Dynamic curvature and stress studies for MBE CdTe on Si and GaAs substrates

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Motivation: Advanced metrology for improved HgCdTe detectors

- IR detector fabrication starts with growth of detector material. (MBE)

- Large area/Low cost substrates are sought to reduce overall manufacturing costs.

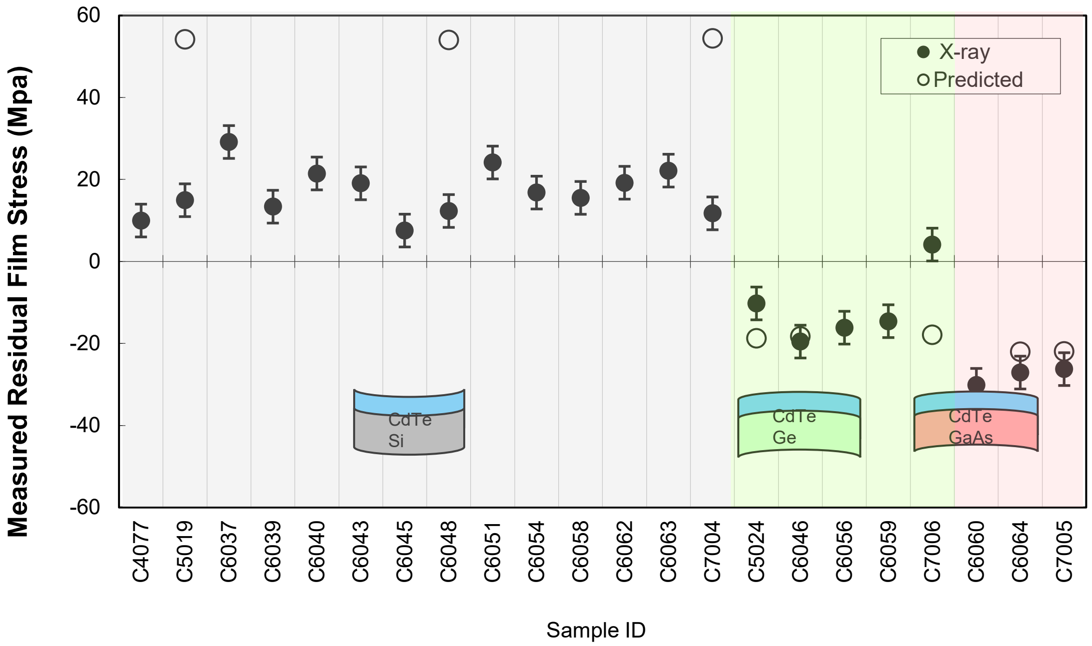
- For Larger substrates: More **Curvature** and **Stress** in heteroepitaxial structure.
  (*especially when film/substrate material properties very different*).

- Potential problems for growth & subsequent processing.

- Case Study: MBE growth of II-VI films on Si and GaAs substrates.
  1. *Ideal materials for de-convolving growth and thermal induced curvature.*
  2. *Differences in lattice parameter & thermal expansion properties.*
  3. *Wide range of temperatures required for epitaxial growth.*

Goal; Achieve better understanding of stress dynamics during molecular beam epitaxy of II-VI materials.

Previous studies: residual stress



Post-growth measurements

- Residual tensile stress in CdTe/Si.
- Residual compressive stress in CdTe/Ge and CdTe/GaAs.
- Thermal mismatch stress dominates after growth

$$\sigma_{res} = \sigma_{misfit} + \sigma_{\alpha}$$

Substrate	Cost ($/cm^2)	Max Available Size (cm^2)	Crystal Structure	EPD (/cm^2)	Lattice Param. (Å)	Lattice Misfit (w/CdTe)	CTE (α) (10^{-6}/C)	α-mismatch (w/CdTe)
CdZnTe	~200	~50	Zinc-Blende	~10^4	6.48	-	5.0	-
Si(211)	~1	~700	Diamond	<10^2	5.43	-19.3%	2.6	-92.3%
Ge(211)	~8	~180	Diamond	<10^3	5.66	-14.6%	5.8	13.8%
GaAs(211)B	~5	~180	Zinc-Blende	<10^3	5.65	-14.6%	5.8	13.8%

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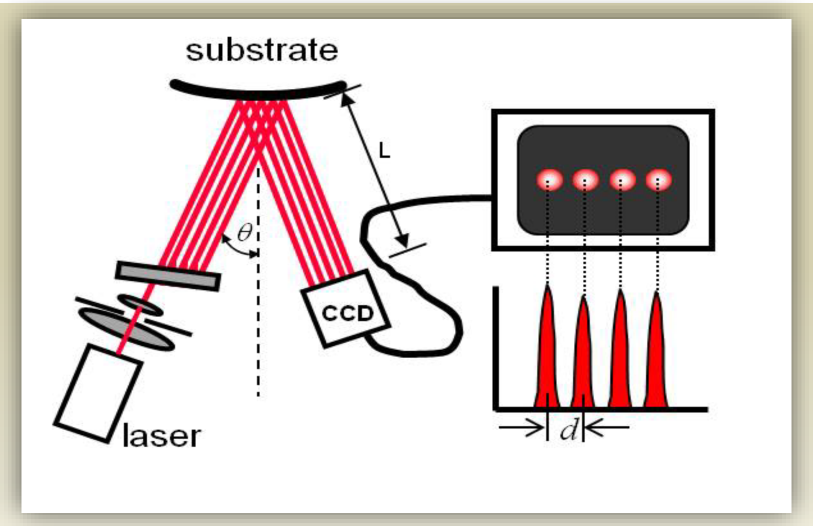
In-situ Stress/curvature monitoring

