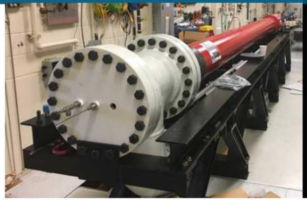
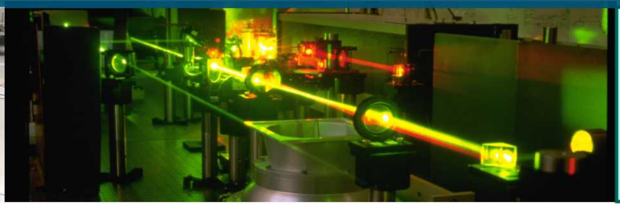
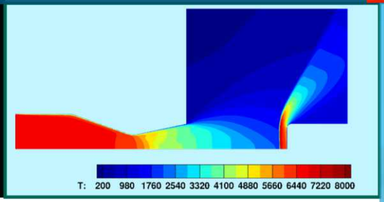
Sandia National Laboratories

SAND2019-11525C

Combined Experimental and Computational Efforts for Hypersonics Validation at Sandia







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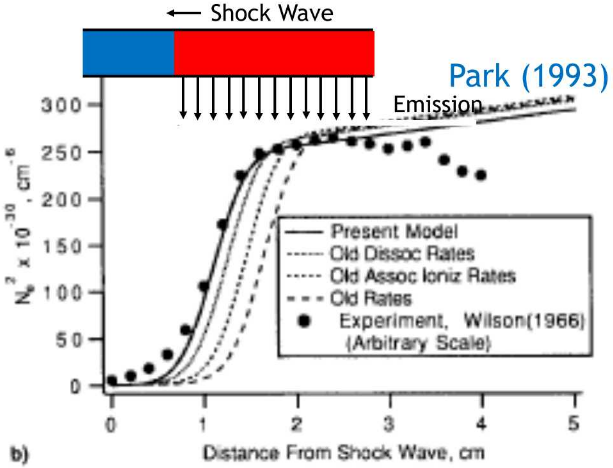
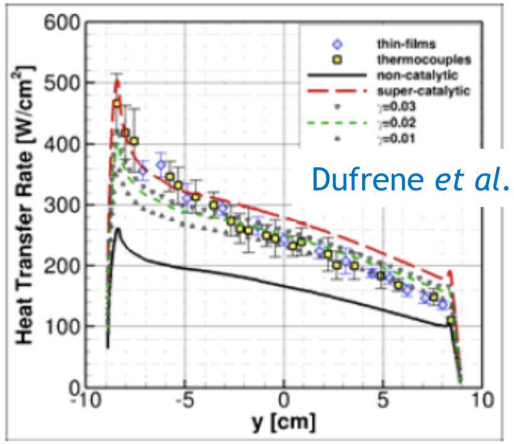
Hypersonic reacting flow modeling: present state-of-the-art

- Thermochemical mechanisms are tuned for ballistic reentry
- Mechanisms derived limited, "integral" experimental data
- Supported by *ab initio* calculations with uncertain potentials



Park (1993)



Dufrene *et al.* (2019)

- Multiple parameters are inferred from single parameter data
- Non-unique, vulnerable to effect of compensating errors

> *".....these parameters cannot necessarily be considered accurate or unique, there could be one or more sets of thermochemical parameters that would lead to an equally good agreement with the experimental data"*
> *–Chul Park, NASA Ames Research Center*

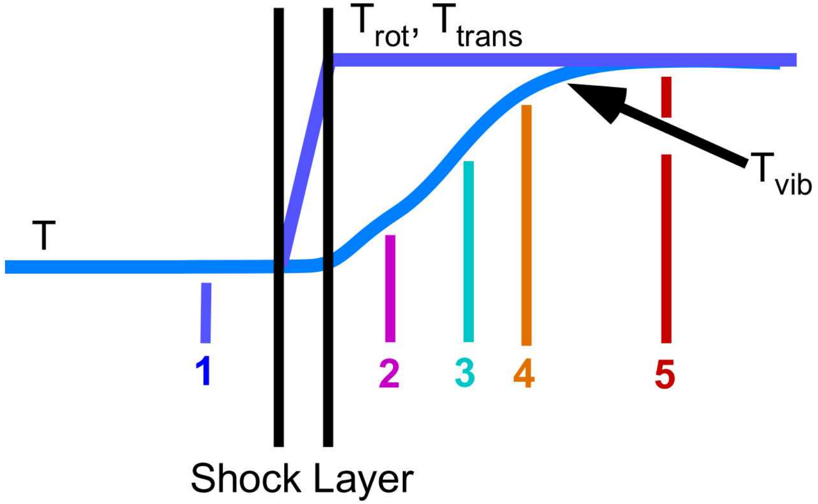
Table 2 Reaction rate coefficients for air (present model)

