Temperature-dependent refractive index of Cleartran® ZnS to cryogenic temperatures

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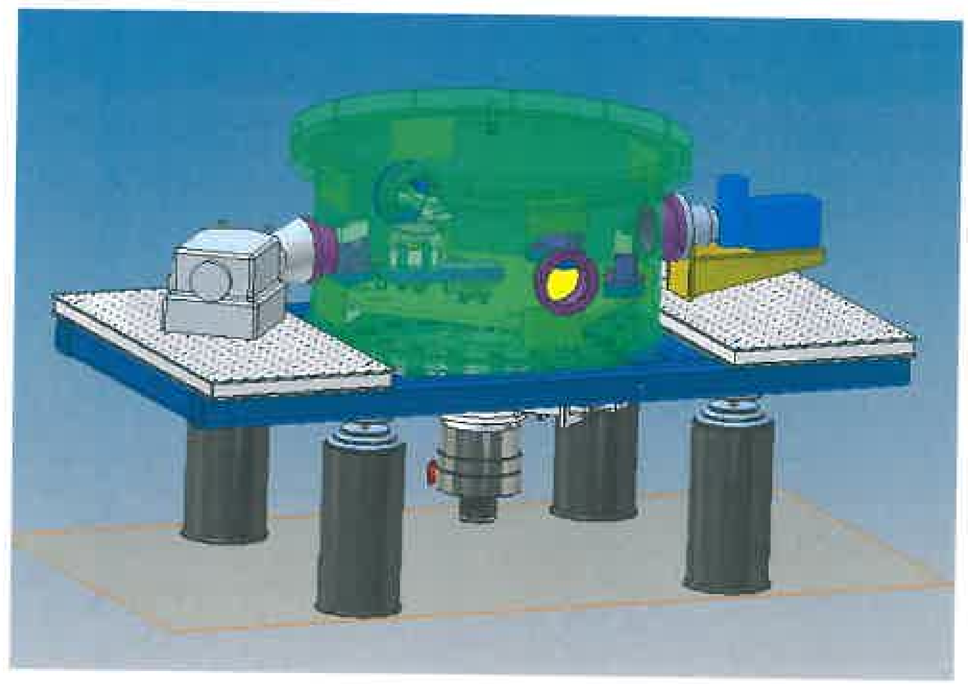
The Cryogenic High-Accuracy Refraction Measuring System (CHARMS) at NASA GSFC

… but first, let's talk about the CHARMS facility at NASA's Goddard Space Flight Center

- Cryogenic, High-Accuracy Refraction Measuring System (CHARMS)
- design features for highest accuracy and precision
- technologies we rely on
- data products and examples
- optical materials for which we've measured cryogenic refractive index

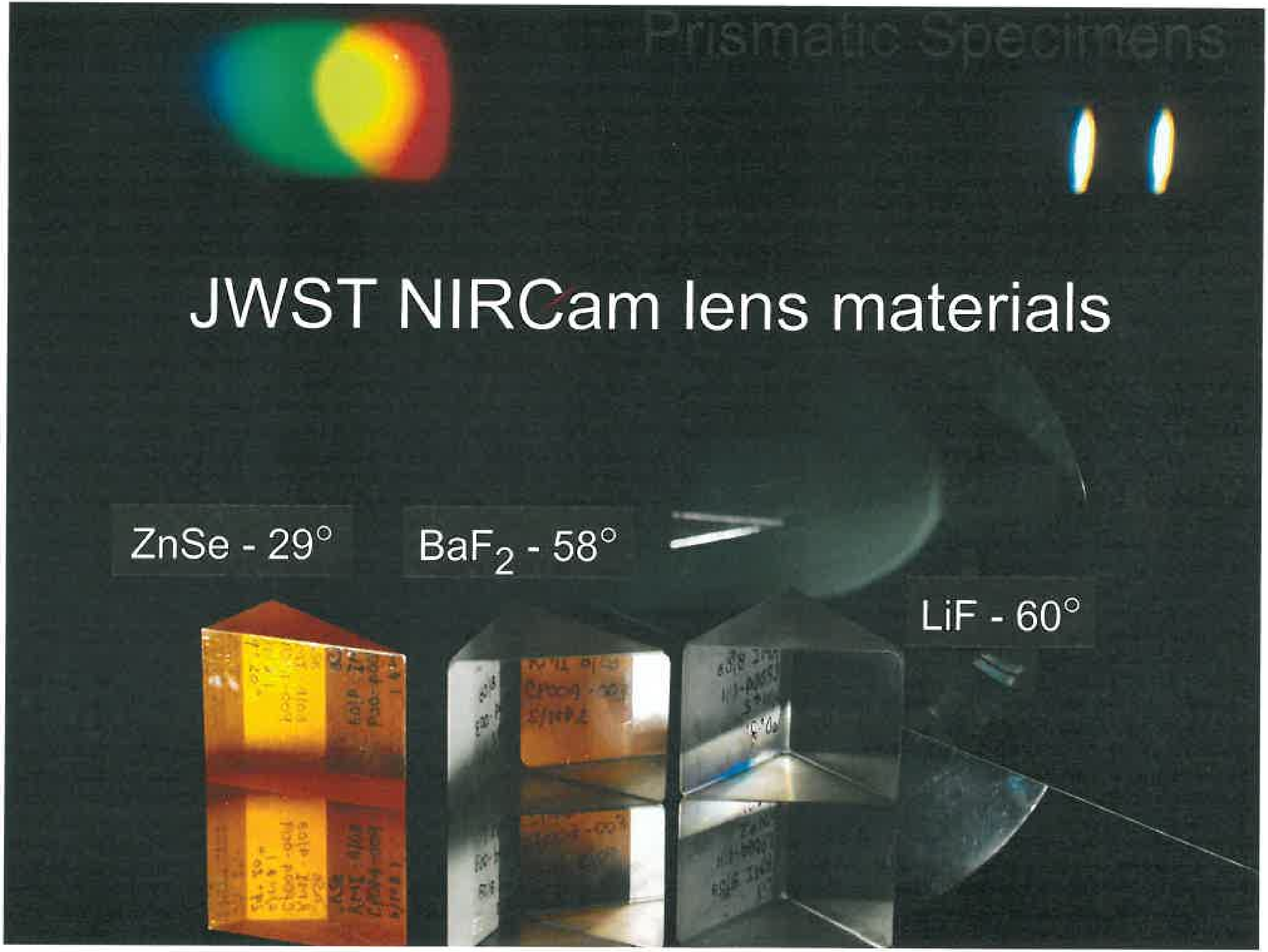


CHARMS fact sheet

- developed in ~2003 to provide design refractive indices of ZnSe, LiF, BaF2 for two triplet lenses in JWST's Near Infrared Camera (NIRCam) at 38 K
- CHARMS is a differential, absolute, minimum deviation refractometer
- provides dense sampling of index in both wavelength and temperature
- wavelength coverage:
  - 400 nm (violet) to 5.6 μm in mid-IR
  - plans to extend range to 120 nm in FUV, and 20 microns in mid-IR
- temperature coverage:

  15 K to 330+ K (60 C)
- accuracy in n(λ,T)

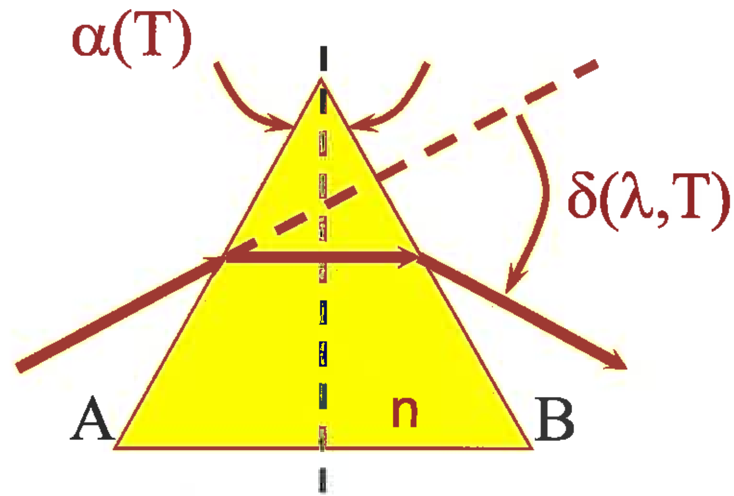
  +/-0.000002 to +/-0.0001 depending on material and temperature


