 1038-1042 (1998).
3. G.W. Charache, D.M. DePoy, J.E. Raynolds, P.F. Baldasaro, K.E. Miyano, T. Holden, F.H. Pollak, P.R. Sharps, M.L. Timmons, C.B. Geller, W. Mannstadt, R. Asahi, A.J. Freeman, W. Wolf, 'Moss-Burstein and plasma reflection characteristics of heavily doped n-type  $In_xGa_{1-x}As$  and  $InP_yAs_{1-y}$ ,' *J. Appl. Phys.* 86, 452-458 (1999).
4. S.J. Spector, D.K. Astolfi, S.P. Doran, T.M. Lyszczarz, J.E. Raynolds, 'Infrared frequency selective surfaces fabricated using optical lithography and phase-shift masks,' *J. Vac. Sci. Technol. B*, 2757-2760 (2001).
5. W.E. Horne, M.D. Morgan, V.S. Sundaram, 'IR Filters for TPV Converter Modules,' *AIP Conf. Proc.* 358, 35-51 (1996).
6. G.W. Charache, D.M. DePoy, P.F. Baldasaro, B.C. Campbell, 'Thermophotovoltaic Devices Utilizing a Back Surface Reflector for Spectral Control,' *AIP Conf. Proc.* 321, 339-350 (1996).
7. N.S. Fatemi, D. M. Wilt, P.P. Jenkins, R.W. Hoffman, Jr., V.G. Weizer, C.S. Murray, D. Riley, 'Materials and Process Development for the Monolithic Interconnected Module (MIM) InGaAs/InP TPV Devices,' *AIP Conf. Proc.* 401, 249-261 (1997).
8. I.-H. Tan, C. Reaves, A. Holmes, Jr., E.L. Hu, J.E. Bowers, S. DenBaars, 'Low-temperature Pd bonding of III-V semiconductors,' *Electron. Lett.* 31, 588-589 (1995).
9. F. Omnes, J.-C. Guillaume, G. Nataf, G. Jager-Waldau, P. Vennegues, P. Gibart, 'Substrate Free GaAs Photovoltaic Cells on Pd-Coated Silicon with a 20% AM1.5 Efficiency,' *IEEE Trans. Electron. Dev.* 43, 1806-1811 (1996).
10. R.H. Horng, D.S. Wuu, S.C. Wei, C.Y. Tseng, M.F. Huang, K.H. Chang, P.H. Liu, K.C. Lin, 'AlGaInP light-emitting diodes with mirror substrates fabricated by wafer bonding,' *Appl. Phys. Lett.* 75, 3054-3056 (1999).
11. H.C. Lin, W.H. Wang, K.C. Hsieh, K.Y. Cheng, 'Fabrication of  $1.55\ \mu m$  VCSELs on Si using metallic bonding,' *Electron. Lett.* 38, 516-517 (2002).
12. J.S. Ward, A. Duda, M.W. Wanlass, J.J. Carapella, X. Wu, R.J. Matson, T.J. Coutts, T. Moriarty, 'A Novel Design for Monolithically Interconnected Modules (MIMs) for Thermophotovoltaic Power Conversion,' *AIP Conf. Proc.* 401, 227-236 (1998).
13. C.A. Wang, H.K. Choi, G.W. Charache, 'Epitaxial growth of GaInAsSb for thermophotovoltaic devices,' *IEE Proc.-Optoelectron.* 147, 193-198 (2000).

---

14. X. Wu, A. Duda, J.J. Carapella, J.S. Ward, J.D. Webb, M.W. Wanlass, 'A Study of Contacts and Back-Surface Reflectors for 0.6-eV  $\text{Ga}_{0.32}\text{In}_{0.68}\text{As}/\text{InAs}_{0.32}\text{P}_{0.68}$  Thermophotovoltaic Monolithically Interconnected Modules,' AIP Conf. Proc. 460, 517-524 (1999).
15. M.A. Schmidt, Proc. IEEE, 'Wafer-to-Wafer Bonding for Microstructure Formation,' Proc. IEEE 86, 1575-1585 (1998).
16. M.B. Clevenger, C.S. Murray, S.A. Ringel, R.N. Sacks, L. Qin, G.W. Charache, D.M. DePoy, 'Optical Properties of Thin Semiconductor Device Structures with Reflective Back-Surface Layers,' AIP Conf. Proc. 460, 327-334 (1999).