Reaction	M	T_x[a]	C	N	T_d	Source
Dissociation reactions						
$N_2 + M \rightarrow N + N + M$	N	T_a	3.0^{22}	−1.60	113,200	Ref. 14
	O		3.0^{22}			
	N_2		7.0^{21}			
	O_2		7.0^{21}			
	NO		7.0^{21}			
	N^+		3.0^{22}			
	O^+		3.0^{22}			
	N_2^+		7.0^{21}			
	O_2^+		7.0^{21}			
	NO^+		7.0^{21}			
	e^-		1.2^{25}			Ref. 9
$O_2 + M \rightarrow O + O + M$	N	T_a	[illegible]	[illegible]	[illegible]	[illegible]
	O		1.0^{22}			
	N_2		2.0^{21}			
	O_2		[illegible]			
	[illegible]		[illegible]			
	N^+		[illegible]			
	O^+		1.0^{22}			
	[illegible]		2.0^{21}			
	[illegible]		2.0^{21}			
	NO^+		[illegible]			
[illegible]	N	[illegible]	[illegible]	0.00	75,500	[illegible] 14
	O		1.1^{17}			
	[illegible]		5.0^{15}			
	[illegible]		[illegible]			
	[illegible]		[illegible]			
	N^+		[illegible]			
	O^+		1.1^{17}			
	[illegible]		[illegible]			
	[illegible]		5.0^{15}			
	[illegible]		5.0^{15}			
NO Exchange reactions						
[illegible]		T	8.4^{12}	0.00	19,450	Ref. 14
[illegible]		T	6.4^{17}	−1.00	38,400	Ref. 14
Associative ionization reactions						
[illegible] $\rightarrow NO^+ + e^-$		T	8.8^{8}	1.00	31,900	This work
[illegible] $+ O \rightarrow O_2^+ + e^-$		T	7.1^{2}	2.70	80,600	This work
$N + N \rightarrow N_2^+ + e^-$		T	4.4^{7}	1.50	67,500	This work
Charge exchange reactions						
$NO^+ + O \rightarrow N^+ + O_2$		T	1.0^{12}	0.50	77,200	Ref. 14
$N^+ + N_2 \rightarrow N_2^+ + N$		T	1.0^{12}	0.50	12,200	Ref. 14
$O_2^+ + N \rightarrow N^+ + O_2$		T	8.7^{13}	0.14	28,600	Ref. 14
$O^+ + NO \rightarrow N^+ + O_2$		T	1.4^{5}	1.90	26,600	Ref. 14
$O_2^+ + N_2 \rightarrow N_2^+ + O_2$		T	9.9^{12}	0.00	40,700	Ref. 14
$O_2^+ + O \rightarrow O^+ + O_2$		T	4.0^{12}	−0.09	18,000	Ref. 14
$NO^+ + N \rightarrow O^+ + N_2$		T	3.4^{13}	−1.08	12,800	Ref. 14
$NO^+ + O_2 \rightarrow O_2^+ + NO$		T	2.4^{13}	0.41	32,600	Ref. 14
$NO^+ + O \rightarrow O_2^+ + N$		T	7.2^{12}	0.29	48,600	Ref. 14
$O^+ + N_2 \rightarrow N_2^+ + O$		T	9.1^{11}	0.36	22,800	Ref. 14
$NO^+ + N \rightarrow N_2^+ + O$		T	7.2^{13}	0.00	35,500	Ref. 14

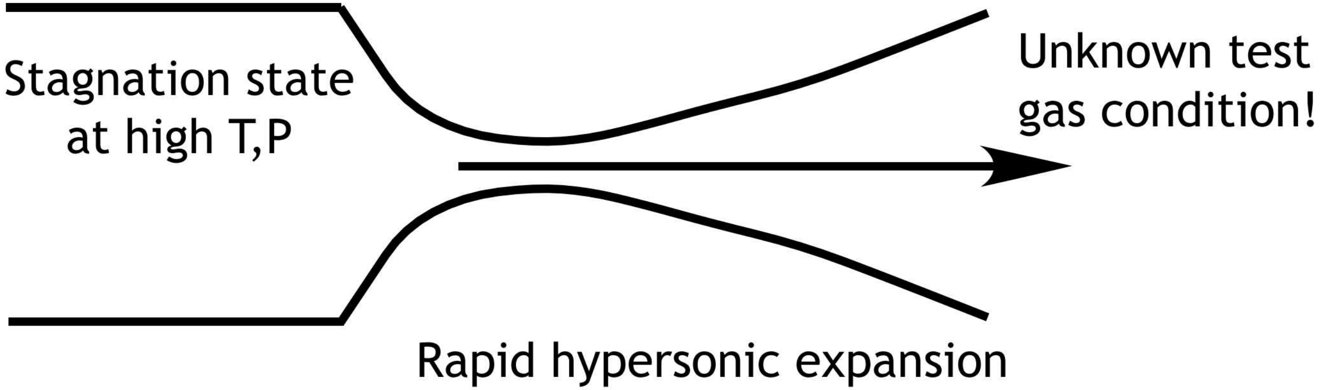
Direct measurements of key reacting species are critical N_2, O_2, NO, O, N…