Prismatic Specimens
JWST NIRCam lens materials
ZnSe - 29°
BaF2 - 58°
LiF - 60°

Minimum deviation refractometry

- apex:
  - measure angle of prism face A
  - measure angle of prism face B
- measure direction of undeviated beam
- measure direction of deviated beam

for each wavelength



$$n(\lambda,T) = \frac{\sin(\alpha/2 + \delta/2)}{\sin(\alpha/2)}$$

Limits on accuracy with minimum deviation method

- $n(\alpha, \delta(\underline{\lambda, T}))$
- dn contains …
  - **$dn/d\alpha \cdot \Delta\alpha$** Prism apex
  - **$dn/d\delta \cdot \Delta\delta$** Deviation angle
  - **$dn/d\lambda \cdot \Delta\lambda$** Spectral dispersion
  - **$dn/dT \cdot \Delta T$** Thermo-optic coefficient
- uncertainty should be listed as a function of both wavelength AND temperature

Bookkeeping error budget

index n apex α deviation δ | dn/dλ dn/dT dn/dα dn/dδ dλ dT dα dδ → dn

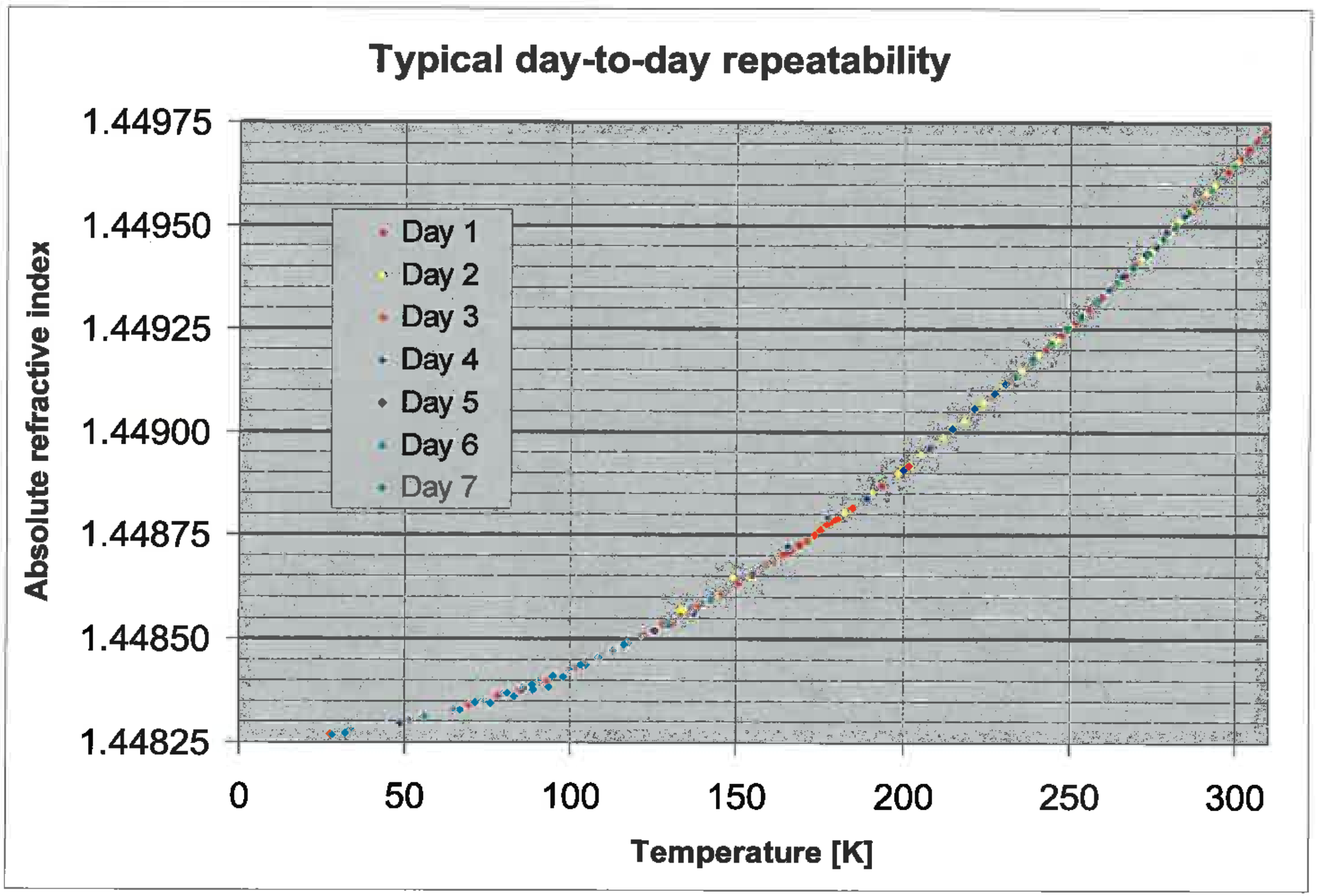
					SENSITIVITIES								FOR SPECIFIED PRISM				FOR SPECIFIED PRISM				
index n	apex a	alpha	delta d		dn/dwv	dn/dT	dn/da	dn/d	dwv	dn(dwv)	dT	dn(dT)	da			dn(da)	dd			dn(dd)	dn r.s.s.
1.4574	10.0 deg	0.175 rads	4.595 deg	0.080 rads	0.00040/nm	0.000120/K	[illegible]	[illegible]	0.10 nm	4.0E-05	0.1 K	[illegible]	0.00014 deg	0.5 sec	#	[illegible]	0.00150 deg	5.4 sec	###	[illegible]	[illegible]
1.4574	20	0.349 rads	9.319 deg	0.163 rads	0.00040/nm	0.000120/K	-1.35/rad	2.786/rad	0.10 nm	4.0E-05	0.1 K	1.2E-05	0.00014 deg	0.5 sec	#	-3.3E-06	0.00150 deg	5.4 sec	###	7.3E-05	9.5E-05
1.4574	30	0.524 rads	14.321 deg	0.250 rads	0.00040/nm	0.000120/K	-0.93/rad	1.789/rad	0.10 nm	4.0E-05	0.1 K	1.2E-05	0.00014 deg	0.5 sec	#	-2.3E-06	0.00150 deg	5.4 sec	###	4.7E-05	7.4E-05
1.4574	40	0.698 rads	19.796 deg	0.346 rads	0.00040/nm	0.000120/K	-0.73/rad	1.267/rad	0.10 nm	4.0E-05	0.1 K	1.2E-05	0.00014 deg	0.5 sec	#	-1.8E-06	0.00150 deg	5.4 sec	###	3.3E-05	6.4E-05
1.4574	50	0.873 rads	26.038 deg	0.454 rads	0.00040/nm	0.000120/K	-0.63/rad	0.932/rad	0.10 nm	4.0E-05	0.1 K	1.2E-05	0.00014 deg	0.5 sec	#	-1.5E-06	0.00150 deg	5.4 sec	###	2.4E-05	5.9E-05
1.4574	58	1.012 rads	31.912 deg	0.557 rads	0.00040/nm	0.000120/K	-0.58/rad	0.730/rad	0.10 nm	4.0E-05	0.1 K	1.2E-05	0.00014 deg	0.5 sec	#	-1.4E-06	0.00150 deg	5.4 sec	###	1.9E-05	5.6E-05
2.6	10	0.175 rads	16.195 deg	0.283 rads	0.00040/nm	0.000120/K	-9.27/rad	5.588/rad	0.10 nm	4.0E-05	0.1 K	1.2E-05	0.00014 deg	0.5 sec	#	-2.3E-05	0.00150 deg	5.4 sec	###	1.5E-04	1.7E-04
2.6	15	0.262 rads	24.677 deg	0.431 rads	0.00040/nm	0.000120/K	-6.27/rad	3.603/rad	0.10 nm	4.0E-05	0.1 K	1.2E-05	0.00014 deg	0.5 sec	#	-1.5E-05	0.00150 deg	5.4 sec	###	9.4E-05	1.2E-04
2.6	20	0.349 rads	33.678 deg	0.588 rads	0.00040/nm	0.000120/K	-4.80/rad	2.569/rad	0.10 nm	4.0E-05	0.1 K	1.2E-05	0.00014 deg	0.5 sec	#	-1.2E-05	0.00150 deg	5.4 sec	###	6.7E-05	9.1E-05
2.6	25	0.436 rads	43.491 deg	0.759 rads	0.00040/nm	0.000120/K	-3.95/rad	1.910/rad	0.10 nm	4.0E-05	0.1 K	1.2E-05	0.00014 deg	0.5 sec	#	-9.7E-06	0.00150 deg	5.4 sec	###	5.0E-05	7.7E-05
2.6	30	0.524 rads	54.587 deg	0.953 rads	0.00040/nm	0.000120/K	-3.42/rad	1.429/rad	0.10 nm	4.0E-05	0.1 K	1.2E-05	0.00014 deg	0.5 sec	#	-8.4E-06	0.00150 deg	5.4 sec	###	3.7E-05	6.7E-05
3.4	10	0.175 rads	24.475 deg	0.427 rads	0.00040/nm	0.000120/K	-13.95/rad	5.479/rad	0.10 nm	4.0E-05	0.1 K	1.2E-05	0.00014 deg	0.5 sec	#	-3.4E-05	0.00150 deg	5.4 sec	###	1.4E-04	1.6E-04
3.4	14	0.244 rads	34.958 deg	0.610 rads	0.00040/nm	0.000120/K	-10.11/rad	3.734/rad	0.10 nm	4.0E-05	0.1 K	1.2E-05	0.00014 deg	0.5 sec	#	-2.5E-05	0.00150 deg	5.4 sec	###	9.8E-05	1.2E-04
3.4	18	0.314 rads	46.265 deg	0.807 rads	0.00040/nm	0.000120/K	-8.03/rad	2.707/rad	0.10 nm	4.0E-05	0.1 K	1.2E-05	0.00014 deg	0.5 sec	#	-2.0E-05	0.00150 deg	5.4 sec	###	7.1E-05	9.6E-05
3.4	22	0.384 rads	58.895 deg	1.028 rads	0.00040/nm	0.000120/K	-6.75/rad	1.994/rad	0.10 nm	4.0E-05	0.1 K	1.2E-05	0.00014 deg	0.5 sec	#	-1.6E-05	0.00150 deg	5.4 sec	###	5.2E-05	8.0E-05
4.0	10	0.175 rads	30.806 deg	0.538 rads	0.00040/nm	0.000120/K	-17.48/rad	5.377/rad	0.10 nm	4.0E-05	0.1 K	1.2E-05	0.00014 deg	0.5 sec	#	-4.3E-05	0.00150 deg	5.4 sec	###	1.4E-04	1.6E-04
4.0	12.5	0.218 rads	39.130 deg	0.683 rads	0.00040/nm	0.000120/K	-14.13/rad	4.134/rad	0.10 nm	4.0E-05	0.1 K	1.2E-05	0.00014 deg	0.5 sec	#	-3.5E-05	0.00150 deg	5.4 sec	###	1.1E-04	1.3E-04
4.0	15	0.262 rads	47.947 deg	0.837 rads	0.00040/nm	0.000120/K	-11.92/rad	3.267/rad	0.10 nm	4.0E-05	0.1 K	1.2E-05	0.00014 deg	0.5 sec	#	-2.9E-05	0.00150 deg	5.4 sec	###	8.6E-05	1.1E-04
4.0	17.5	0.305 rads	57.461 deg	1.003 rads	0.00040/nm	0.000120/K	-10.39/rad	2.608/rad	0.10 nm	4.0E-05	0.1 K	1.2E-05	0.00014 deg	0.5 sec	#	-2.5E-05	0.00150 deg	5.4 sec	###	6.8E-05	9.5E-05