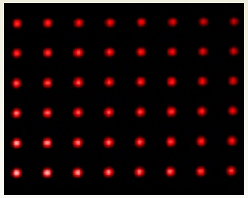
Multibeam Optical Stress Sensor(MOS). -k-Space Associates

- Array of laser beams are reflected off wafer surface during growth.
- The reflected spots are measured in a CCD, and curvature determined by the change in spot spacing.
- Multi-beam array moves uniformly during substrate vibration, so that measurement is relatively insensitive to external “noise.”
- Thin film stress determined from radius curvature.

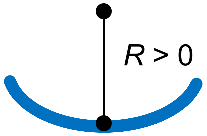


$$\Delta k = \left(\frac{\Delta d}{d_0}\right)\frac{\cos\theta}{2L}$$

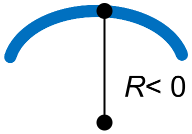
$^{*}\Delta k_{\mathrm{res}}$: $2\mathrm{x}10^{-4}$ m^{-1}



Simultaneous vertical and horizontal measurement.



Tensile curvature/stress



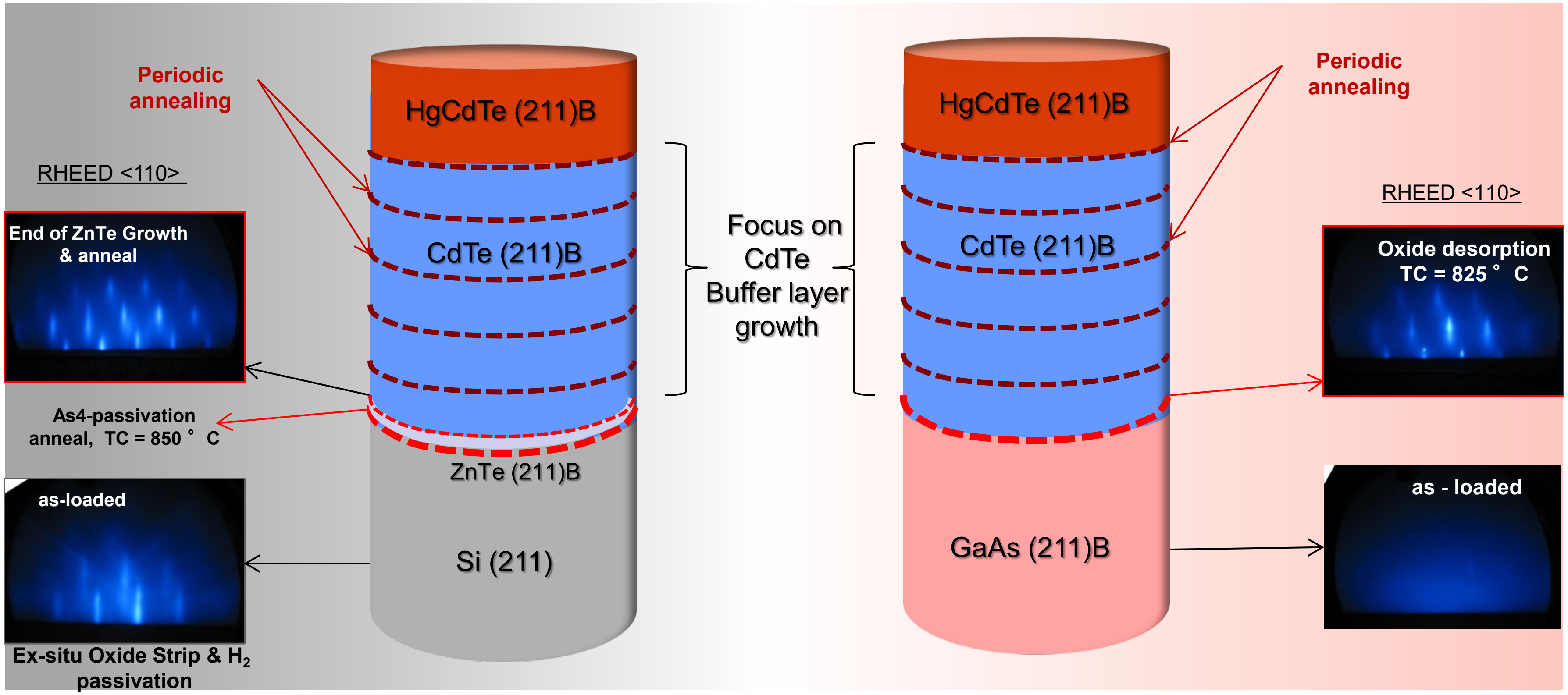
Compressive curvature/stress

$$\sigma_{residual} = \frac{\Delta k E_s h_s^2}{6(1-\nu_s)h_f}$$

$^{*}\sigma_{\mathrm{res}}$: < 1 MPa

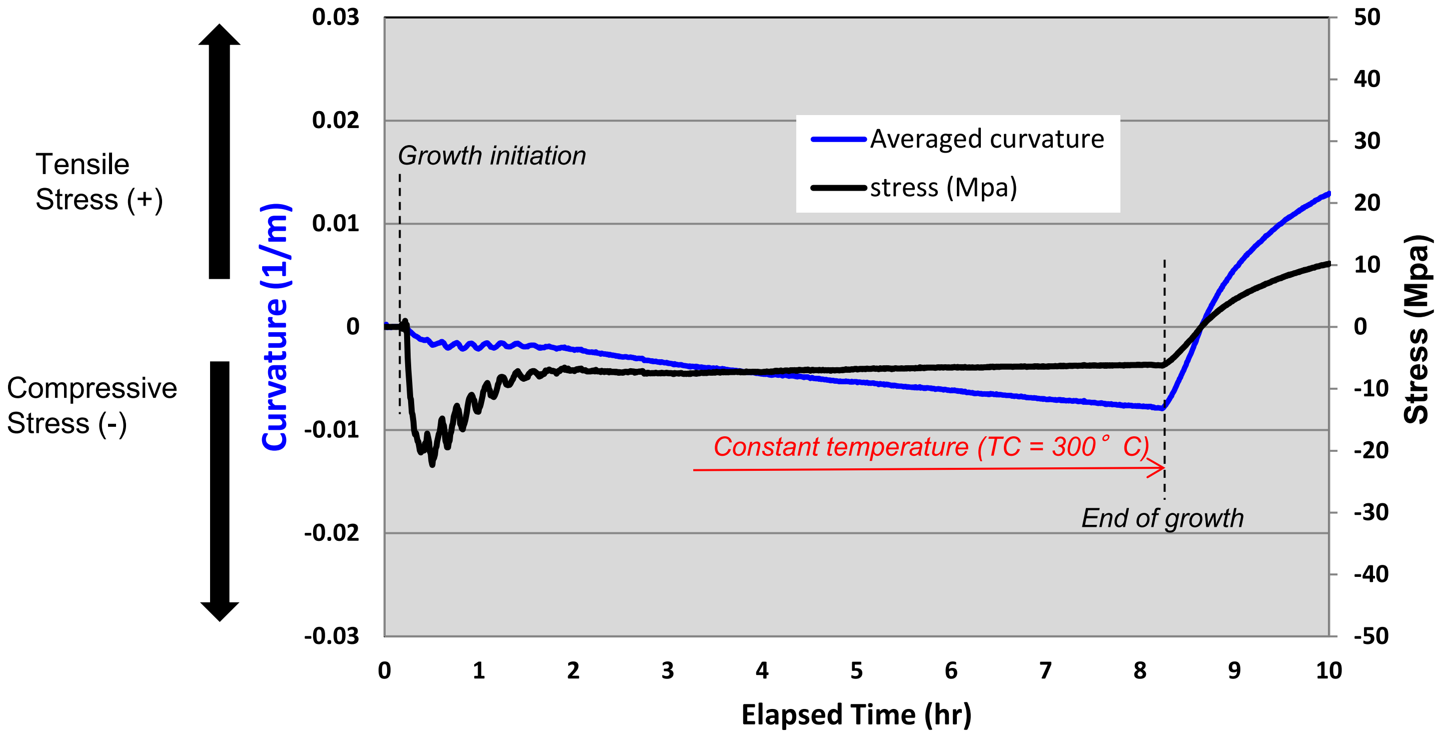
*For our configuration

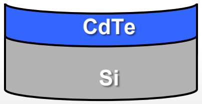
MBE Growth procedures



- High temperature (TC = 850 ° C) surface preparation prior to growth.
- Similar crystallinity and surface quality prior to CdTe growth procedure.
- Periodic annealing incorporated during CdTe growth on both Si and GaAs.
- Initial stress studies focus on CdTe layer growth and in-situ annealing.