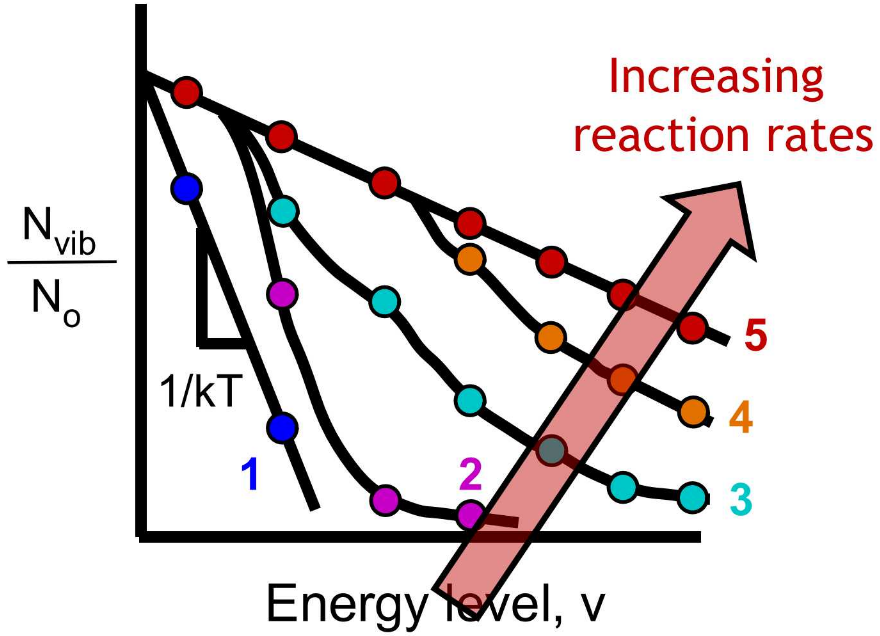
Importance of nonequilibrium conditions

- Chemical mechanisms are valid “near equilibrium”
- Reaction rates are modified using ***thermodynamic distributions*** which are frequently assumed
- Vibrational excitation has significant impact on rates
- Internal ⟷ translational energy exchange affects flow processes like transition to turbulence



Nonequilibrium conditions can be significant in ground-test facilities





Sandia validation paradigm for hypersonic reacting flow

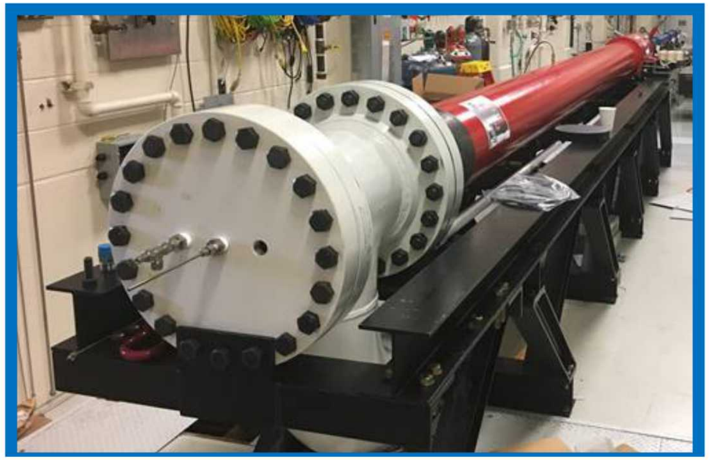
- Co-location and integration
  - modeling
  - high-enthalpy test facilities
  - diagnostics

- High-speed diagnostic development
  - Temperatures & distribution functions
  - Quantitative reacting species data

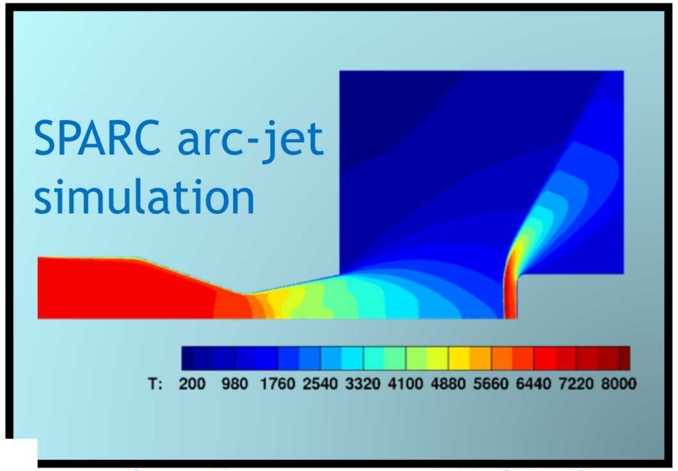
- Shift hypersonic validation paradigm
  - Reduce compensating errors
  - Extrapolate models to real flight conditions