• uncertainty governed by all eight quantities in the red box for each measurement for a given specimen (green box)

So, refractometers should not list just a single number for accuracy

On precision ...

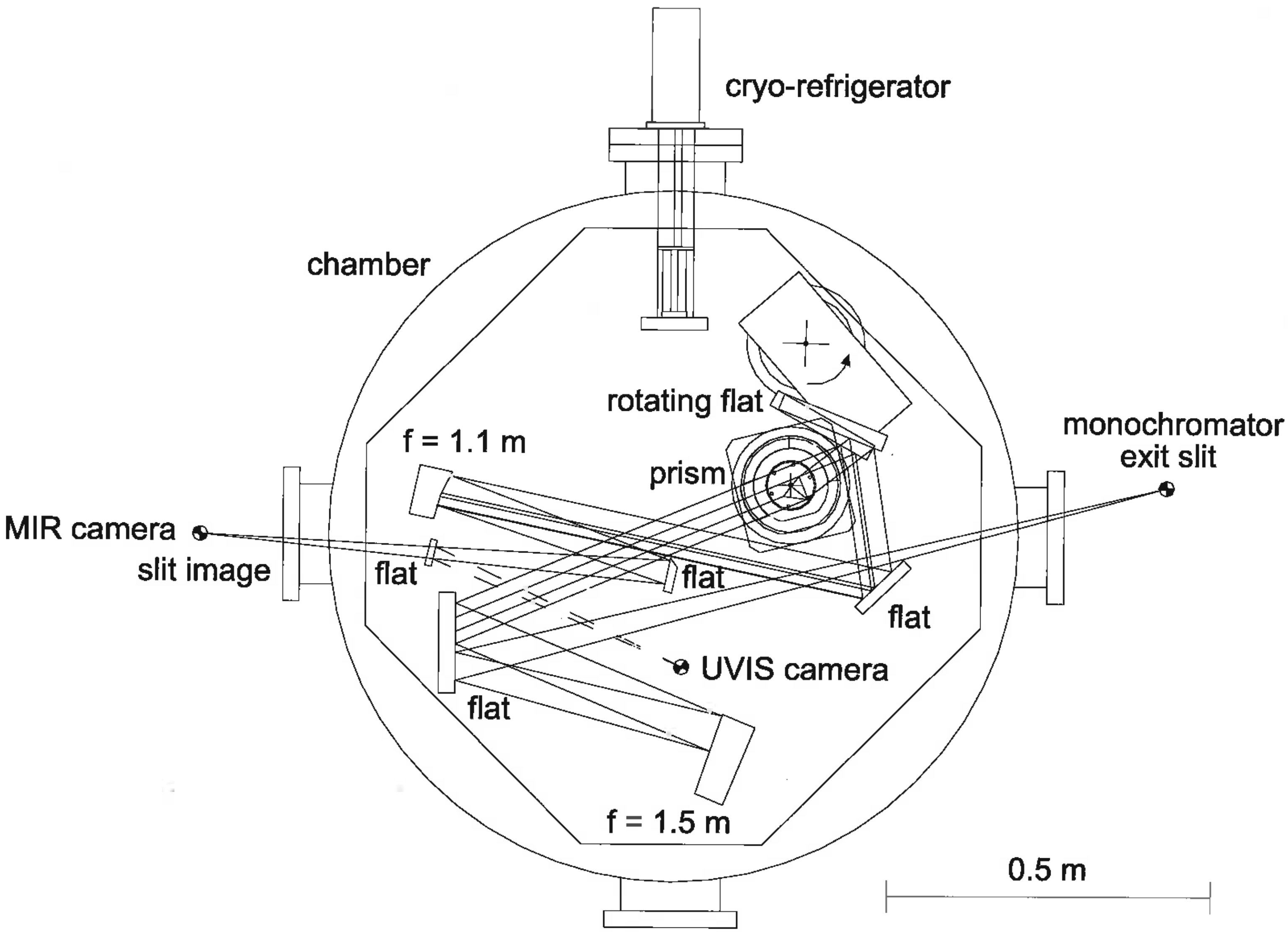
- precision often well exceeds accuracy; do not confuse with accuracy
- CHARMS precision for fused silica at a given wavelength is ~1E-7



