NREL
NATIONAL RENEWABLE ENERGY LABORATORY

Opportunities in low-cost (yet high quality!) III-V materials and devices

Solar University-National Lab Ultra-Effective Program (SUN UP)

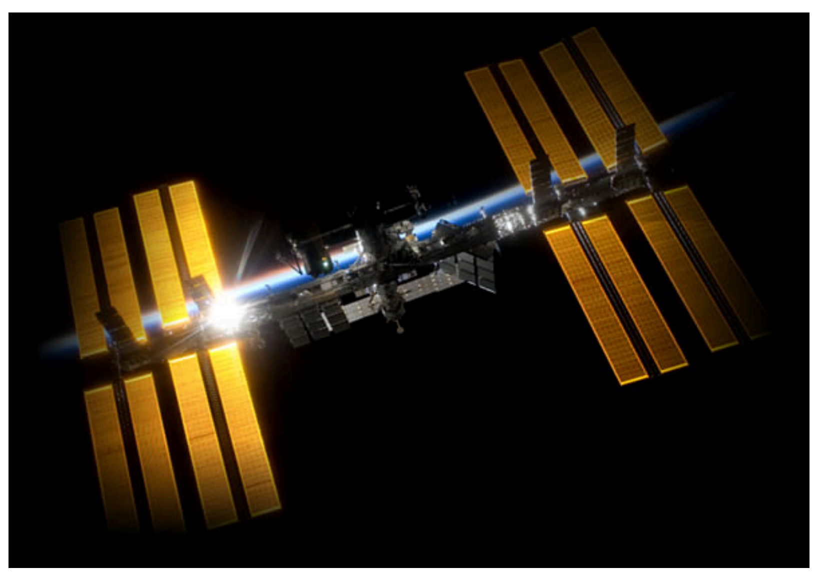
October 6, 2016

Outline

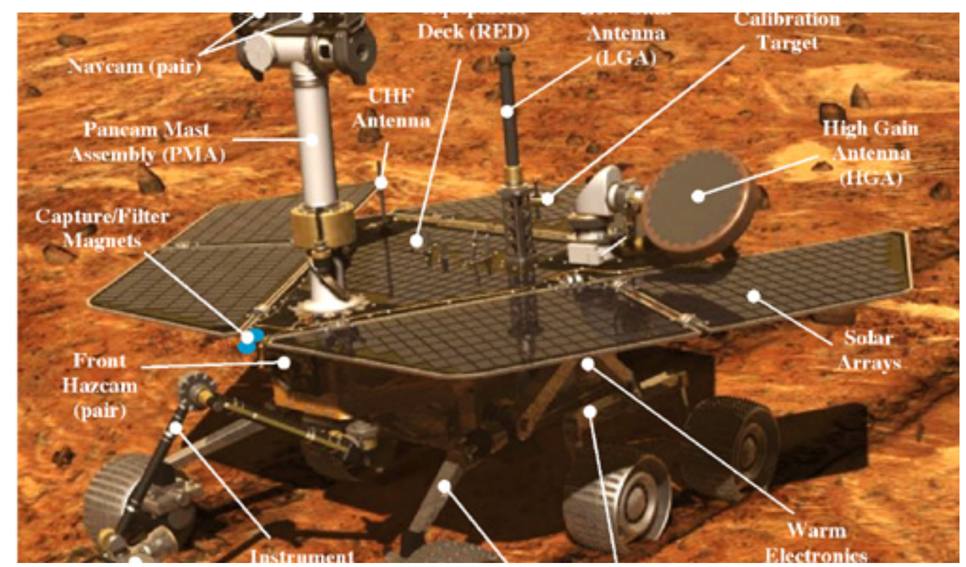
- Why we do what we do
- What we do
- What else we could do with talented students