- Detailed validation facility characterization with quantifiable uncertainties

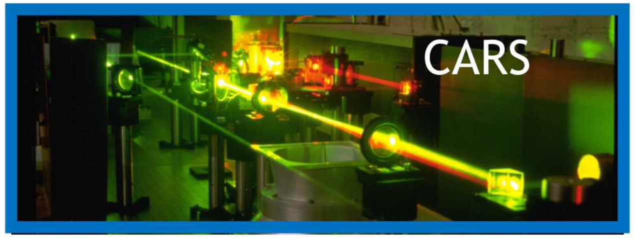
- Capability demonstration
  - Canonical normal shock (SPARTA DSMC)
  - 'Capstone' high-enthalpy experiment (SPARC)

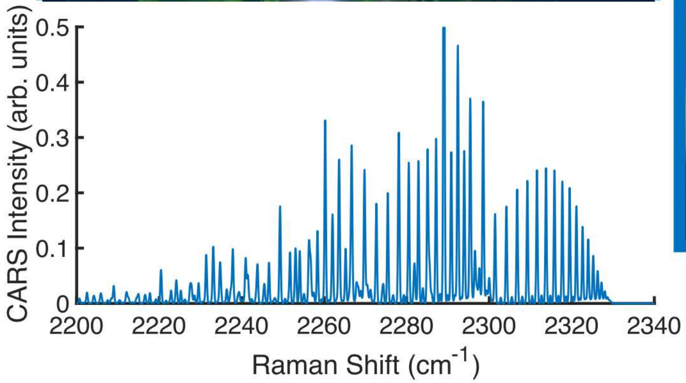


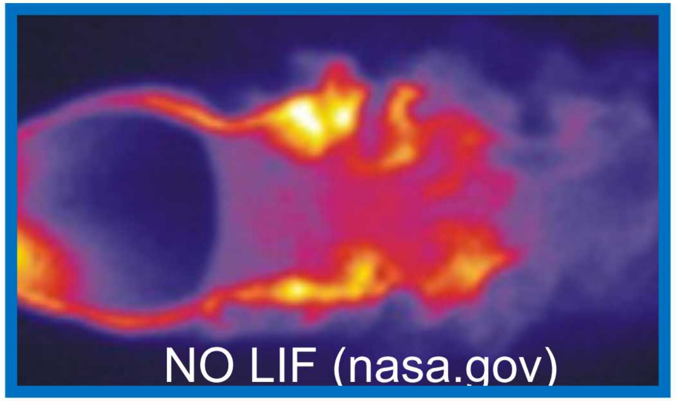
High-enthalpy ground-test facilities



Continuum and DSMC modeling on large-scale compute platforms







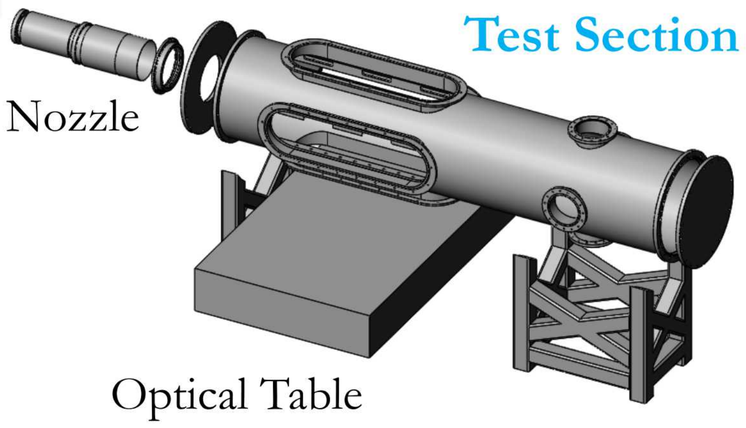
Advanced diagnostic methods

Sandia's Free-Piston High-Temperature Shock Tube (HST)

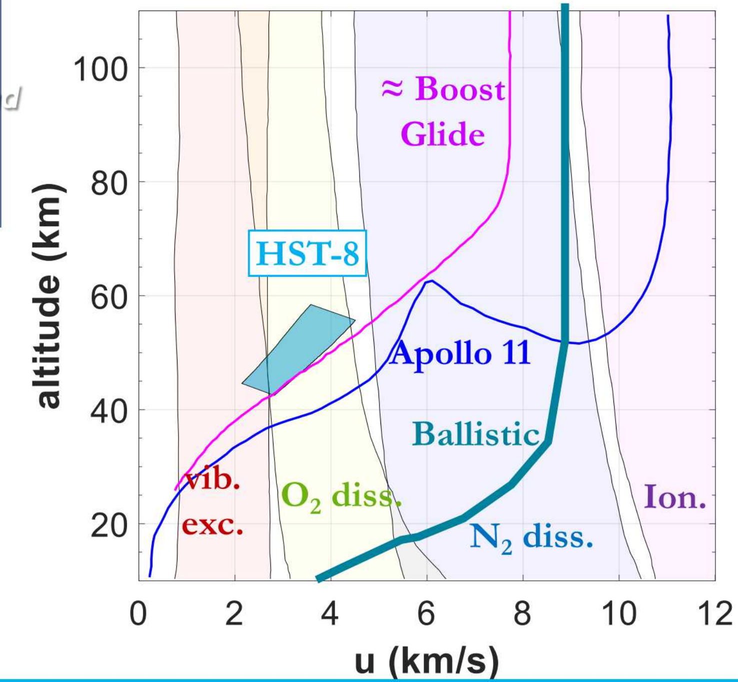
Design shock tunnel for hypersonic, *reacting* flight environments