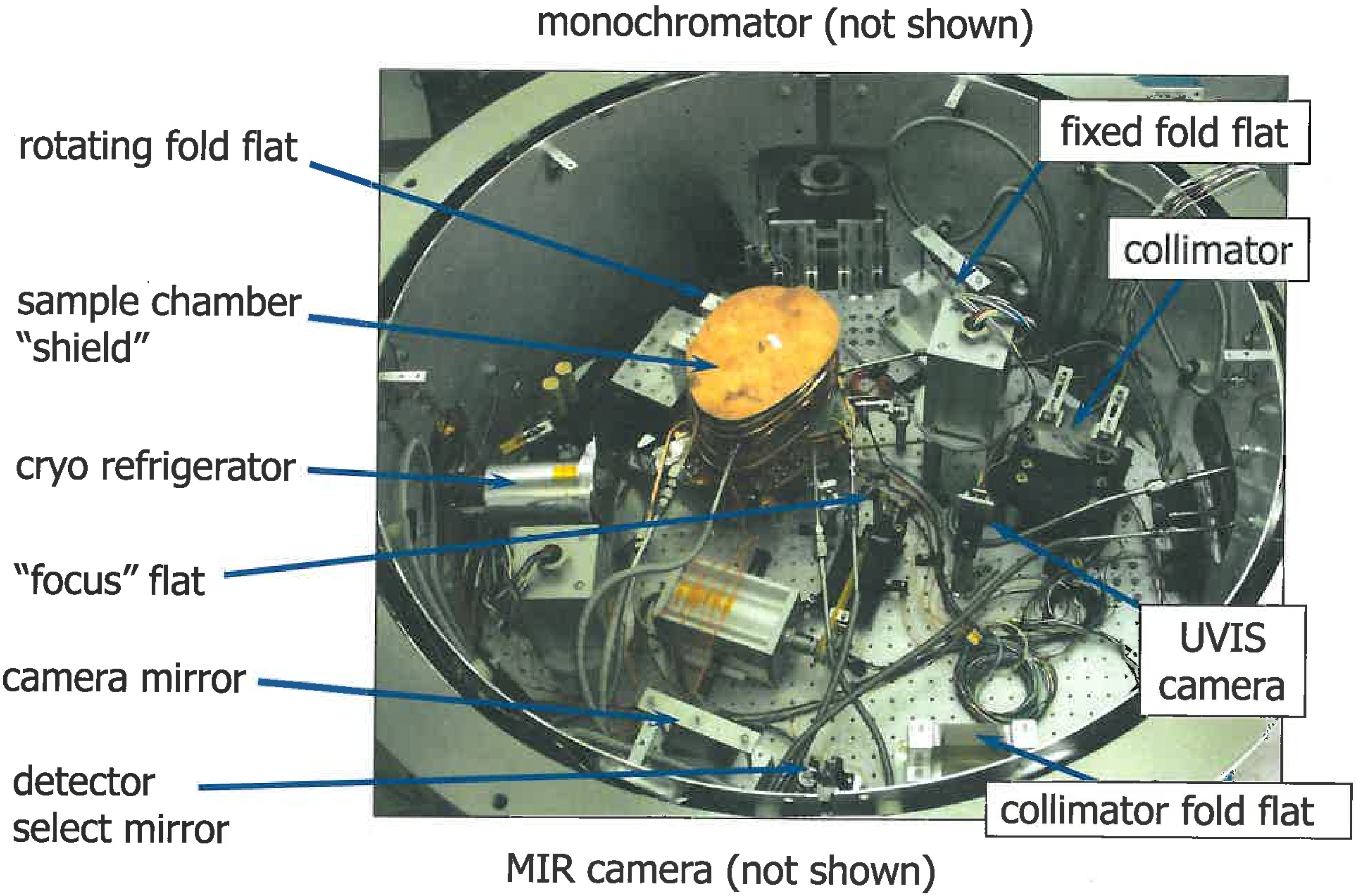
CHARMS design approach / measurement technique

- limit contribution of each error source by design / know each contributor well
  - automate to eliminate human factor
  - build best practical machine for measuring apex angle
  - use similar hardware for measuring beam direction in refractometer
  - use multiple, calibrated high accuracy temperature sensors on prism
  - calibrate monochromator carefully with laser lines and measure only at wavelengths for calibrated (order number x wavelength)
- make differential measurements
  - have access to undeviated beam and refer to it frequently !
  - measure spectral index over and over as temperature of sample slowly drifts in temperature – builds rich data set for fitting
- immerse entire refractometer in vacuum
  - measurements thus absolute
  - no window effects
  - eliminates most environmental effects
  - all reflective design is broadband and achromatic