III-Vs currently used in high-value applications

https://www.researchgate.net/figure/253863517_fig3

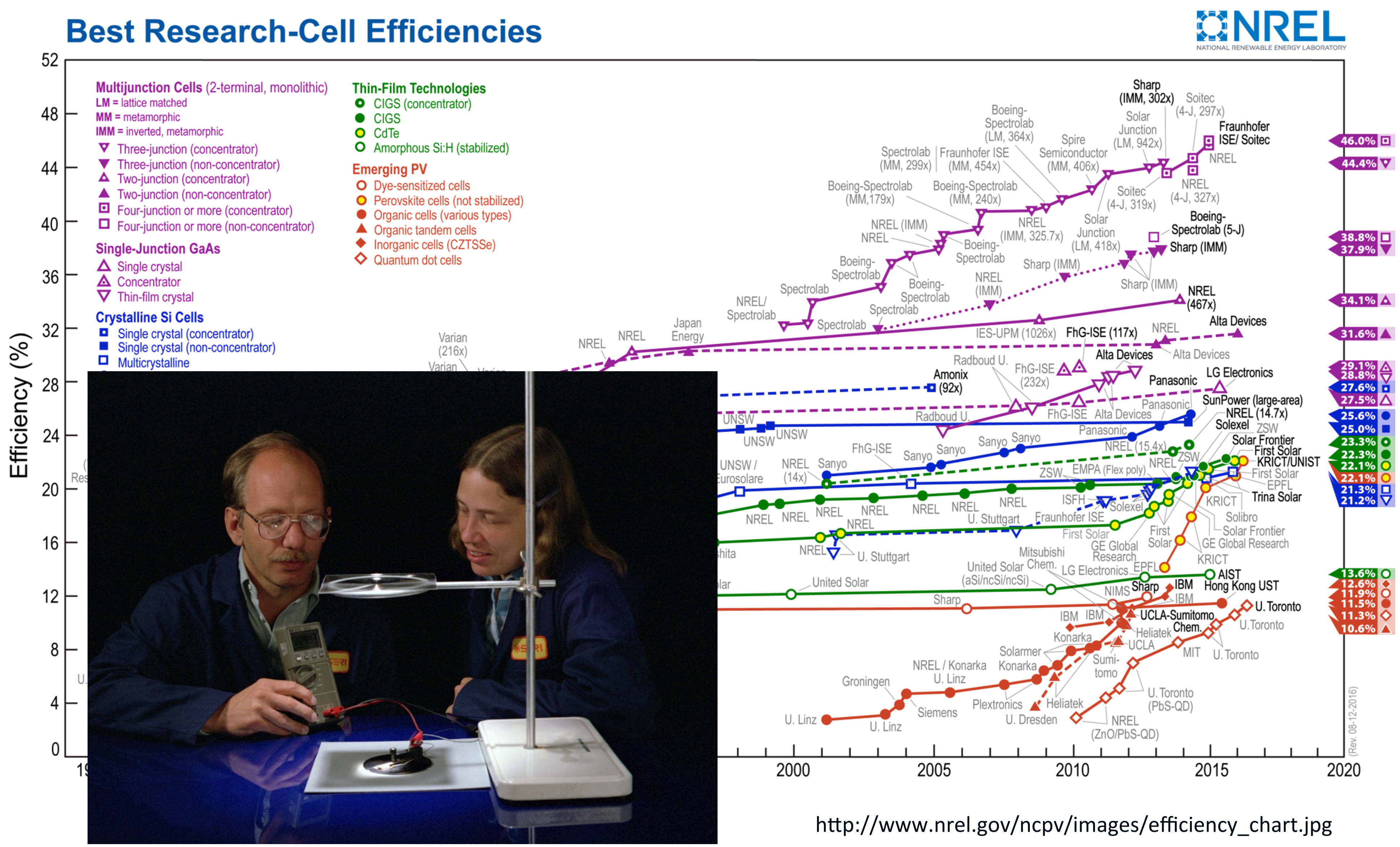


http://www.spectrolab.com/space.htm#



http://mars.nasa.gov/mer/mission/spacecraft_surface_rover.html

III-V efficiencies continue to climb



http://www.nrel.gov/ncpv/images/efficiency_chart.jpg

More motivation

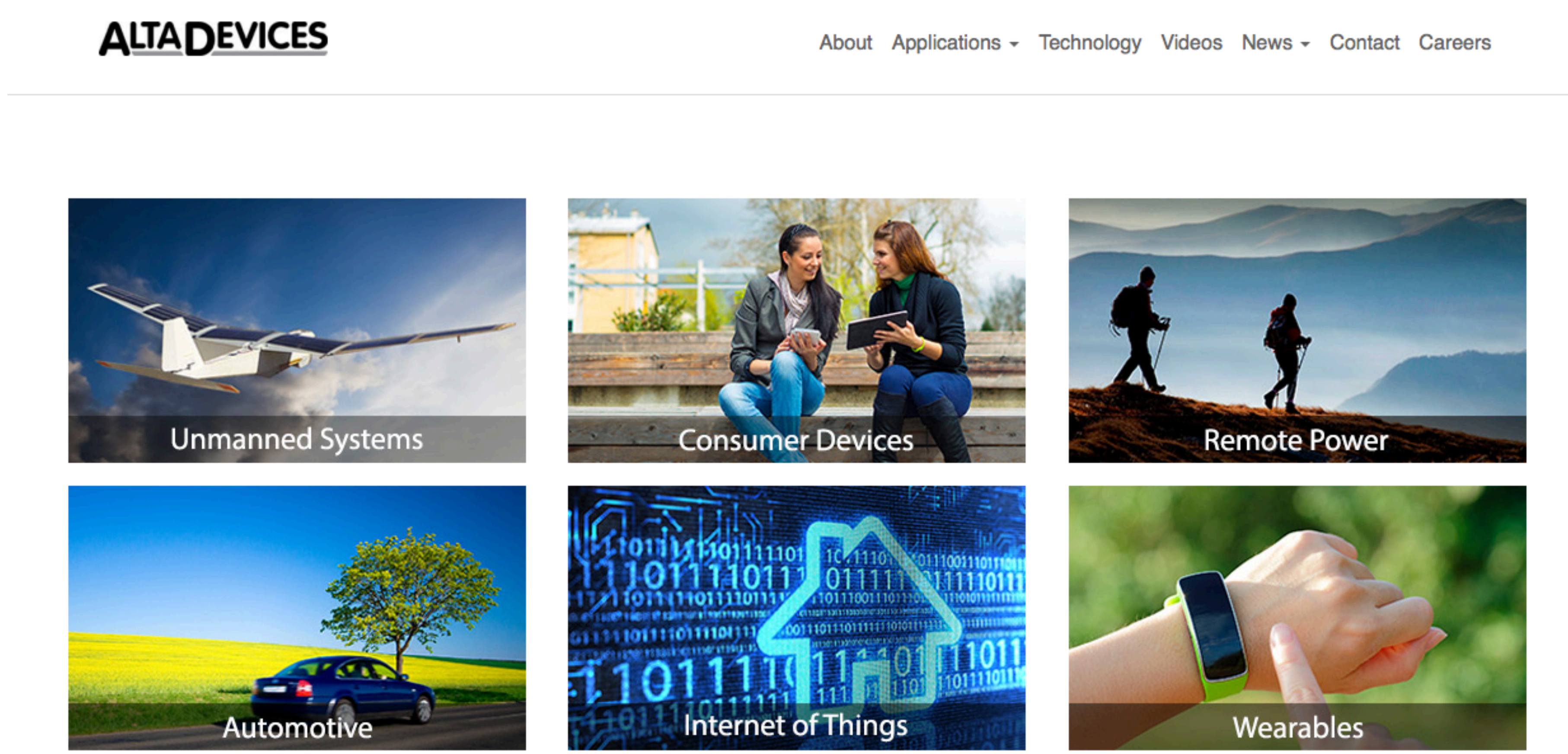
The case for one-sun terrestrial III-Vs:

- High efficiency, leading to high areal power densities (W/m^2) and low BOS costs.