Dynamic curvature: continuous growth

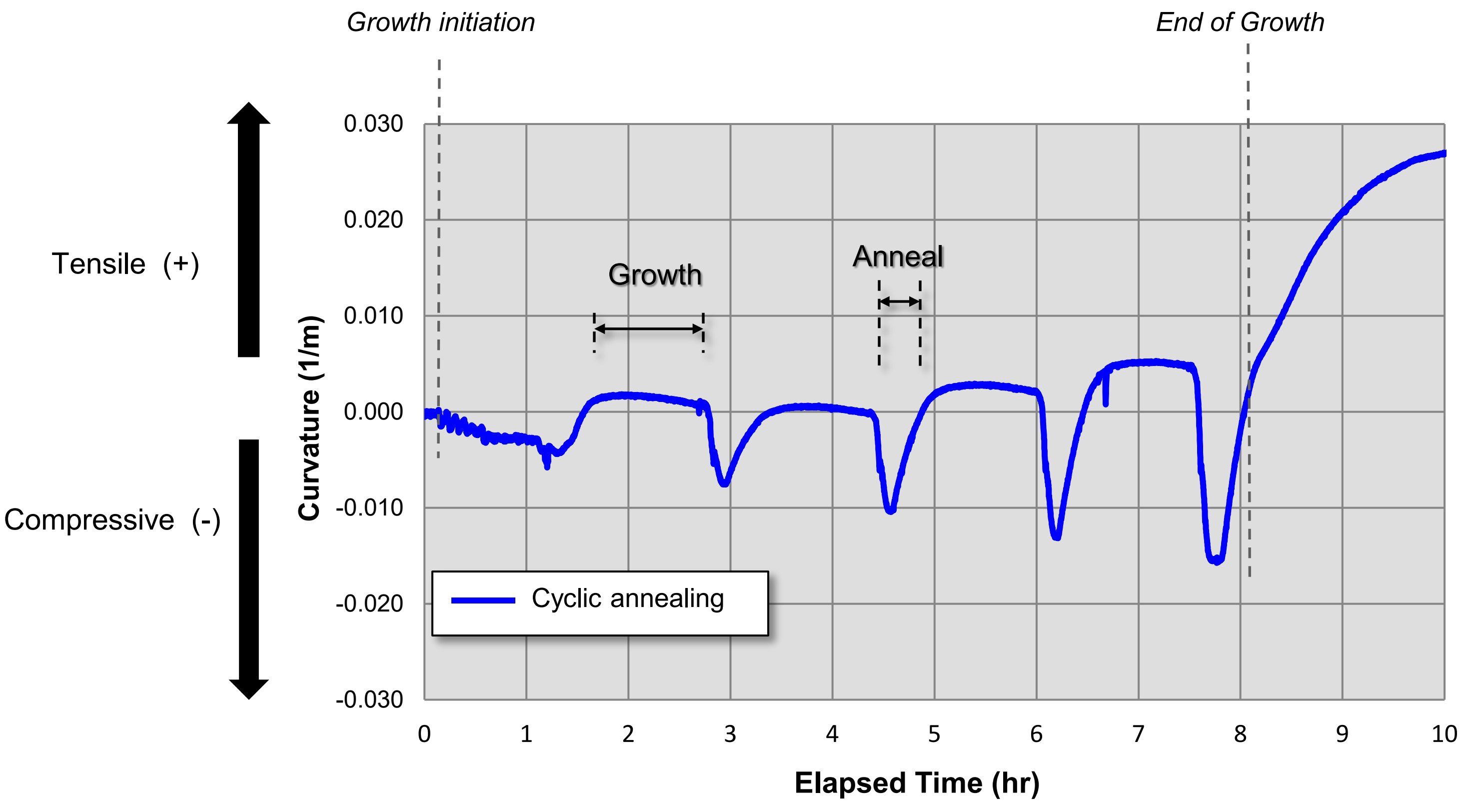

CdTe/Si: continuous growth

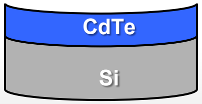


Residual Tensile curvature/stress produces "bowl" shaped substrate.

- Initial curvature/stress is compressive…., due to lattice misfit.
- Gradual decrease in curvature due to residual misfit.
- Overall tensile stress after cooling to room temperature.