CHARMS optical layout



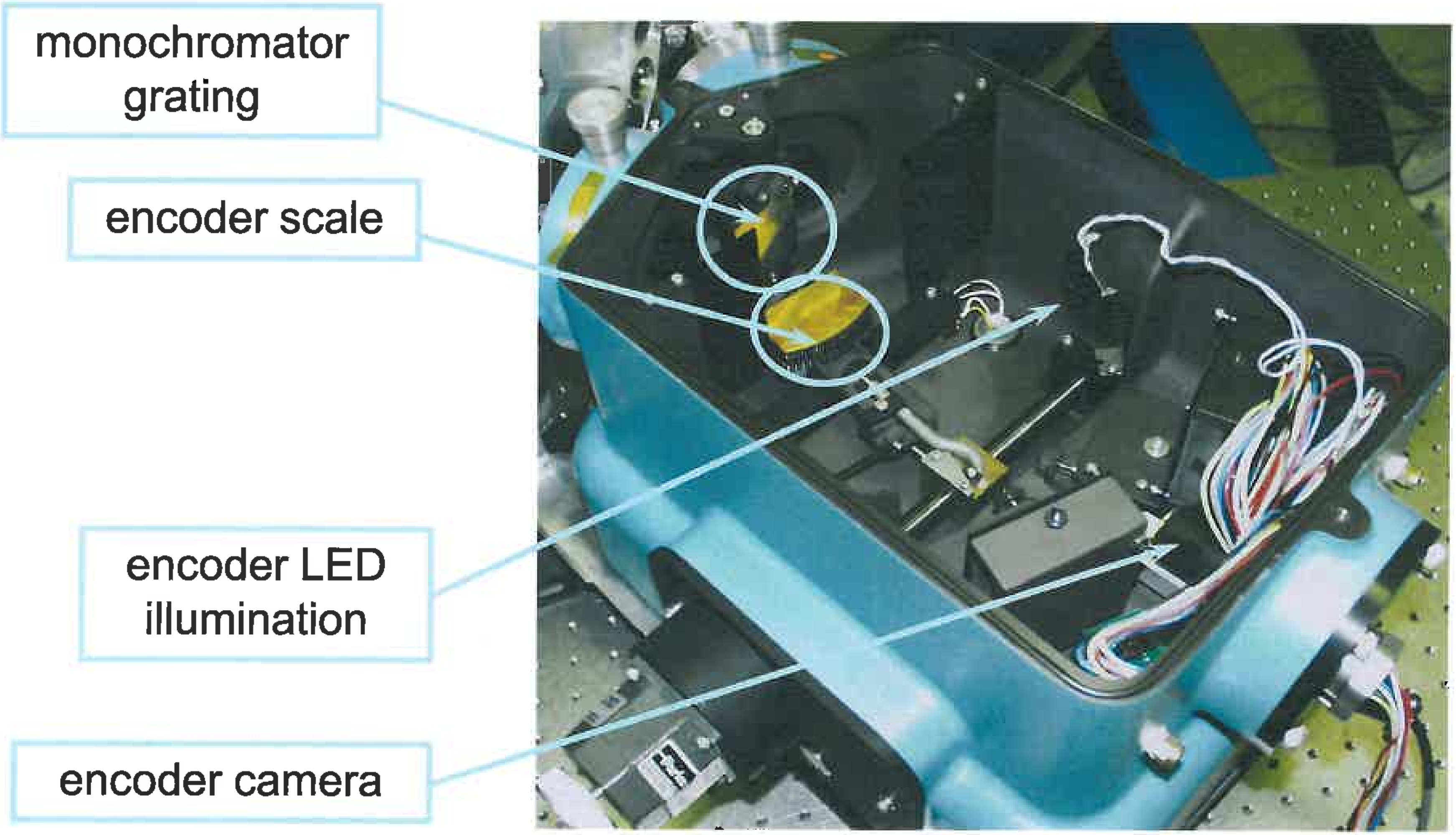
CHARMS opto-mechanical layout



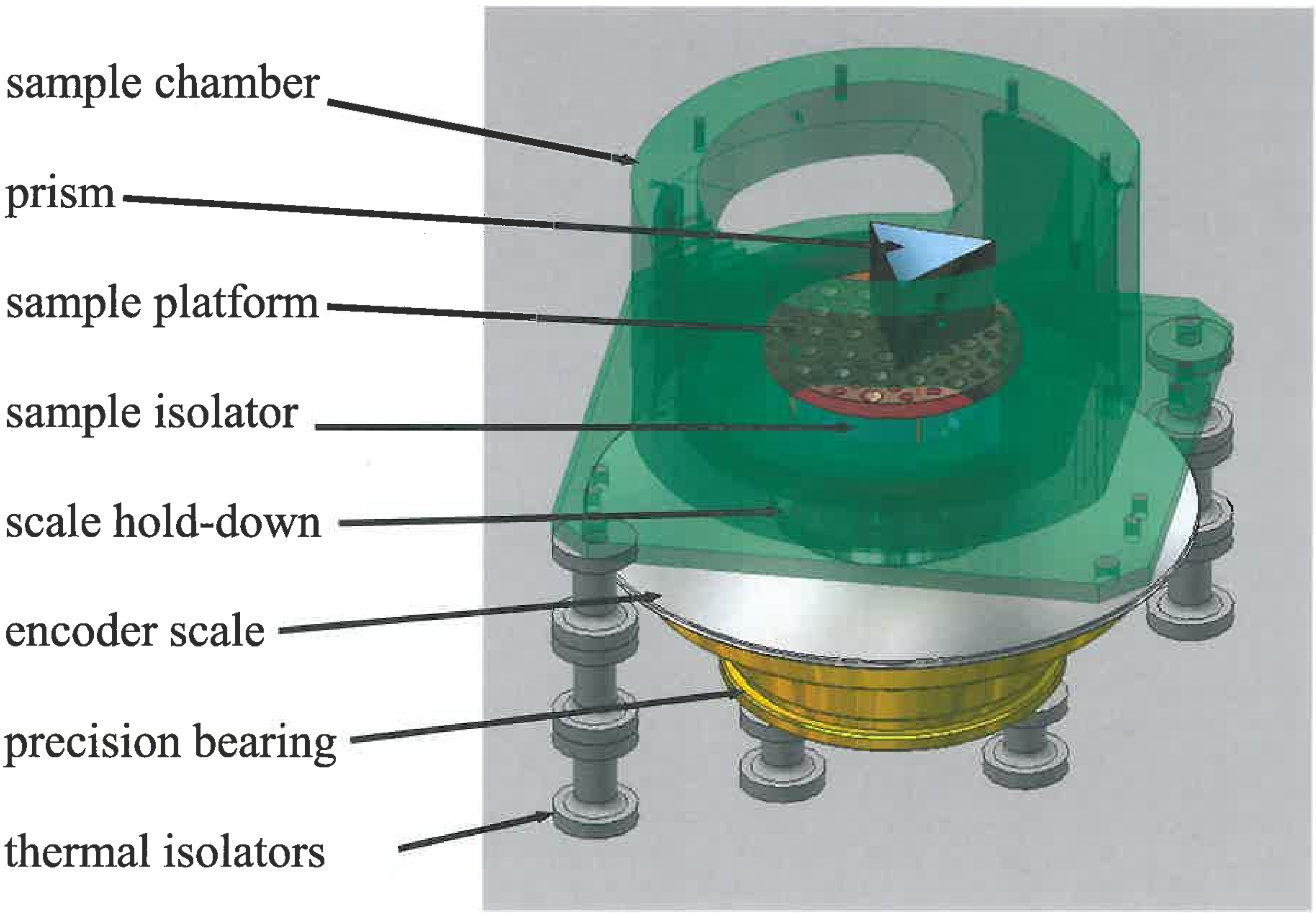
Technologies we rely on

- high accuracy, high resolution, absolute Leviton encoders installed on
  - apex measuring setup (0.3 arcsecond apex accuracy)
  - rotating fold mirror spindle (0.8 arcsecond deviation accuracy)
  - sample stage
  - monochromator grating shaft
- absolute electronic autocollimator
- long focal length collimating and camera mirrors
- high accuracy calibrated Si diode temperature sensors
- CCD for NUV / Vis / NIR wavelengths
- InSb array camera for NIR to mid-IR wavelength
- QTH and globar light sources
- numerous order sorting filters

Calibrated monochromator



Windowless prism assembly



CHARMS automation

Rack contains:

- control PC
- motor controllers
- encoder readouts
- temperature monitors
- programmed power supplies
- turbopump control
- pressure gauges
- monochromator control

Measurement campaigns to date

- JWST / NIRCam
  - ZnSe, $BaF_{2,}$ LiF, Si, Ge, Cleartran ZnS(2 prisms each)
- Ball Aerospace / Kepler Photometer
  - Corning 7980 fused silica (5 samples from 1 m corrector boule)
- ESO / ESA
  - ZnSe
- UC Lick Observatory
  - $CaF_{2,}$ S-FTM16 (2 prisms), S-FPL15
- Harvard College Observatory
  - S-TIM28
- University of Oxford
  - BaLKN3, E-SF03, N-BK7, SF15
- NASA proposals
  - Corning 7940, CaF2, Infrasil 301, SF4, SF6, S-TIH1
- Lockheed Martin
  - Infrasil 301, ZnSe

20 different materials and counting

Cleartran ZnS

- Cleartran (ZnS) is a water-clear form of CVD ZnS
- made by Rohm and Haas (formerly CVD, Inc.), now a subsidiary of Dow Corporation
- different from conventional CVD ZnS by about 0.001 to 0.002 in index

Noteworthy applications for Cleartran ZnS

- Infrared Array Camera (IRAC) on the Spitzer Space Telescope
- Near-InfraRed Imager and Slitless Spectrograph (NIRISS) (replacement for Tunable Filter Imager (TFI) for James Webb Space Telescope
- Gemini Planet Imager (GPI) for the Gemini South telescope

What previous cryogenic index studies are there ?