- Low temperature coefficients, allowing efficiencies to stay high even as the operating temperature of a real-world device rises. This leads to high annual energy harvesting efficiency.*
- Low material usage (single-junction device thickness <2 µm, triple-junctions ~5–7 µm).
- Flexibility with small radius-of-curvature.
- High specific power (W/kg).

The catch: $30,000 – 50,000/$m^2$

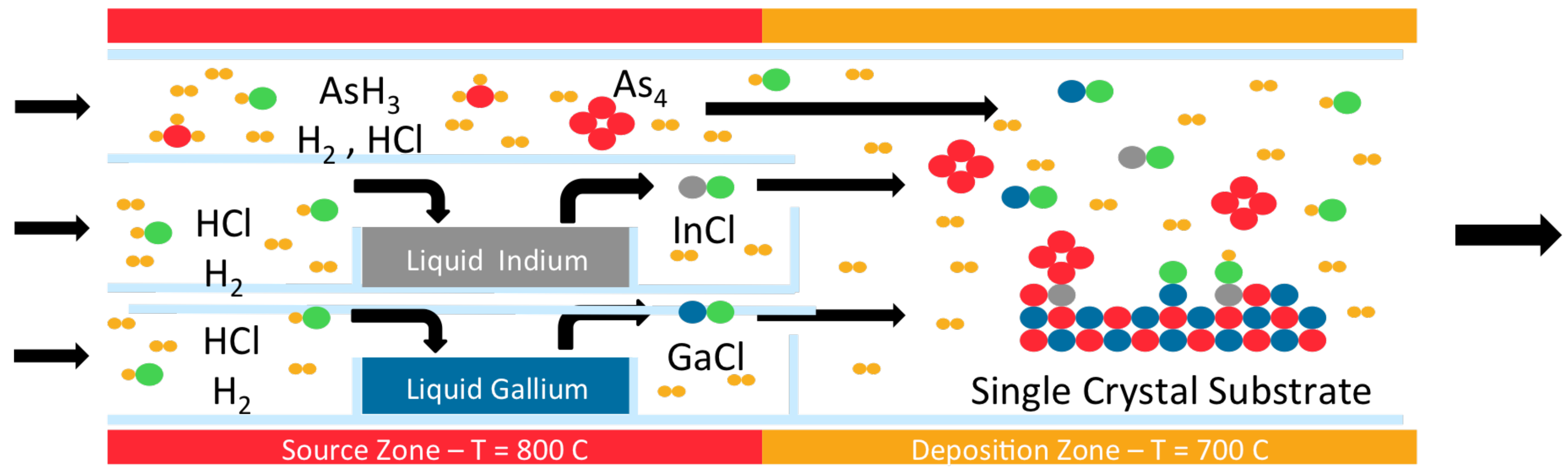
* T. J. Silverman, M. G. Deceglie, B. Marion, S. Cowley, B. Kayes and S. Kurtz, in *Photovoltaic Specialists Conference (PVSC), 2013 IEEE 39th* (2013), pp. 0103-0108.