Dynamic curvature: CdTe/Si Periodic Annealing

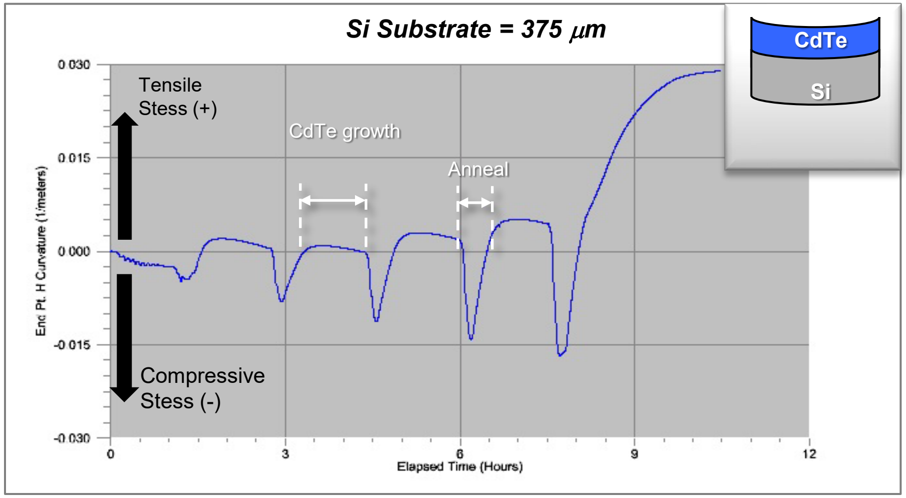


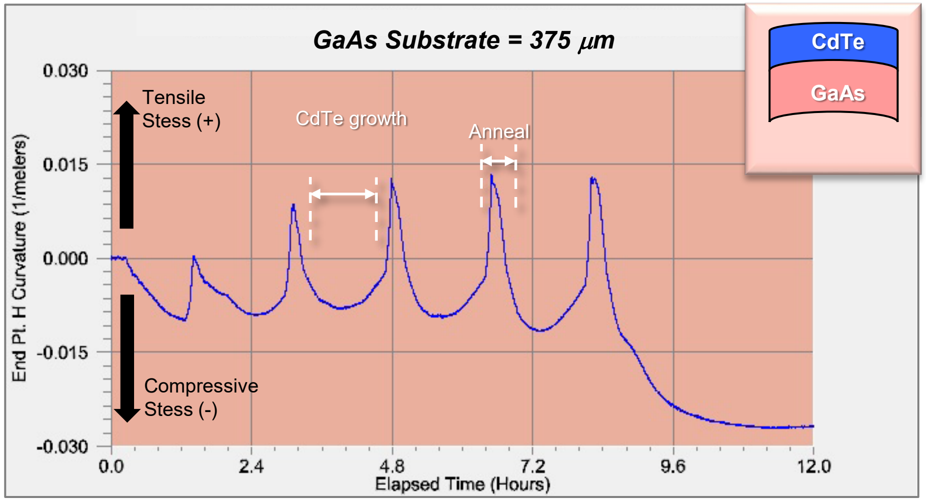


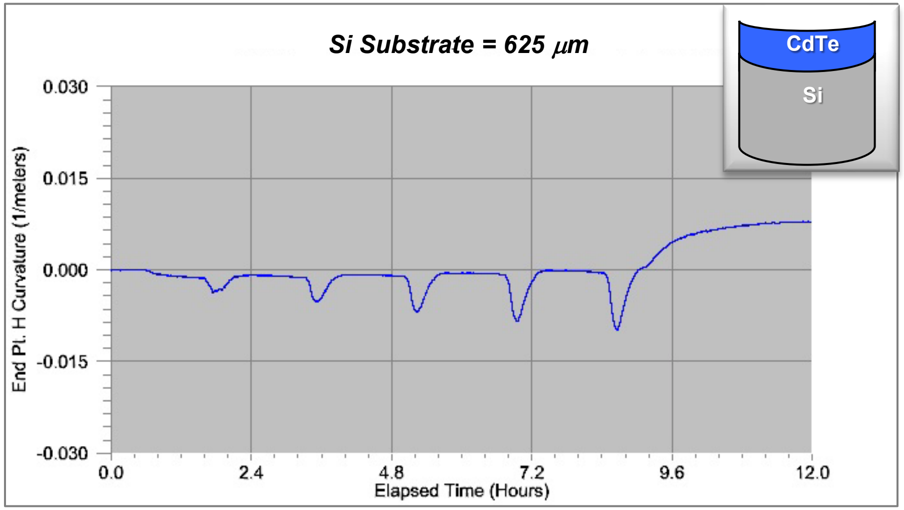
Residual Tensile curvature/stress produces “bowl” shaped substrate.

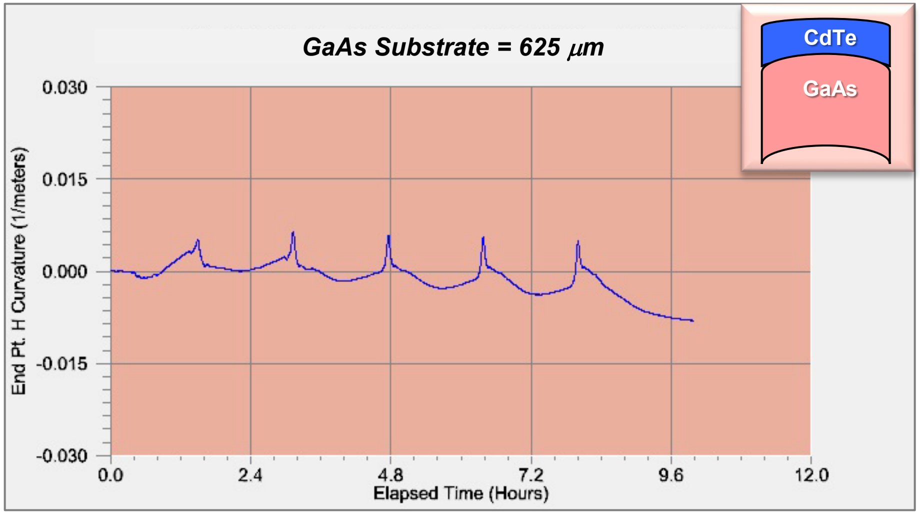
- •Initial compressive curvature due to lattice misfit.
- •Annealing: compressive during ramp up, tensile during ramping down.
- •Gradually compressive during 1 hr growth cycles.
- •Thermally induced curvature increases with thickness.
- •Overall Tensile Curvature after cool down to room temperature.