## FIGURES

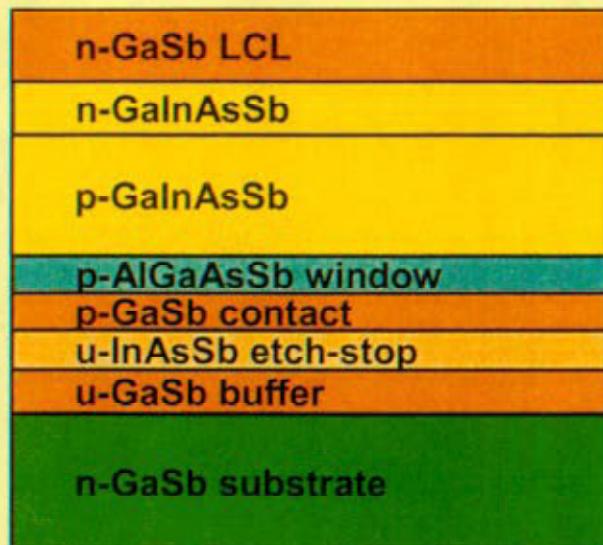


Figure 1(a). Inverted GaInAsSb/GaSb TPV device structure grown on n-GaSb for wafer bonding.



Figure 1(b). Wafer-bonded GaInAsSb/GaSb TPV structure on GaAs handle substrate. GaSb device layers exposed after GaSb substrate and InAsSb etch-stop layer removed.

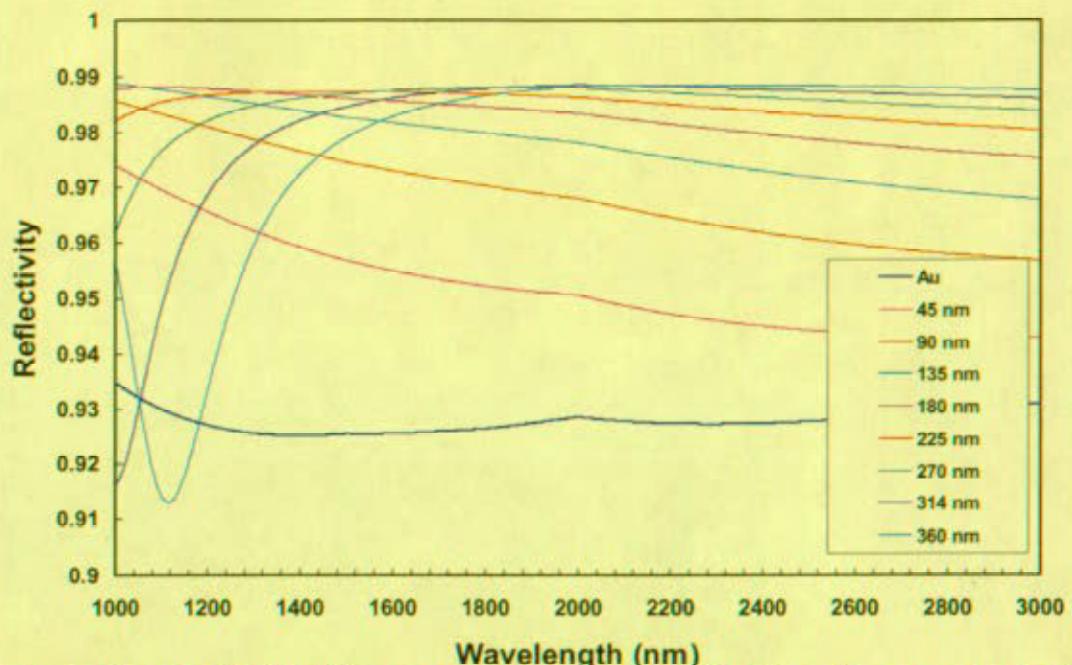


Figure 2. Simulated reflectivity at normal incidence for  $\text{SiO}_2/\text{Au}$  reflector on GaAs. No absorption in GaAs is assumed.