Where we want cost-effective III-V solar



http://www.altadevices.com/applications/applications-overview/

Hydride Vapor Phase Epitaxy (HVPE)



Overall Deposition Process:

Source reaction: $Ga(l) + HCl \rightarrow GaCl + HCl + \frac{1}{2} H_2$

Deposition: $\frac{1}{2} H_2 + GaCl + \frac{1}{4} As_4 \rightarrow GaAs(s) + HCl$

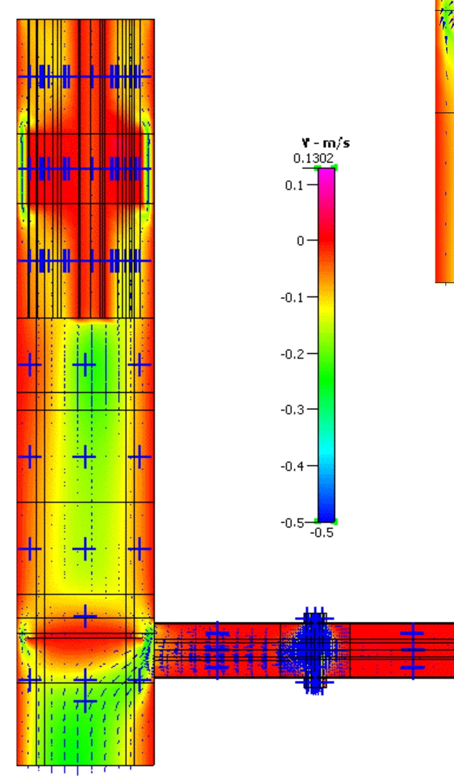
- Atmospheric pressure, hot wall process
- Near thermodynamic equilibrium growth process, relatively low gas-phase supersaturation
- Typical reactant partial pressures ~ 10^{-3} atm

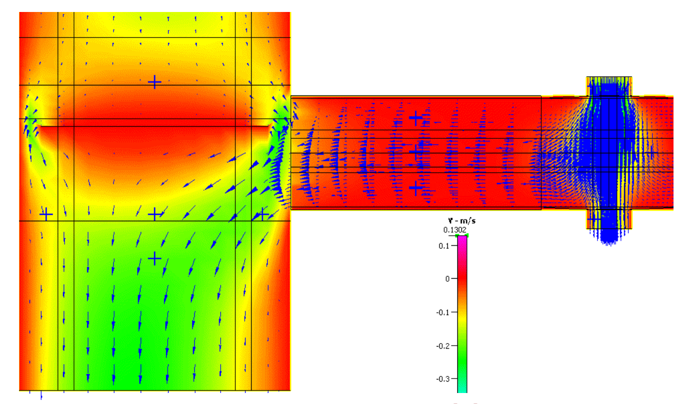
Low cost III-V growth using HVPE

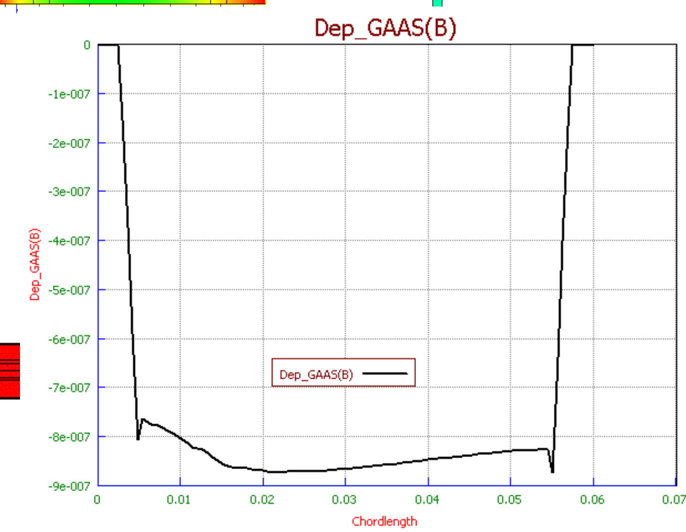
	MOCVD	HVPE
Growth rate (μm/min)	0.10 – 0.15*	1 – 2
Ga cost ($/g)	> 4**	0.3
V/III ratio	60 – 80	3 – 4
Source utilization (%)	??	70***

* See Schmieder, *et al.*, "Effect of Growth Temperature on GaAs Solar Cells at High MOCVD Growth Rates", next presentation in this session.
** On a per Ga basis.
*** 70% Ga utilization measured in our custom research HVPE reactor