Si vs. GaAs substrates (Effect of substrate thickness)


Si Substrate = 375 μm

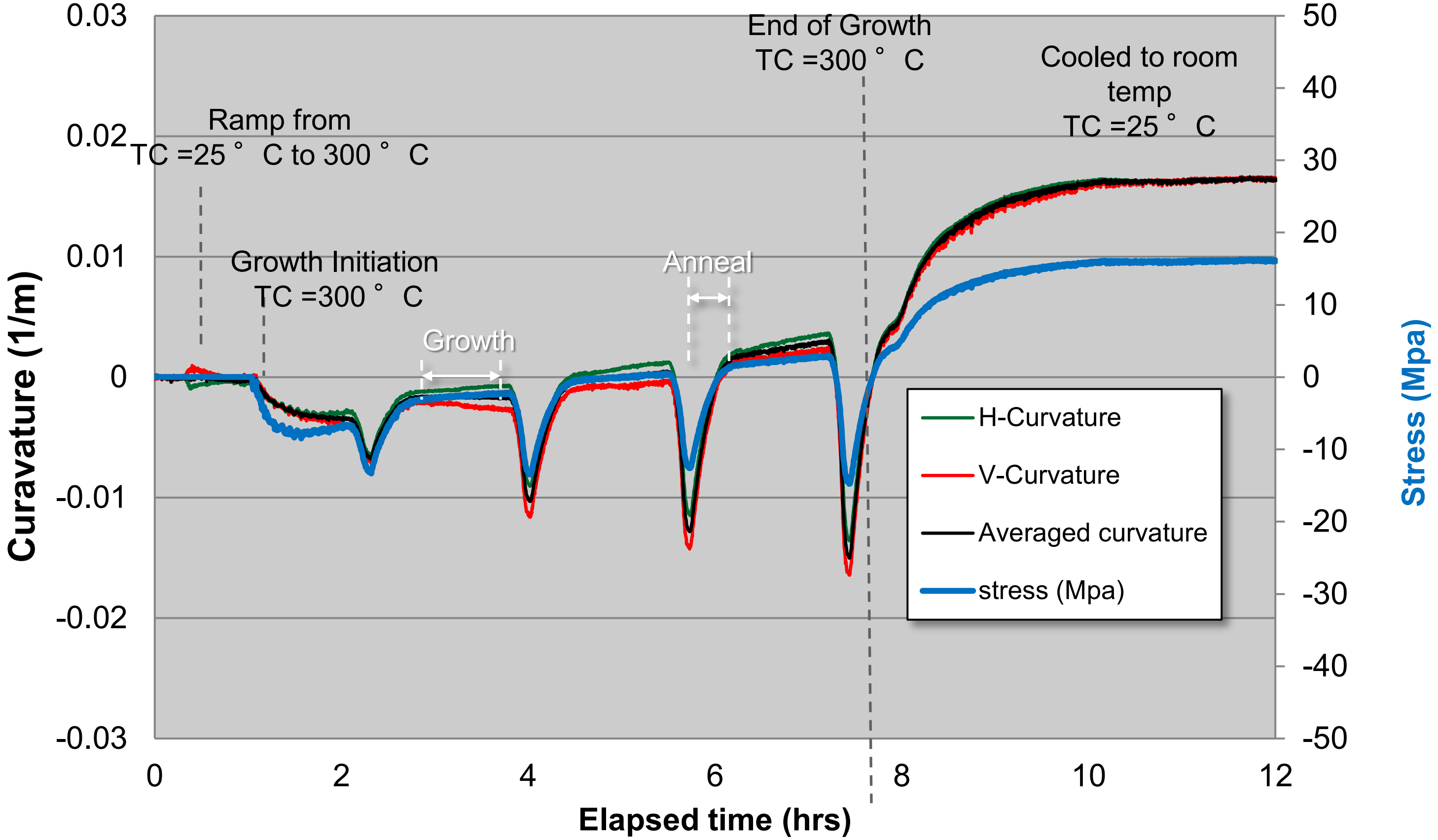

GaAs Substrate = 375 μm


Si Substrate = 625 μm


GaAs Substrate = 625 μm

- CdTe/GaAs: tensile during ramp up, and compressive during ramp down. (Contrary to CdTe/Si).
- Curvature profiles consistent with opposite TEC mismatch for CdTe/Si and CdTe/GaAs.
- In-situ and residual curvature suppressed for growth on thicker Substrates.