HST becomes 2nd free-piston tube to ever fire in the U.S.

Commission Shock Tunnel



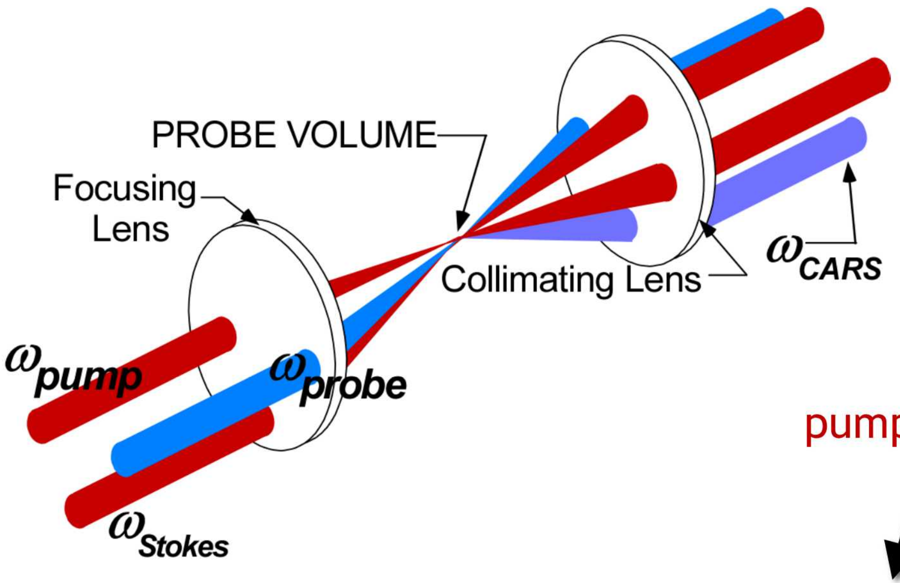
Estimated Operating Map



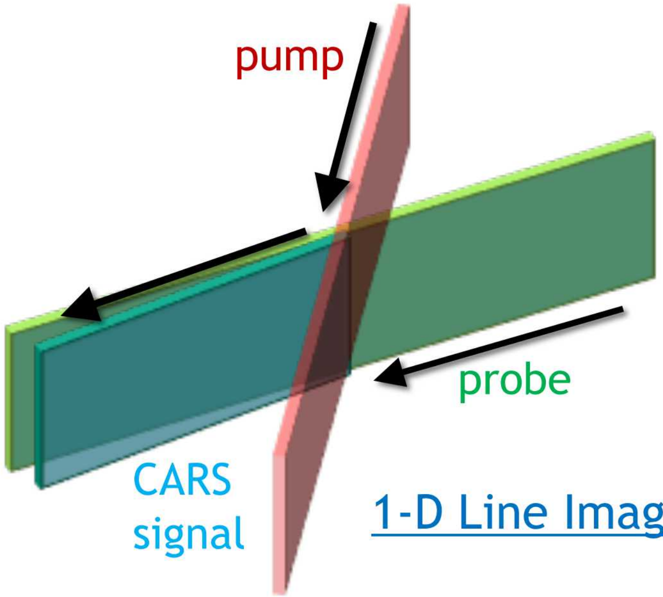
- Freestream Mach number of 8 and velocities > 4 km/s
- Enthalpies of order 10 MJ/kg and stagnation temperatures ≈ 6000 K
- Conditions are in regions of significant thermodynamic and chemical non-equilibrium

Coherent anti-Stokes Raman scattering (CARS)

- Powerful laser spectroscopic tool
  - Major species (N_2, O_2)
  - Temperature
  - Nonequilbrium states (T_{rot}, T_{vib})
  - **Distribution functions**