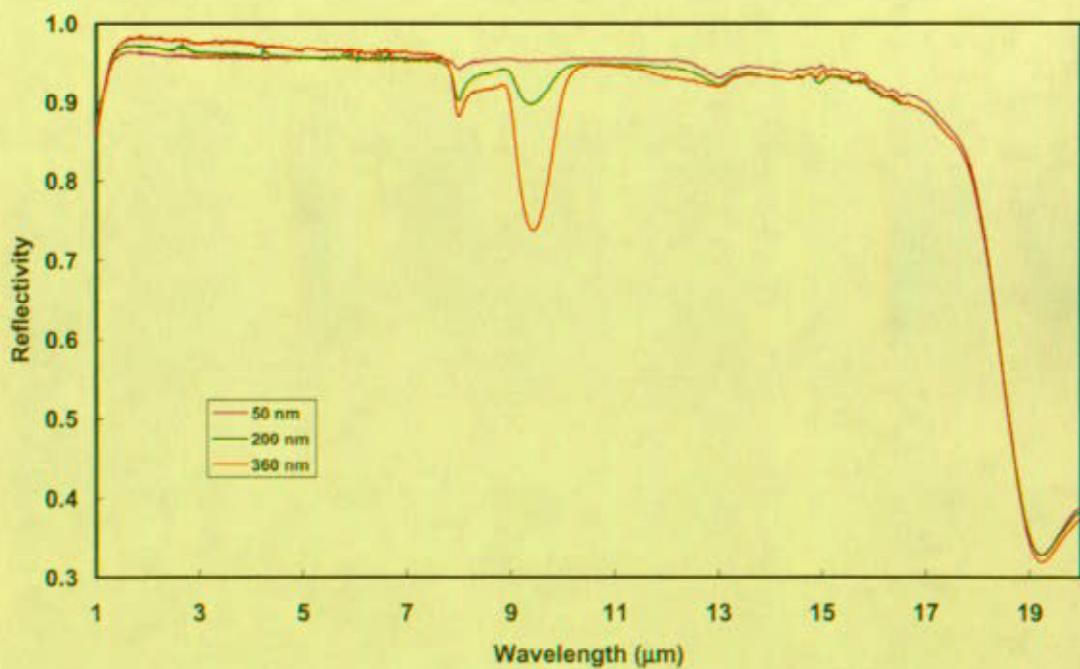
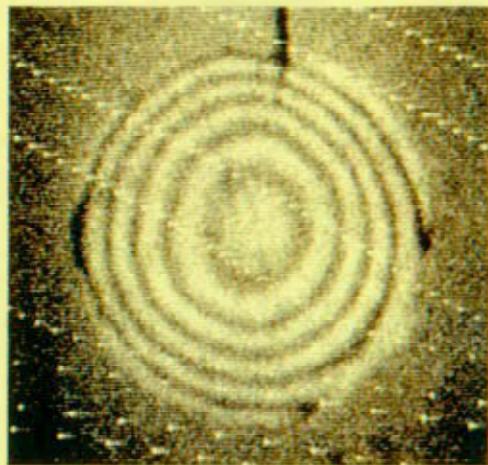
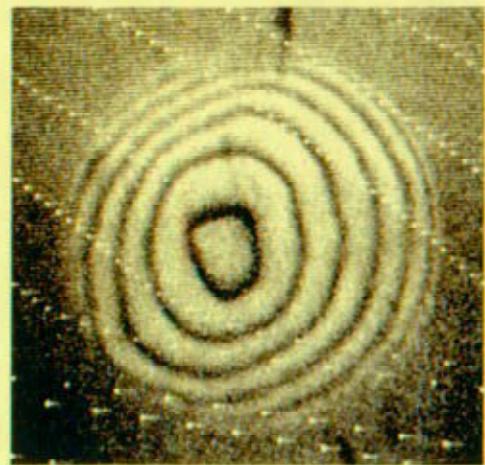


Figure 3. Measured reflectivity of  $\text{SiO}_2/\text{Au}$  reflector layers on GaAs.

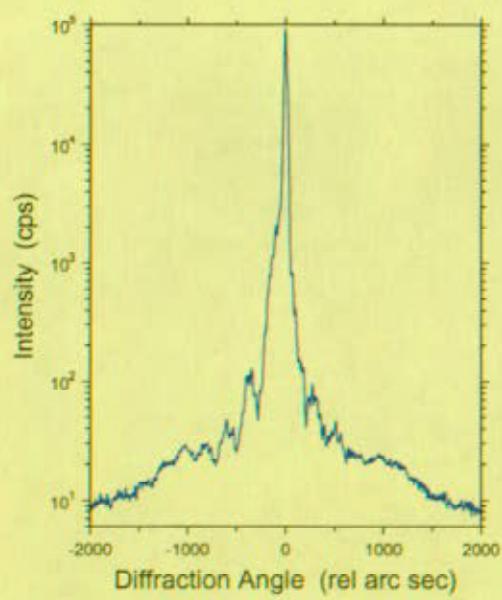


(a)