Curvature: Ramp from room temp



- Initial ramping from 25 C to Growth temperature.
- Substrate flexes (H vs. V) upon ramp up to growth temperature.
- Overall, this ramp evokes little change.

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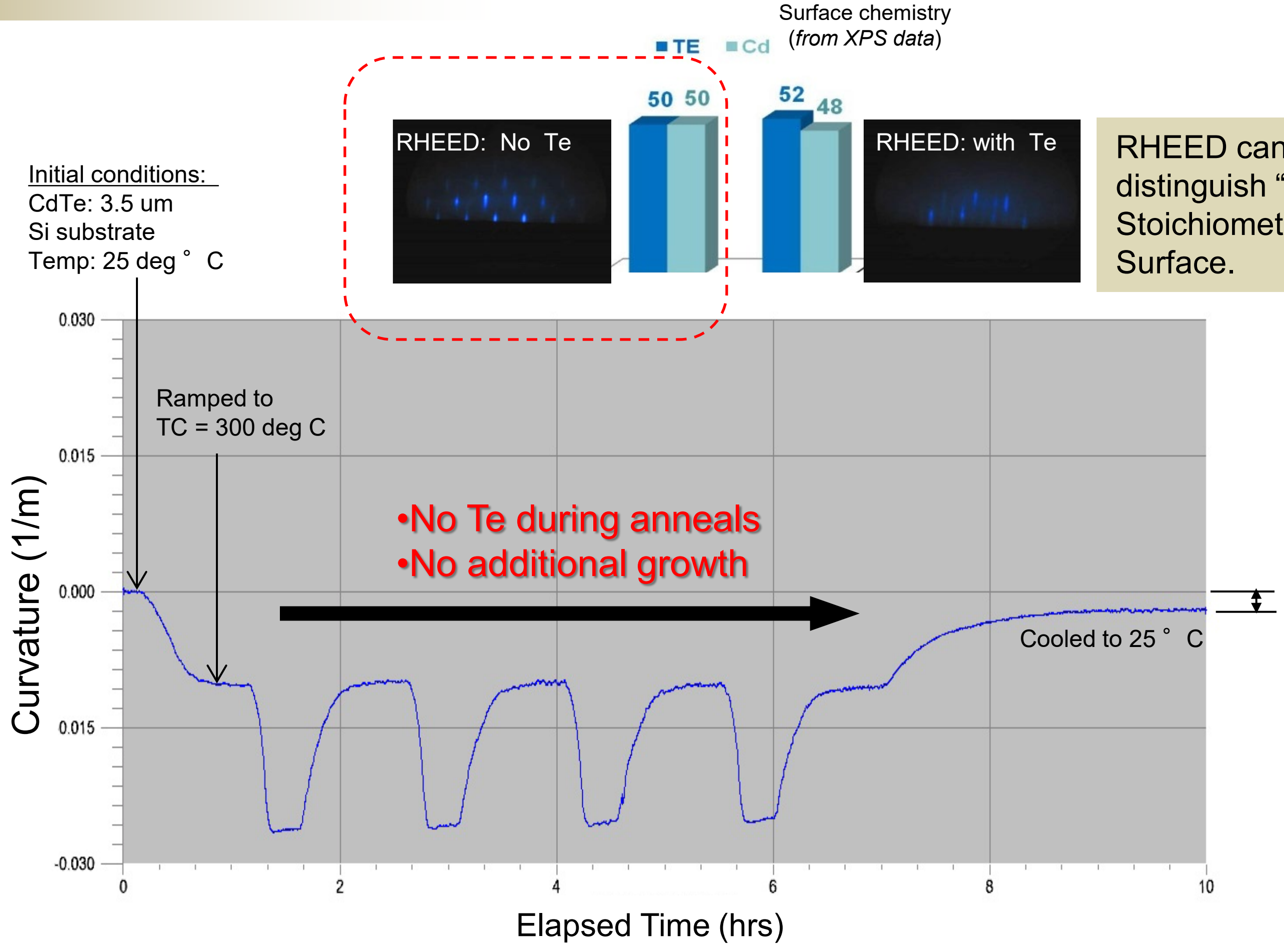
Study of Te saturated annealing



RHEED can be used to distinguish “Te-Rich” from Stoichiometric CdTe Surface.

Residual curvature= -2.1×10^{-3} 1/m

(ΔR= -476 m)

- Initial conditions: ~3.5 um thick CdTe film on Si at room temperature.
- Four Annealing cycles performed without Te overpressure, (and no additional CdTe growth).
- Small residual curvature reveals **material desorption**.
- A loss of 0.2 um (per annealing cycle) is estimated from curvature data.

-(confirmed by ex-situ thickness measurement).