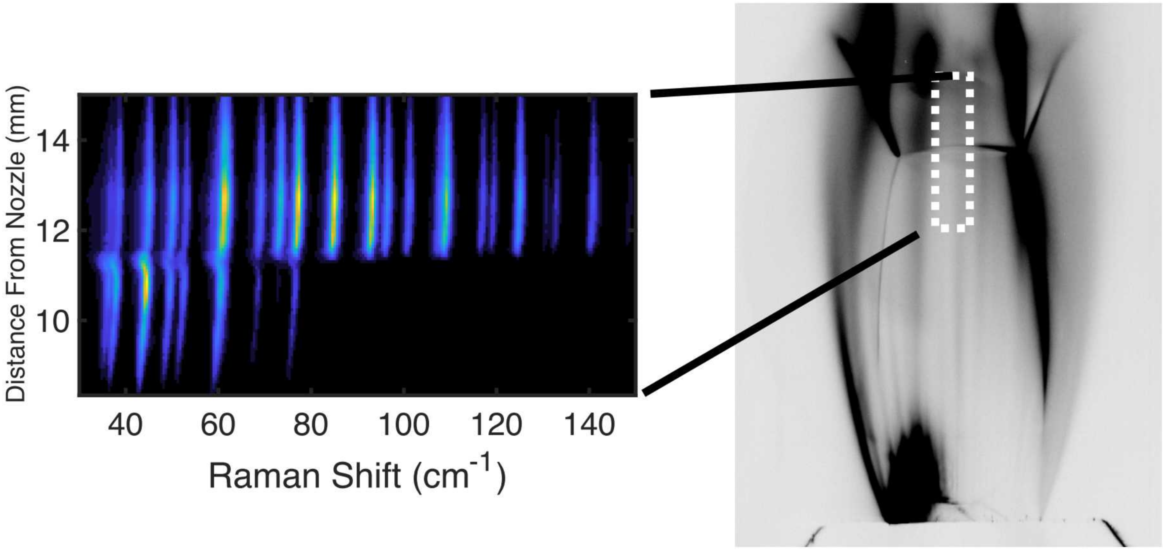
Point Measurements



1-D Line Imaging

Coherent anti-Stokes Raman scattering (CARS)

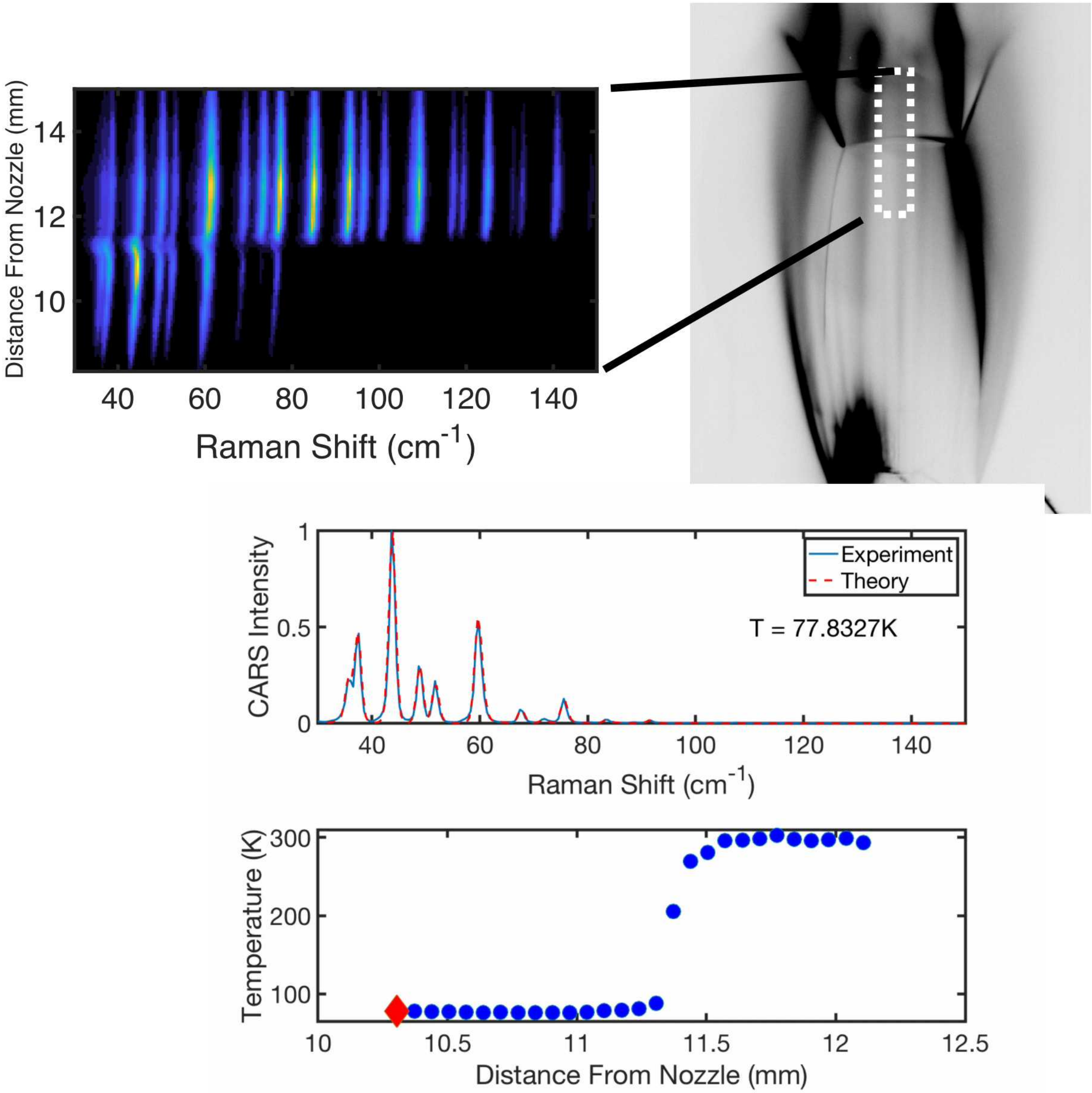
- Powerful laser spectroscopic tool
  - Major species (N_2, O_2)
  - Temperature
  - Nonequilbrium states (T_{rot}, T_{vib})
  - **Distribution functions**