The HVPE reactor at NREL

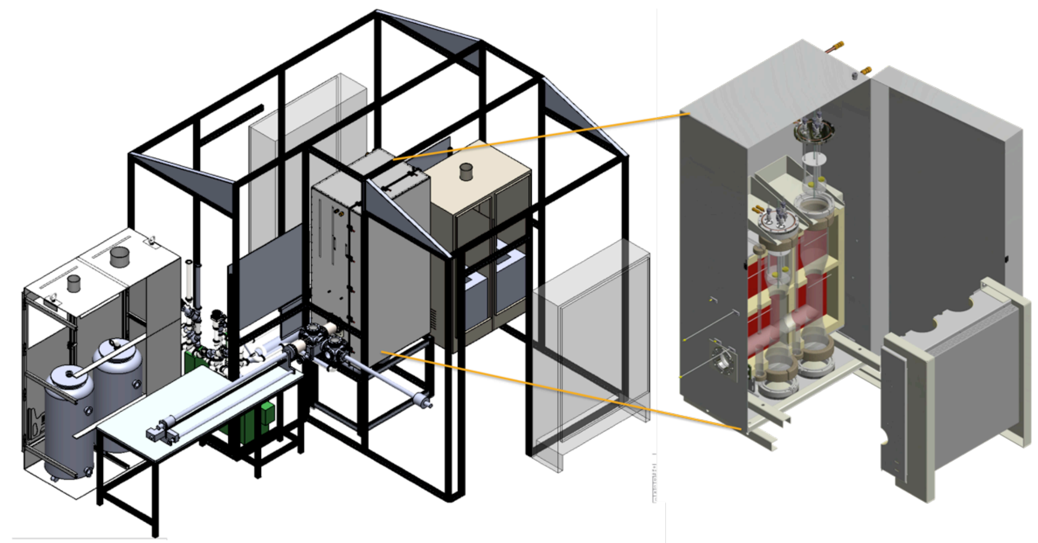






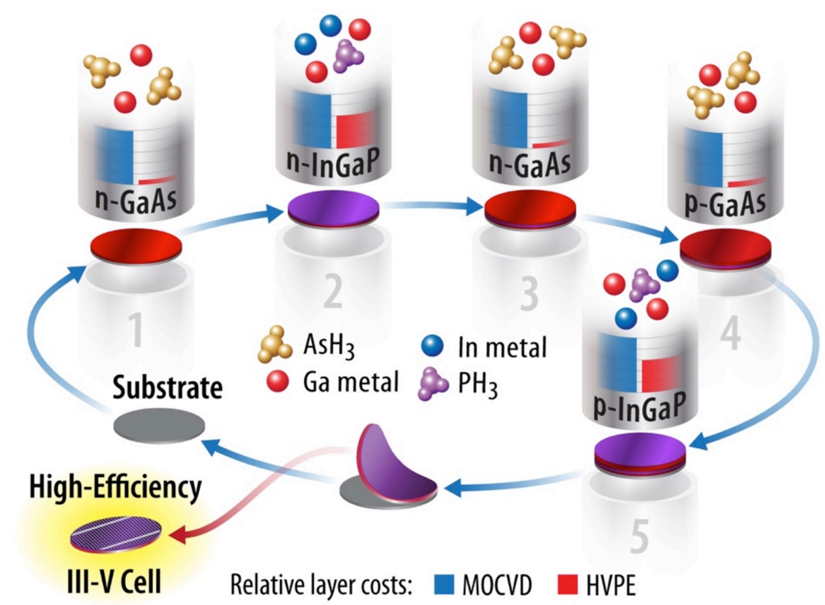
Computational Fluid Dynamics modeling used to design our 2nd generation HVPE reactor

The HVPE reactor at NREL



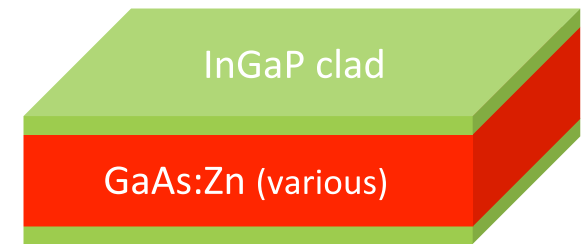
Currently operating at NREL since Feb. 2014

Schematic of an in-line HVPE reactor with continual substrate reuse that eliminates metal-organic sources and uses cheap elemental metals. The bar charts show the relative materials costs for each layer.