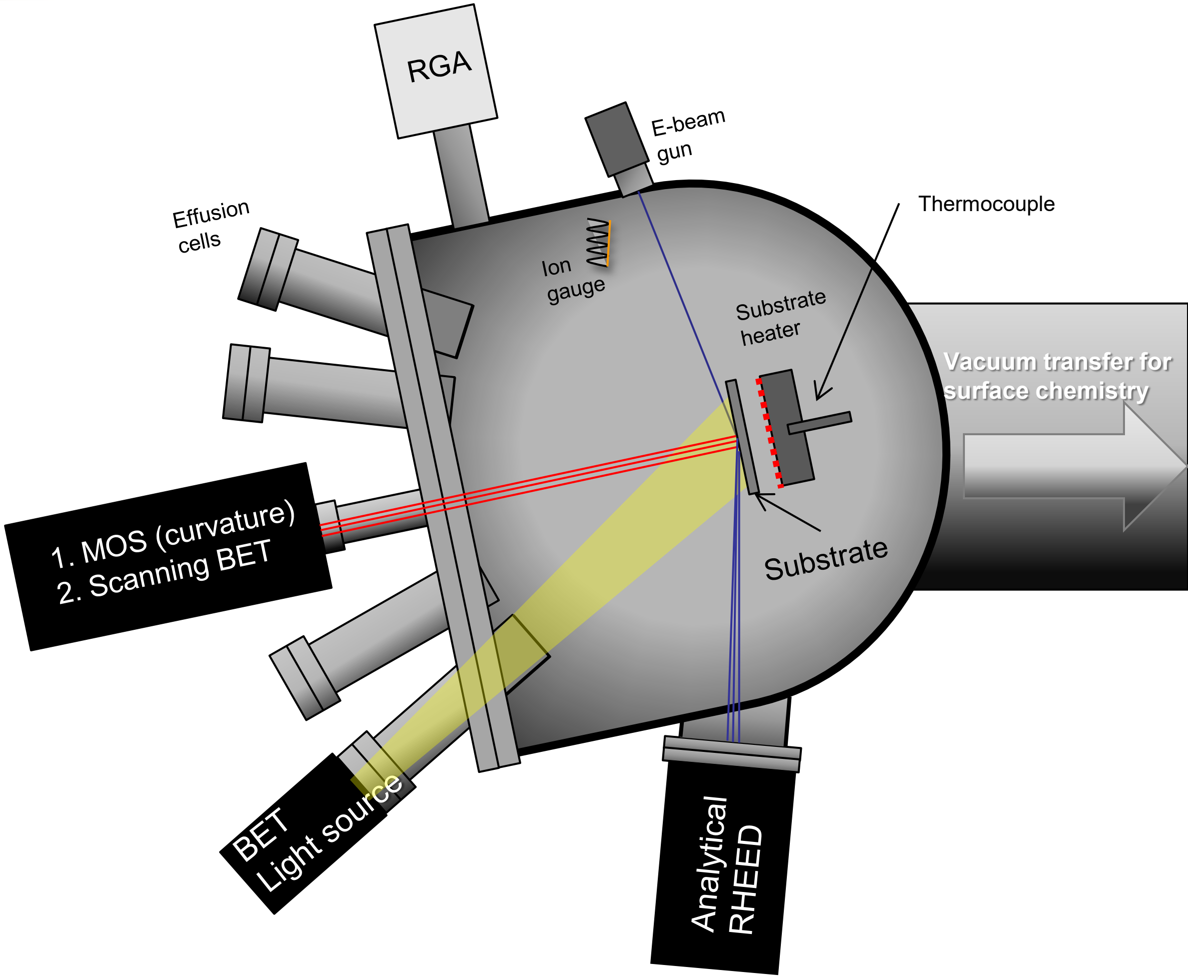
Integrated Metrology for MBE

Standard in-situ metrology:

- **Thermocouple/pyrometer**
  -Subst. temperature
- **Ion gauge**
  -chamber pressure
  -Beam equivalent pressure
- **RHEED**
  -Qualitative surface structure.
- **Residual Gas Analyzer (RGA)**
  -Partial pressures

Recently acquired at NVESD:

- **Curvature monitoring (MOS)**
  - **Curvature/Stress**
  - **Substrate bowing**
- **Band-edge thermometry (BET)**
  - *Substrate temperature mapping*
  - *Thickness/growth rate*
  - *Roughness*
- **Analytical RHEED**
  - *Quantitative diffraction patterns*
  - *Lattice param. Monitoring*
  - *Compliments MOS (surface vs Bulk)*



Summary and Conclusions

- Demonstrated MOS technique for dynamic curvature measurement during CdTe MBE on GaAs and Si substrates.

- Confirmed results of previous x-ray diffraction-based studies on residual stress & curvature.

- Observed predicted tensile and compressive properties in-situ and after growth.

- In-situ studies deconvolved lattice-mismatch induced from thermal-mismatch induced stress.

- Near term (ongoing) Studies:
    - *Incorporate BET and MOS techniques to examine effect of substrate backing plates (used during growth of HgCdTe over-layers).*
    - *Evaluate new annealing schedules for stress-reduction.*

- Dynamic curvature studies for MBE III-V SLS materials.