1-D CARS imaging across a Mach-4 shock

Coherent anti-Stokes Raman scattering (CARS)

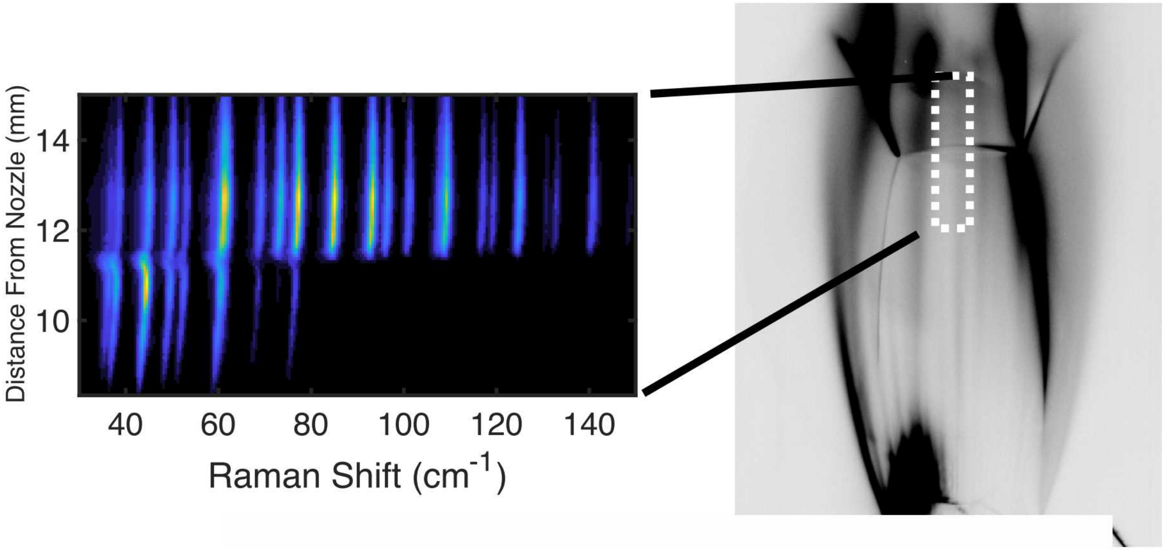
- Powerful laser spectroscopic tool
  - Major species (N_2, O_2)
  - Temperature
  - Nonequilbrium states (T_{rot}, T_{vib})
  - **<u>Distribution functions</u>**



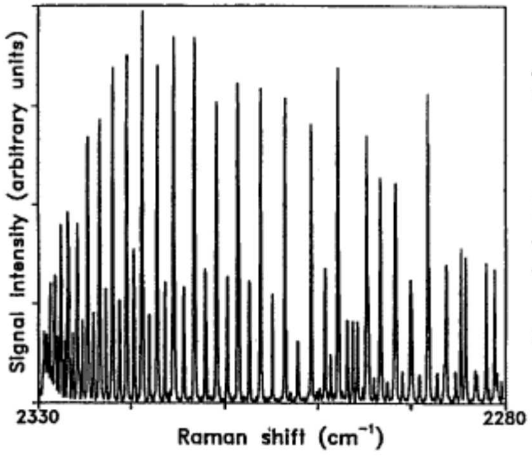
1-D CARS imaging across a Mach-4 shock

Coherent anti-Stokes Raman scattering (CARS)