- None for Cleartran ZnS at cryogenic temps :~(
- Room temperature for conventional CVD ZnS
  - "Refractive indices of zinc sulfide in the 0.405–13-μm wavelength range," Debenham, M., Appl. Opt. **23**, 2238–2239, (1984)
  - "Optical materials characterization," Feldman, A., Horowitz, D., Waxler, R., Dodge, M., NBS (US) Tech Note **993**, 63 (1979)
  - "Refractive index of ZnS, ZnSe, and ZnTe and its wavelength and temperature derivatives," Li, H.H., J. Phys. Chem. Ref Data, **13**(1), 103-150, (1984)
  - W.J. Tropf, "Temperature-dependent refractive index models for BaF2, CaF2, MgF2, SrF2, LiF, NaF, KCl, ZnS, and ZnSe," Optical Engineering, **34**(5), pp. 1369-1373, (1995)

CHARMS data products

- spectral index over temperature from 20 to 300 K, and wavelength from 0.5 to 5.6 μm
- 3-term Sellmeier fits to measured data with 4th order temperature dependence
- spectral dispersion tables over temperature
- spectral thermo-optic coefficient tables over temperature

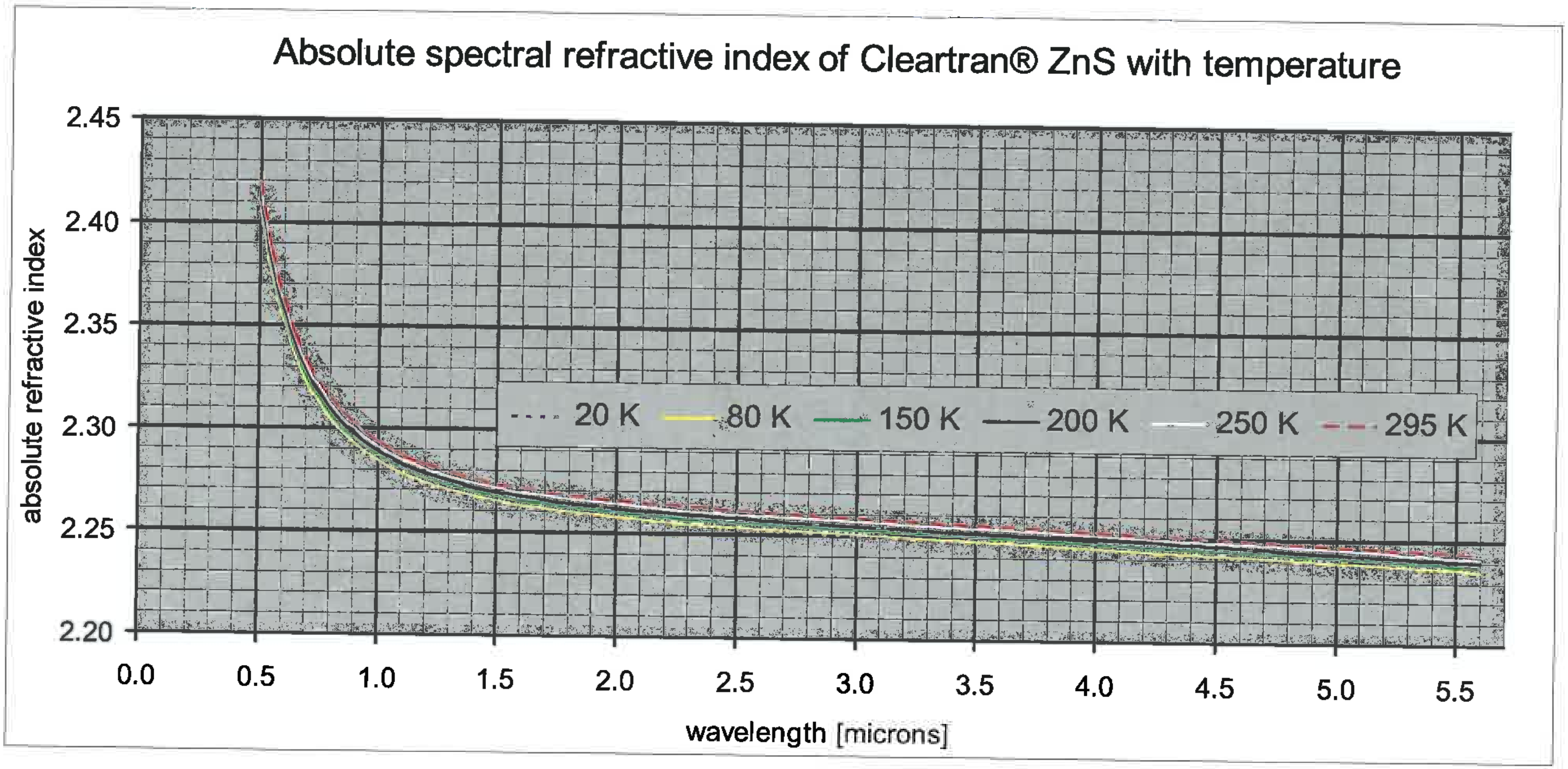
$$n^2(\lambda,T)-1 = \sum_{i=1}^{3} \frac{S_i(T)\cdot\lambda^2}{\lambda^2-\lambda_i^2(T)}$$ ← this functional form

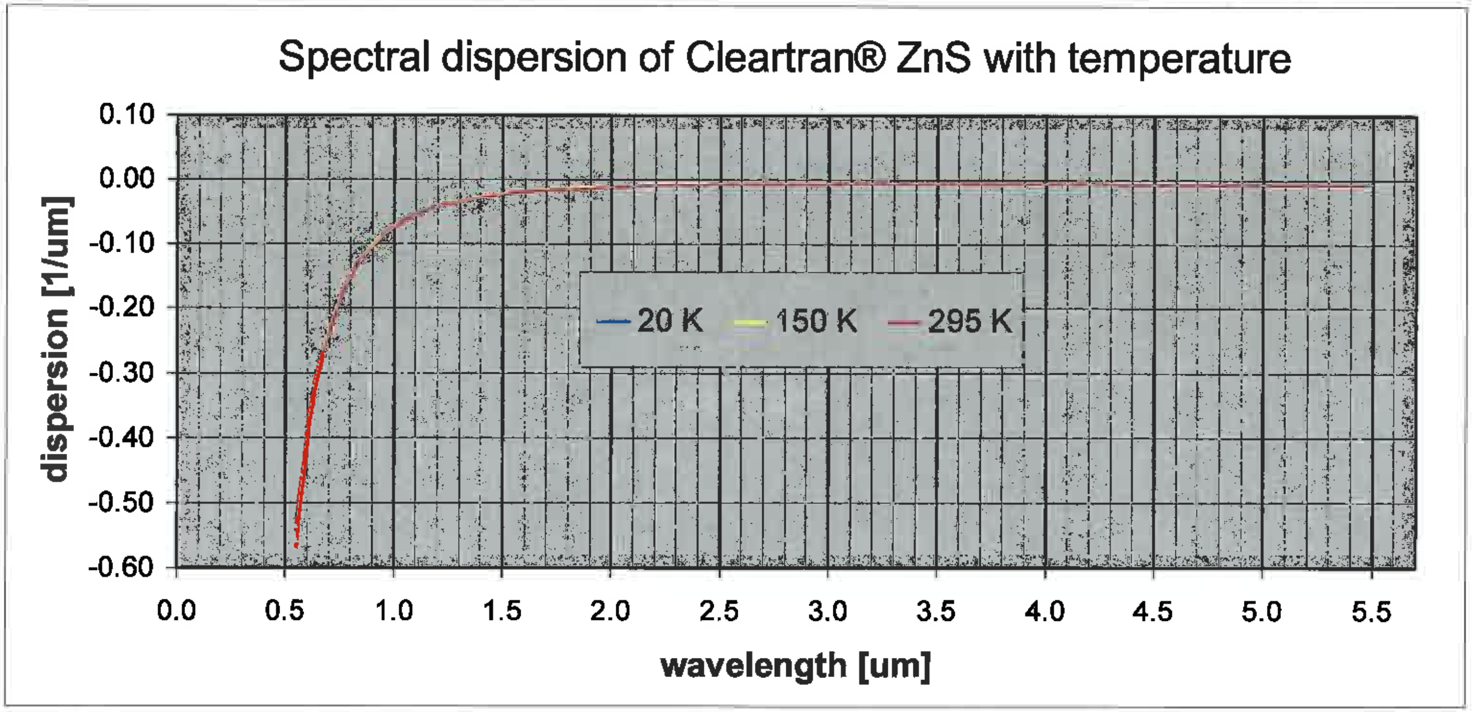
these coefficients →
$$S_i(T) = \sum_{j=0}^{4} S_{ij}\cdot T^j$$