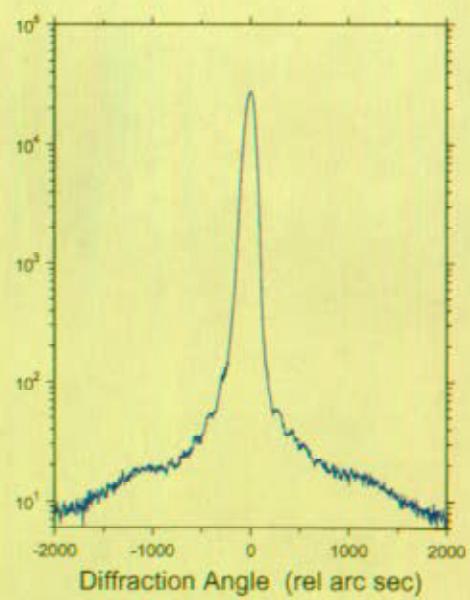


(b)

Figure 4. Interferograms of (a) back side of GaSb substrate bonded to GaAs handle substrate; (b) back side of GaAs handle substrate. One fringe corresponds to 4.83  $\mu$ m.



(a)



(b)

Figure 5. X-ray diffraction of (a) control GaInAsSb/GaSb TPV wafer and (b) wafer-bonded GaInAsSb/GaSb TPV structure.

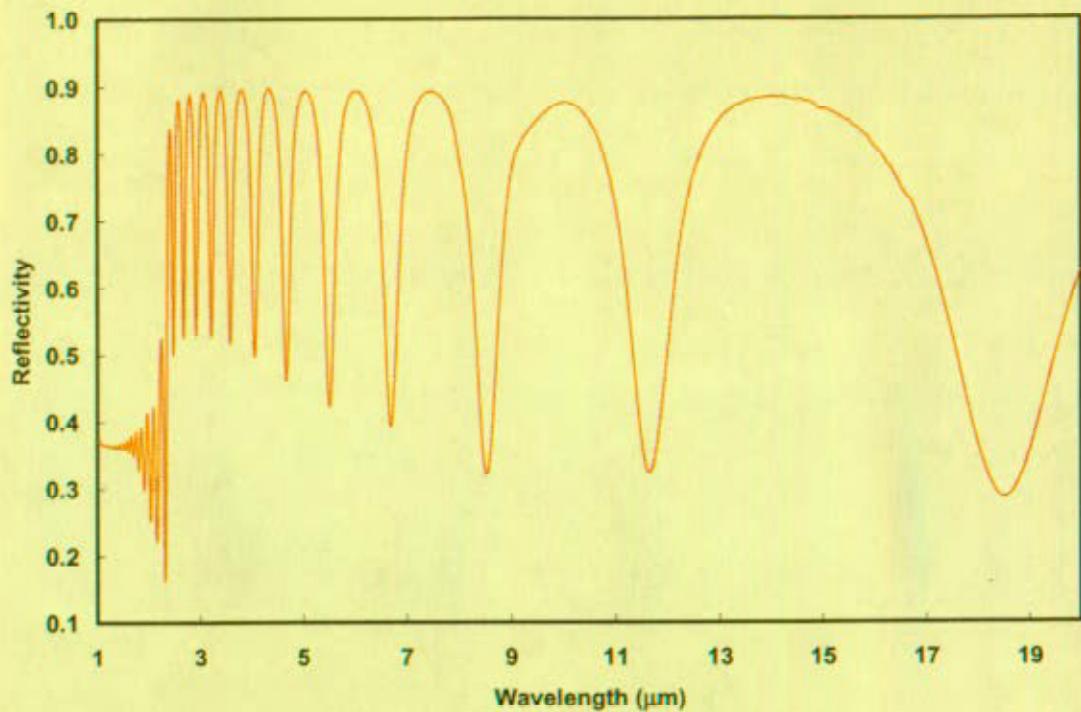


Figure 6. Reflectivity spectrum of uncoated wafer-bonded GaInAsSb/GaSb TPV structure with internal BSR on GaAs substrate. The TPV device structure is 4  $\mu\text{m}$  thick. Thinner device structures will increase the resonant fringe spacing.