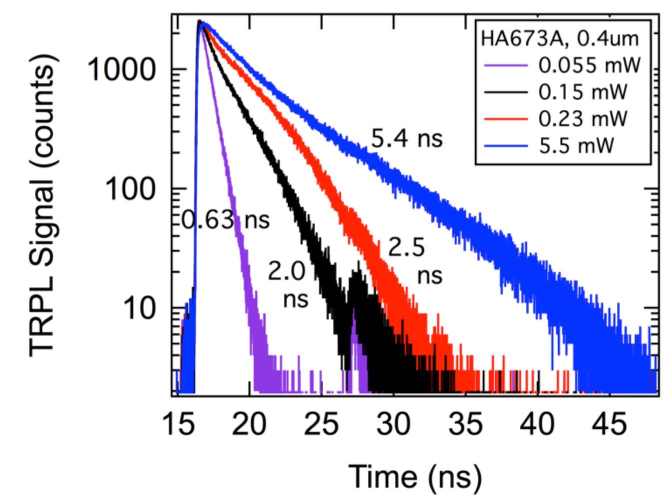


Heterojunction formation

Developed InGaP/GaAs/InGaP double heterostructures for the measurement of bulk lifetime and interface recombination velocity



	Acceptor doping (cm^{-3})	Where the layer was grown: GaAs	Where the layer was grown: InGaP	Growth pause?
Set #1	$2x10^{16}$	GC2	GC2	Yes
Set #2	$1x10^{17}$	GC1	GC2	No
Set #3	$2x10^{16}$	GC2	GC1	No



Conclusions

- **Use of growth interrupts leads to reduced lifetime**
  - Also true in solar cell structures, likely due to high surface recombination velocity
- **Structures with base grown in GC1 exhibit SRH dominated signal**
- **Structures with base grown in GC2 exhibit significantly improved lifetime**
  - Effect SRH recombination significantly reduced relative to GC1 but not zero
  - Determination of precise bulk lifetime complicated by injection dependence, but likely ~20 ns at 2e16 cm^{-3} doping
  - Most importantly, we've learned that our material is bulk limited, and know where to apply future effort

Growth kinetics

Postulated Reaction Steps

1) $GaCl + S \overset{K_1}{\leftrightarrow} GaCl(s),\ \ K_1 = \frac{\theta_{GaCl}}{P_{GaCl}\theta_v}$

2) $\frac{1}{4}As_4 + S \overset{K_2}{\leftrightarrow} As(s),\ \ K_2 = \frac{\theta_{As}}{P_{As_4}^{1/4}\theta_v}$

3) $GaCl(s) + As(s) \overset{K_3}{\leftrightarrow} AsGaCl(s) + S,$

$$K_3 = \frac{\theta_{AsGaCl}\theta_v}{\theta_{GaCl}\theta_{As}}$$

4) $AsGaCl(s) + \frac{1}{2}H_2 \overset{K_4}{\leftrightarrow} GaAs(s) + HCl + S,$

*rate limiting step

$$K_4 = \frac{P_{HCl}\theta_v}{\theta_{AsGaCl}P_{H_2}^{1/2}} = \frac{k_4^+}{k_4^-}$$

Develop a rate law for GaAs growth by HVPE…

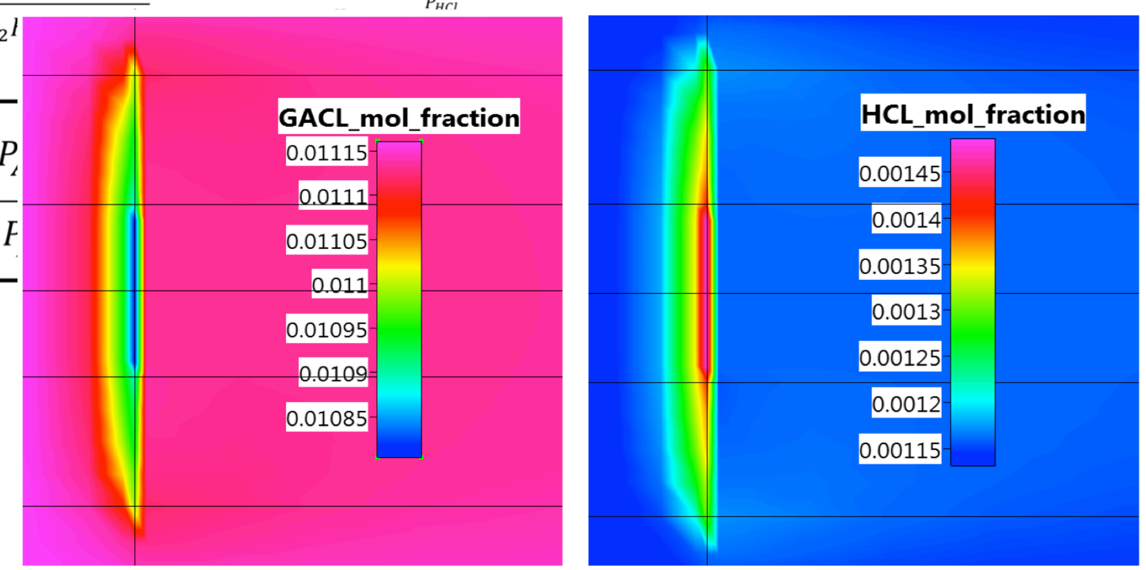
Mass action rate law from rate limiting step (step 4): $r = k_4^+\theta_{AsGaCl}P_{H_2}^{1/2} - k_4^- P_{HCl}\theta_v$ **=>** $r = k_f\left(P_{GaCl}P_{As_4}^{1/4}P_{H_2}^{1/2} - \frac{P_{HCl}}{K_{eq}}\right)\theta_v$

