Molecular Beam Epitaxy of Wide-Bandgap InAlAsSb

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Triple-junction solar cells, lattice-matched to InP, have recently gained interest as an alternative to traditional GaAs-based devices [1]. To maximize efficiency, this design requires a top subcell with bandgap (E_g) of 1.74 eV, thus motivating the development of the widest direct-gap material lattice-matched to InP, $In_xAl_{1-x}As_ySb_{1-y}$. Both the immaturity and mixed group-V nature of this alloy pose significant challenges, requiring in depth investigation. Initial attempts at molecular beam epitaxy (MBE) of $In_xAl_{1-x}As_ySb_{1-y}$ resulted in anomalously low photoluminescence (PL) emission energies, compared with energies extracted from variable angle spectroscopic ellipsometry (referred to as ellipsometry herein) [2]. To further investigate the cause of this discrepancy, in this work we have performed a systematic study of the substrate temperature (T_{sub}) and V/III of $In_{0.26}Al_{0.24}As_{0.28}Sb_{0.22}$ (expected E_g=1.64 eV).

We grew seven samples of $In_xAl_{1-x}As_ySb_{1-y}$ (x≈0.26, y≈0.28) on InP by solid source MBE with valved crackers supplying cracked As and Sb. We investigated T_{sub} (measured via bandedge thermometry) ranging from 325 to 455 °C and V/III ratios (beam equivalent pressure) of 16 and 30. Given that the alloy composition varies with T_{sub}, we re-calibrated the group-V fluxes for each growth, using energy extracted from ellipsometry (E=1.69 ± 0.05 eV) and lattice matching (to within 0.1% mismatch) via x-ray diffractometry as our compositional guide. Room temperature PL yielded emission from only four of the seven samples and we again found that it underestimates the energies extracted from ellipsometry (Figure 1). Low-temperature PL will be performed to inform the remaining three samples. Furthermore, we hypothesize that phase separation and clustering is responsible for this behavior and will probe this via power- and temperature-dependent PL measurements as in [3] and transmission electron microscopy. By quantifying phase separation in this way, we can relate degree of phase separation to growth conditions, guiding us toward the appropriate conditions for $In_xAl_{1-x}As_ySb_{1-y}$ yielding the least phase separation and widest E_g.

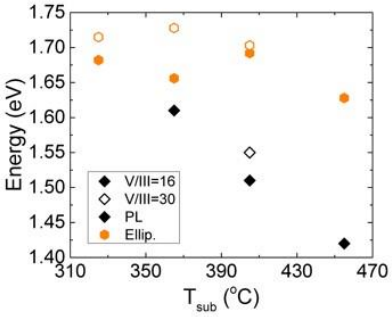

Figure 1 PL emission energy (black symbols) as a function of T_{sub} and V/III compared with energy extracted from ellipsometry (orange symbols).

[1] R. J. Walters et al., *37th IEEE Photovoltaic Specialists Conference*, pp. 000122-000126 (2011).
[2] M. P. Lumb et al., *40th IEEE Photovoltaic Specialist Conference (PVSC)*, pp. 0243-0246 (2011).
[3] L. C. Hirst et al., *J. Appl. Phys.* **117**, 215704 (2015).

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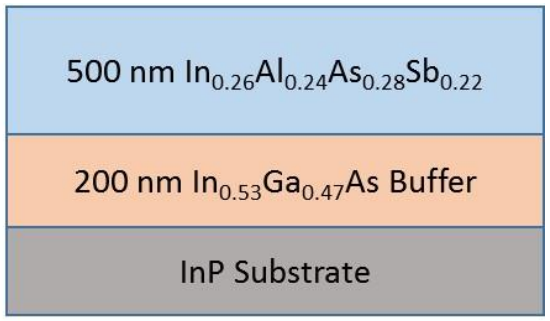
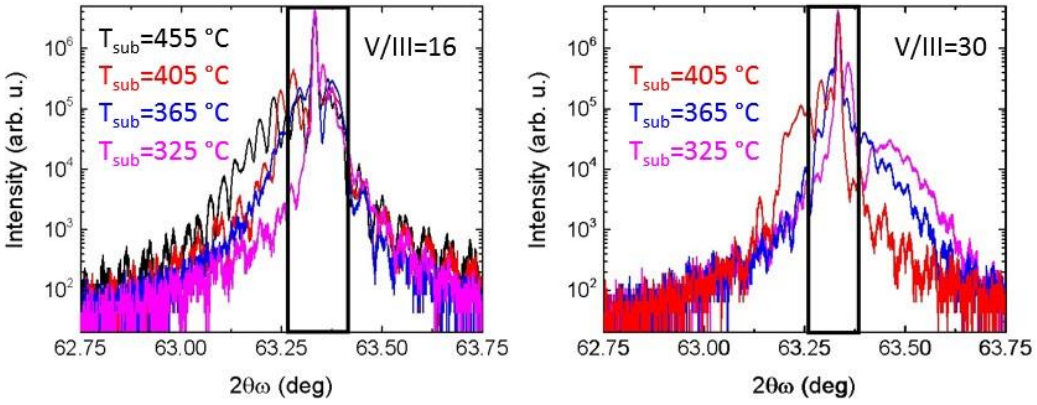
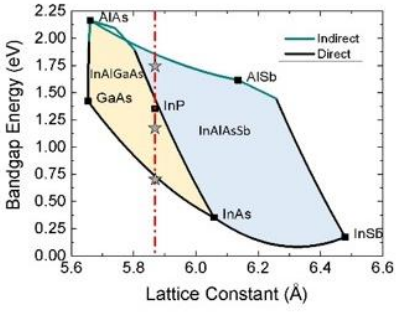
T_{sub} (°C)	V/III=16	V/III=30
455	✓	
405	✓	✓
365	✓	✓
325	✓	✓



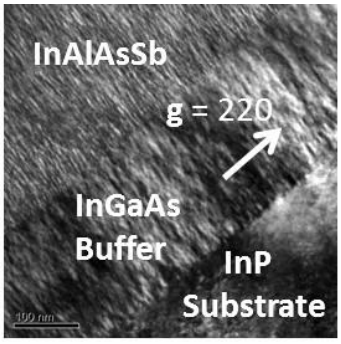
Left: Summary of growth conditions explored here. Right: Cross-sectional schematic of sample structure.



X-ray diffraction spectra for all samples explored here, black boxes represent ±0.1% lattice mismatch. Left: Samples grown with V/III=16 showing film peaks within ±0.1% mismatch as well as thickness fringes indicating high material quality. Right: Samples grown with V/III=30 showing film peaks within ±0.1% mismatch as well as additional broad, unidentified peaks and degraded thickness fringes, implying a high V/III may not be desirable for $In_xAl_{1-x}As_ySb_{1-y}$.



Bandgap v. lattice-constant for relevant III-V materials. Stars represent bandgap combinations that result in maximized triple-junction solar cell efficiency lattice-matched to InP. From [1].



Cross-sectional TEM image with **g**=220 revealing phase separation in previously grown InAlAsSb, represented as striations in contrast modulation.

[1] Tomasulo et al., *42nd IEEE Photovoltaic Specialists Conference*, pp. 1-4 (2015).