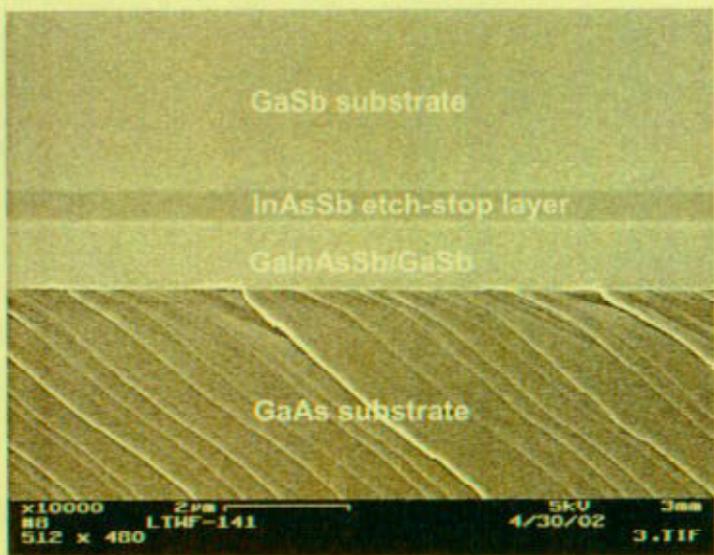


Figure 7. Cross-section scanning electron micrograph of GaInAsSb/GaSb fused to directly to GaAs substrate. The GaSb substrate and InAsSb etch-stop layer can be removed as described for structures with an internal BSR.

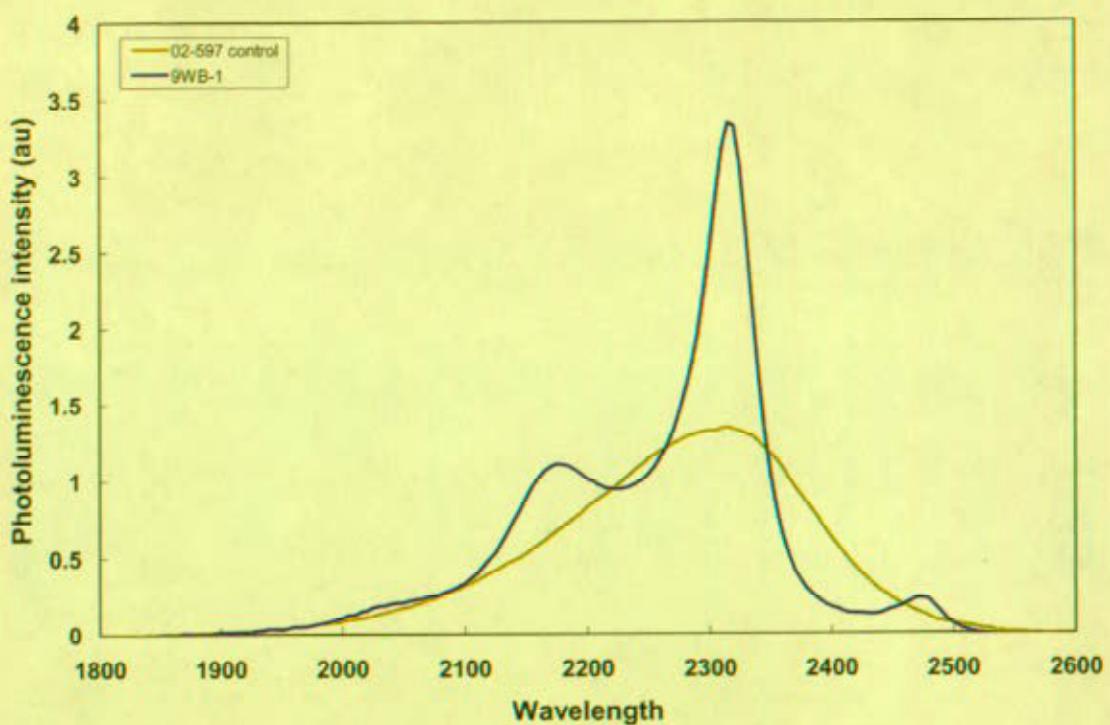


Figure 8. 300 K photoluminescence of control (02-597) and wafer bonded (9WB-1)  $\text{GaInAsSb}/\text{GaSb}$  TPV structure.