Expression for surface coverage: $\theta_v = \frac{1}{1 + K_1P_{GaCl} + K_2P_{As_4}^{1/4} + K_1K_2 \ldots}$

Rate law in terms of only partial pressures (P_i) or constants:

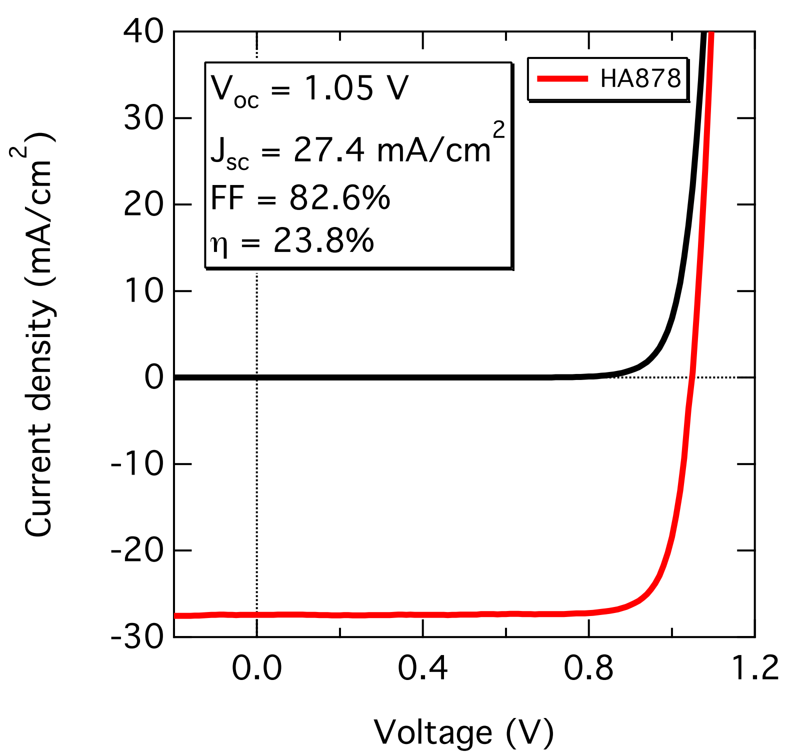
$$r = \frac{k_f\left(P_{GaCl}P \ldots\right.}{1 + K_1P_{GaCl} + K_2P \ldots}$$

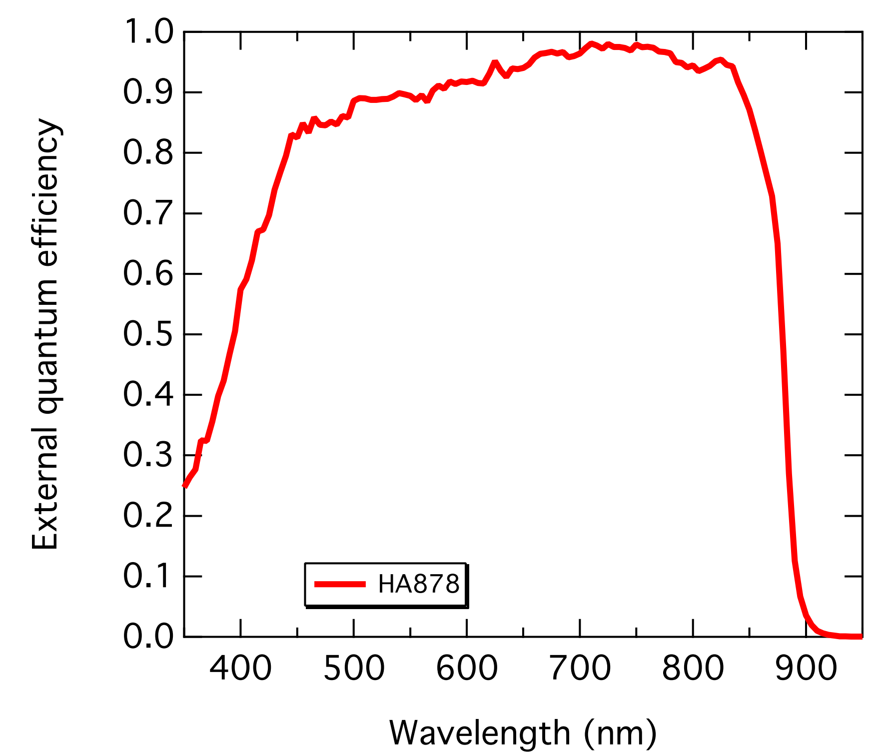
… and couple it to CFD models of the reactor to predict composition and growth rate.