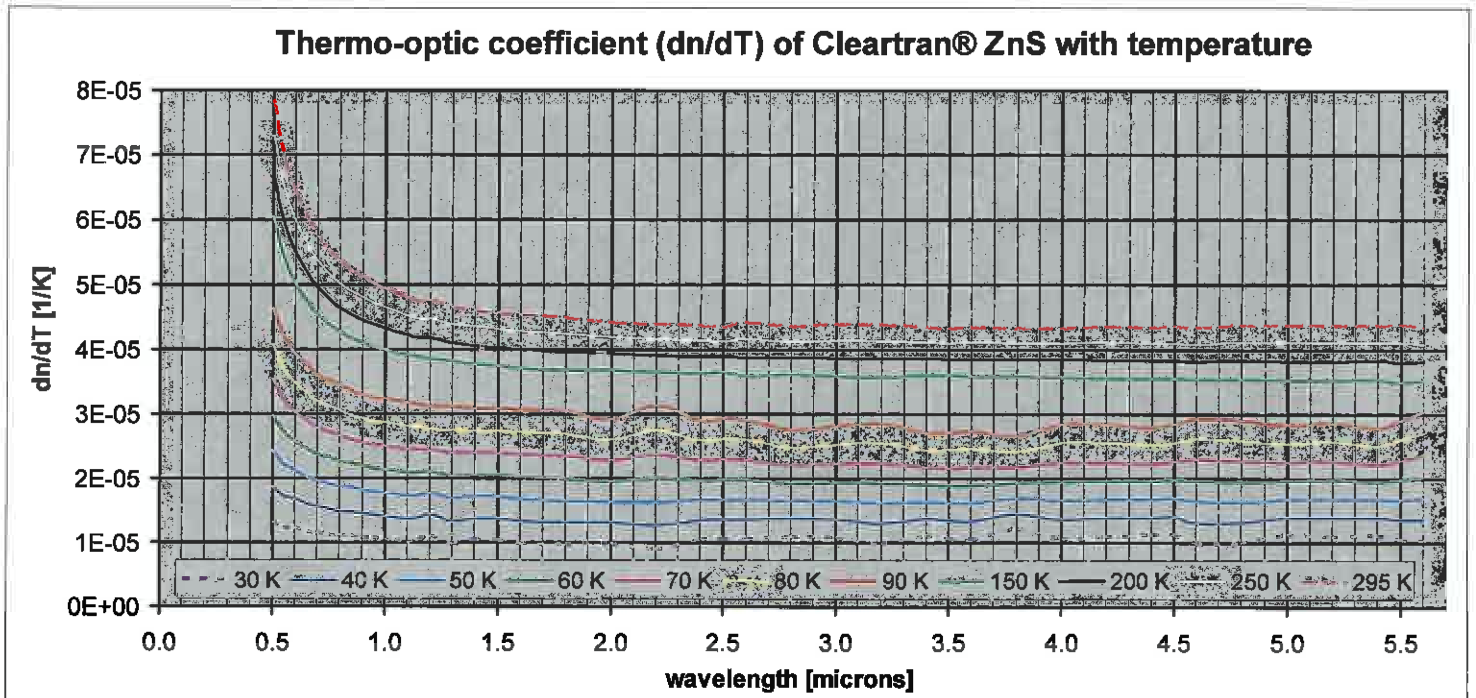
→
$$\lambda_i(T) = \sum_{j=0}^{4} \lambda_{ij}\cdot T^j$$

Index uncertainties

Wavelength [μm]	30 K	75 K	100 K	150 K	200 K	295 K
0.5	1.1E-04	1.3E-04	1.2E-04	1.1E-04	1.0E-04	1.1E-04
1.0	4.7E-05	6.4E-05	5.0E-05	4.2E-05	3.8E-05	4.7E-05
3.0	3.8E-05	5.2E-05	3.8E-05	2.8E-05	2.3E-05	3.8E-05
5.0	3.9E-05	5.2E-05	3.8E-05	2.8E-05	2.3E-05	3.9E-05


Absolute spectral refractive index of Cleartran® ZnS with temperature
absolute refractive index
2.45
2.40
2.35
2.30
2.25
2.20
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
5.0
5.5
wavelength [microns]
20 K
80 K
150 K
200 K
250 K
295 K


Spectral dispersion of Cleartran® ZnS with temperature
dispersion [1/um]
wavelength [um]
0.10
0.00
-0.10
-0.20
-0.30
-0.40
-0.50
-0.60
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
5.0
5.5
20 K
150 K
295 K


Thermo-optic coefficient (dn/dT) of Cleartran® ZnS with temperature
dn/dT [1/K]
wavelength [microns]
8E-05
7E-05
6E-05
5E-05
4E-05
3E-05
2E-05
1E-05
0E+00
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
5.0
5.5
30 K
40 K
50 K
60 K
70 K
80 K
90 K
150 K
200 K
250 K
295 K

Coefficients of wavelength and temperature-dependent Sellmeier fit

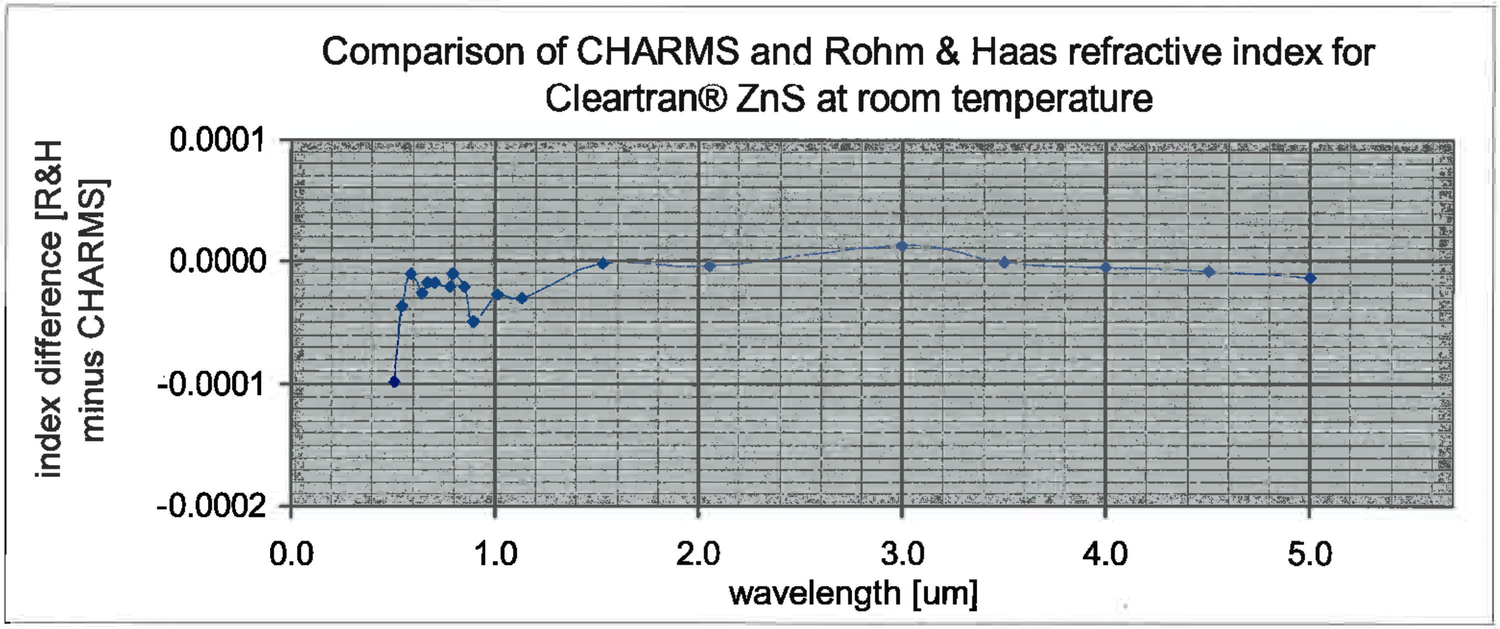
Coefficients for temperature dependent Sellmeier equation for Cleartran ZnS
Applicability: 20 K ≤ T ≤ 300 K; 0.50 μm ≤ λ ≤ 5.6 μm