Concentration of GaCl (left) and HCl (right) immediately adjacent to the wafer surface. The view is rotated 90° relative to Fig. x, with the fluid flowing from left to right. The wafer is the thin vertical line on the left.

Rear heterojunction results

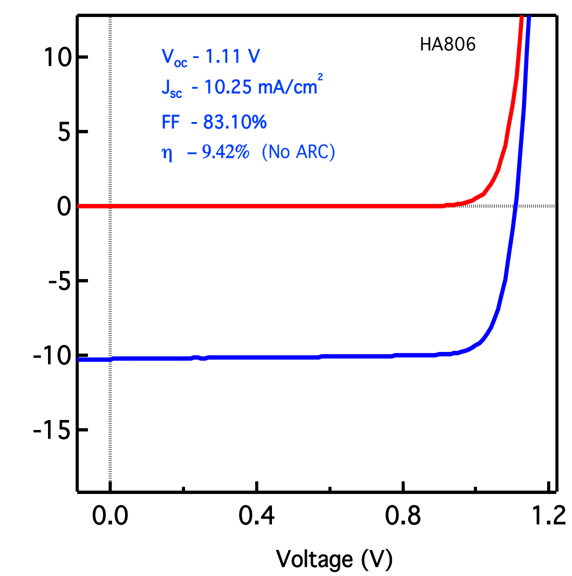




- Growth rate = 1 µm/min
- V_{oc}'s as high as 1.06 V (W_{oc} ~ 0.36 V) obtained using the RHJ structure
- External radiative efficiency measurements being performed
- Devices submitted for certification

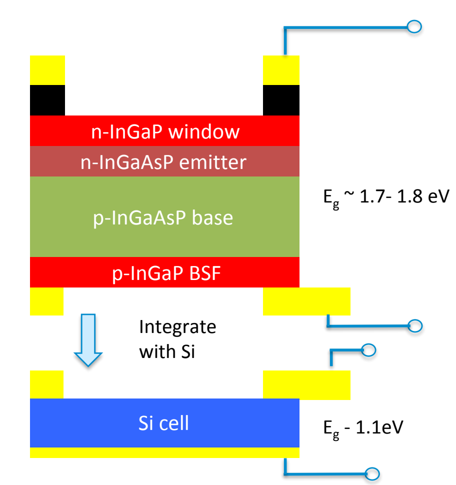
III-V integration with Si

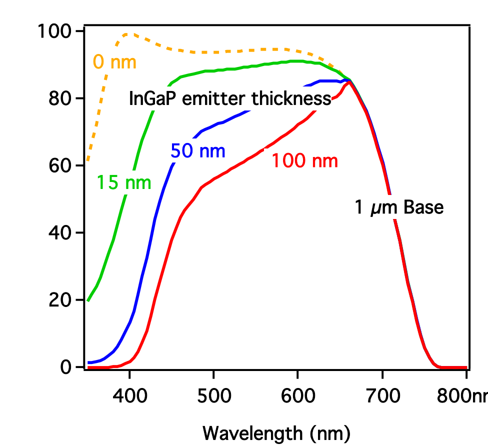
- Develop high growth rate lattice-matched InGaAsP alloys via HVPE
  - Bandgap ~ 1.7 eV
  - ~0.73 μm/min (or ~44 μm/h)
- Preliminary HVPE heterojunction InGaAsP solar cells
  - No window
  - V_{OC} ~ 1.1 eV
  - AM1.5G efficiency ~9.5% (w/o ARC)
- Path for 20% InGaAsP cells
  - Improvement in J_{SC}
    - Homo-junction cell development
    - Incorporation of window layer
  - Improvement in V_{OC} and FF
    - Bulk material quality (eg. temp.)
    - Sheet resistance and grid design



AM1.5G spectrum

InGaAsP hetero-junction cells
- No window
- No ARC
- Grown at ~ 44 μm/h





Possible projects and activities

- Growth
  - Pushing the limits of HVPE
    - What is the ultimate growth rate before epitaxy breaks down?
    - How do we simultaneously optimize growth rate and spatial uniformity in our reactor, and what are the implications for the next-generation reactor?
- Processing
  - Back texturing of III-Vs to increase light absorption
  - Integration of III-Vs with Si
  - Epitaxial liftoff using HVPE-compatible materials
- Modeling
  - Development of a new rate law that more accurately depicts our current growth parameters
  - Realistic optical modeling of III-Vs on Si and all III-V multijunctions
- Market and economics
  - Technoeconomic analysis of HVPE growth
  - Interfacing with industry to understand market entry, opportunities, etc.

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