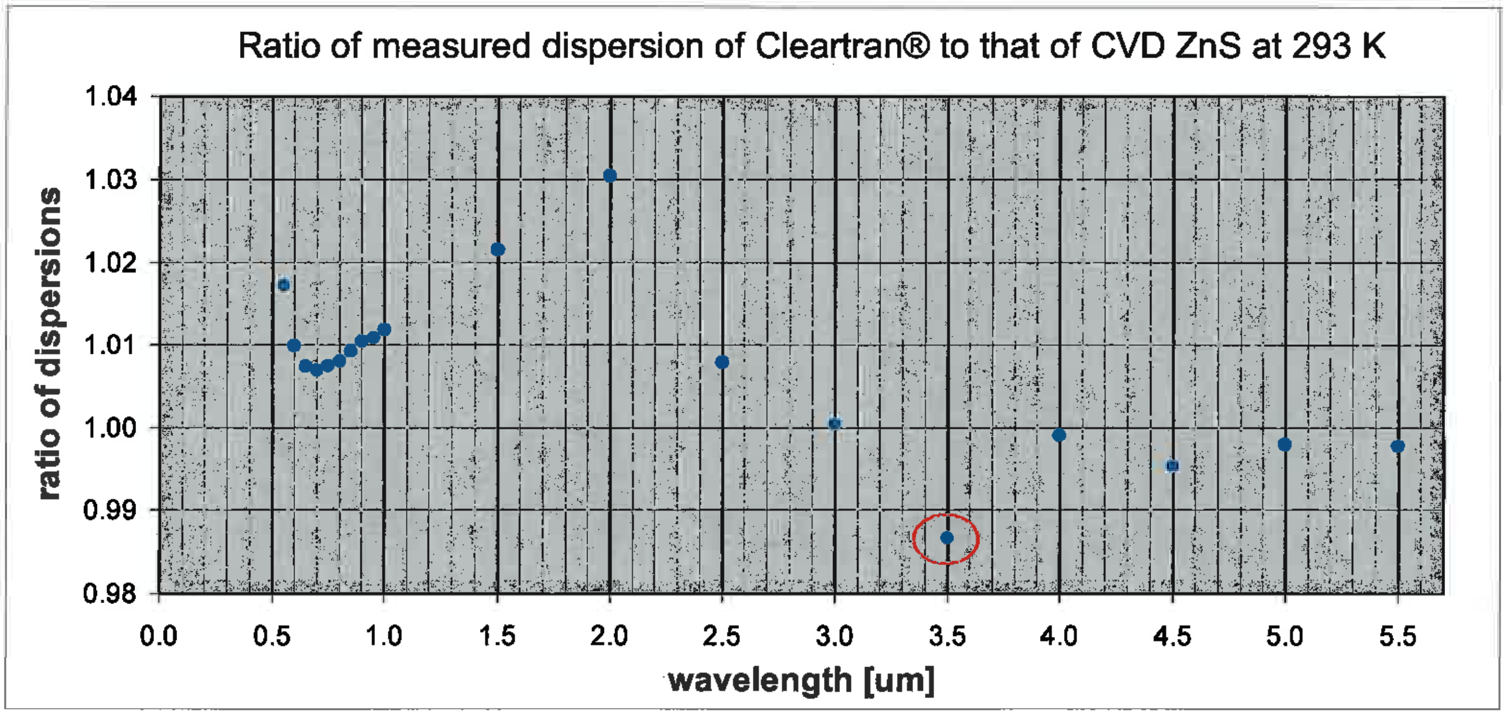
	S_1	S_2	S_3	λ_1	λ_2	λ_3
Constant term	3.35933	0.706131	4.02154	0.161151	0.282427	41.1590
T term	-5.12262E-04	4.89603E-04	-2.93193E-02	-8.93057E-06	-4.66636E-05	-0.161010
T^2 term	1.01086E-05	-8.91159E-06	2.31080E-04	2.73286E-07	7.55906E-07	1.23906E-03
T^3 term	-4.14798E-08	3.81621E-08	-7.57289E-07	-1.23408E-09	-2.77513E-09	-3.95895E-06
T^4 term	6.91051E-11	-6.54805E-11	8.31188E-10	2.29917E-12	4.35237E-12	4.16370E-09

wavelength [um]	20 K	30 K	40 K	50 K	60 K	70 K	80 K	100 K	150 K	200 K	250 K	295 K
0.50	2.40515	2.40524	2.40539	2.40561	2.40590	2.40623	2.40662	2.40751	2.41026	2.41347	2.41700	2.42037
0.60	2.35088										.36075	2.36351
0.70	2.32154										.33049	2.33297
0.80	2.30359										.31202	2.31433
0.90	2.29171										.29980	2.30201
1.00	2.28338										.29125	2.29339
1.50	2.26390										.27127	2.27324
2.00	2.25659										.26380	2.26571
2.50	2.25247										.25961	2.26150
3.00	2.24942										.25652	2.25840
3.50	2.24672										.25380	2.25567
4.00	2.24407										.25114	2.25300
4.50	2.24133										.24838	2.25024
5.00	2.23841										.24545	2.24731
5.60	2.23462	2.23467	2.23477	2.23493	2.23512	2.23535	2.23560	2.23615	2.23777	2.23964	2.24163	2.24348

Three rules for using these coefficients:

1. Do not use outside the identified range of applicability, i.e. do not extrapolate
2. Use all listed significant figures for each coefficient
3. Make sure you can reproduce all of the index value in acommpanying table which were generate with the fit


Comparison of CHARMS and Rohm & Haas refractive index for
Cleartran® ZnS at room temperature
index difference [R&H minus CHARMS]
0.0001
0.0000
-0.0001
-0.0002
0.0
1.0
2.0
3.0
4.0
5.0
wavelength [um]


Ratio of measured dispersion of Cleartran® to that of CVD ZnS at 293 K
ratio of dispersions
1.04
1.03
1.02
1.01
1.00
0.99
0.98
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
5.0
5.5
wavelength [um]

Conclusions

1. first cryogenic measurements of Cleartran ZnS refractive index
2. dispersion and thermo-optic coefficient of Cleartran quite similar to conventional CVD ZnS
3. CHARMS measurements agree very well with those of material manufacturer at room temperature
4. would be prudent to measure more than one sample before concluding that we know Cleartran at cryo (boule-to-boule variability