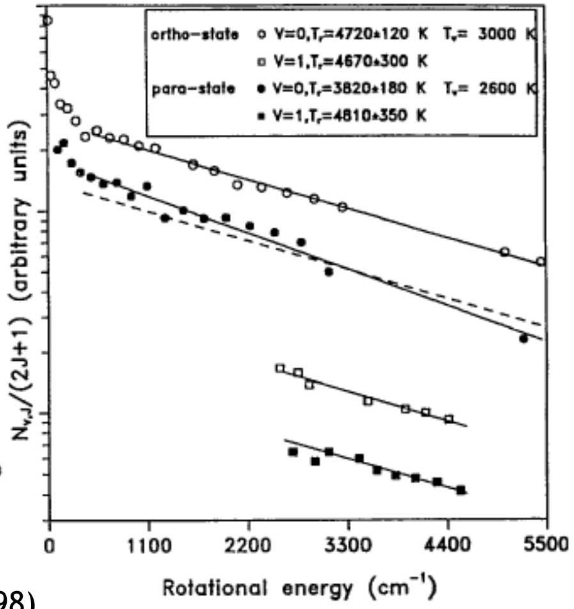
- Powerful laser spectroscopic tool
  - Major species (N_2, O_2)
  - Temperature
  - Nonequilbrium states (T_{rot}, T_{vib})
  - **Distribution functions**



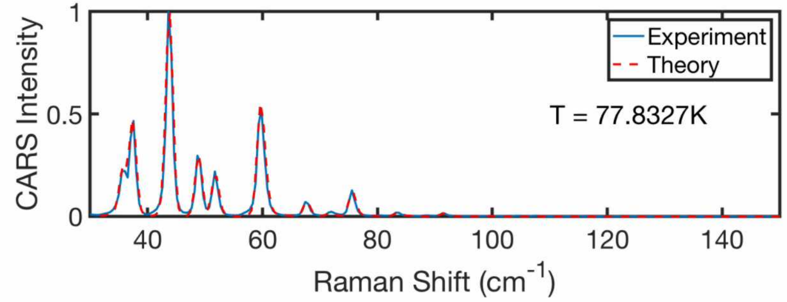
CARS measurements in nonequilibrium shock layer

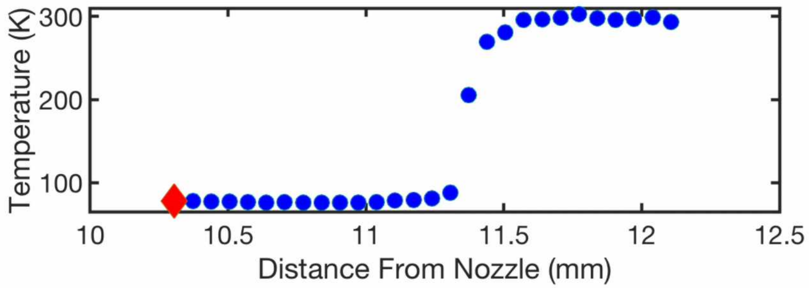


nitrogen CARS spectrum



Bonnet *et al., Ann. Rev. Fluid Mech.* (1998)



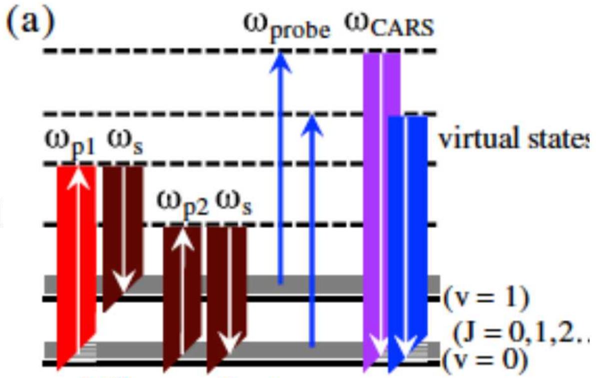


1-D CARS imaging across a Mach-4 shock

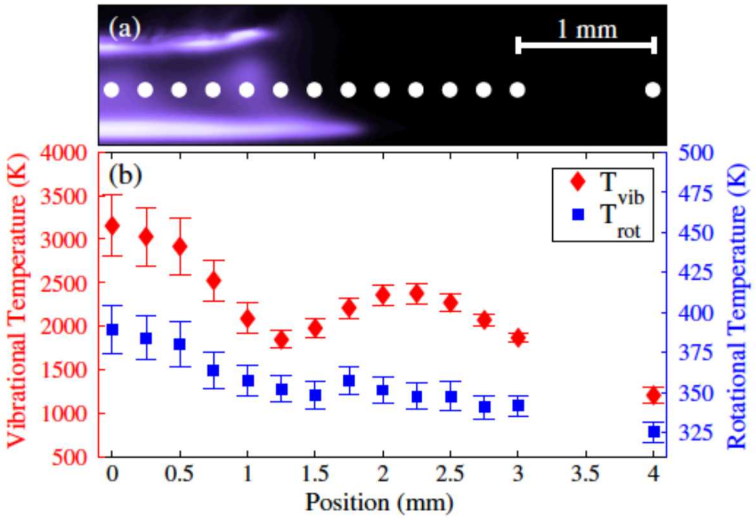
CARS Measurements in a nonequilibrium plasma

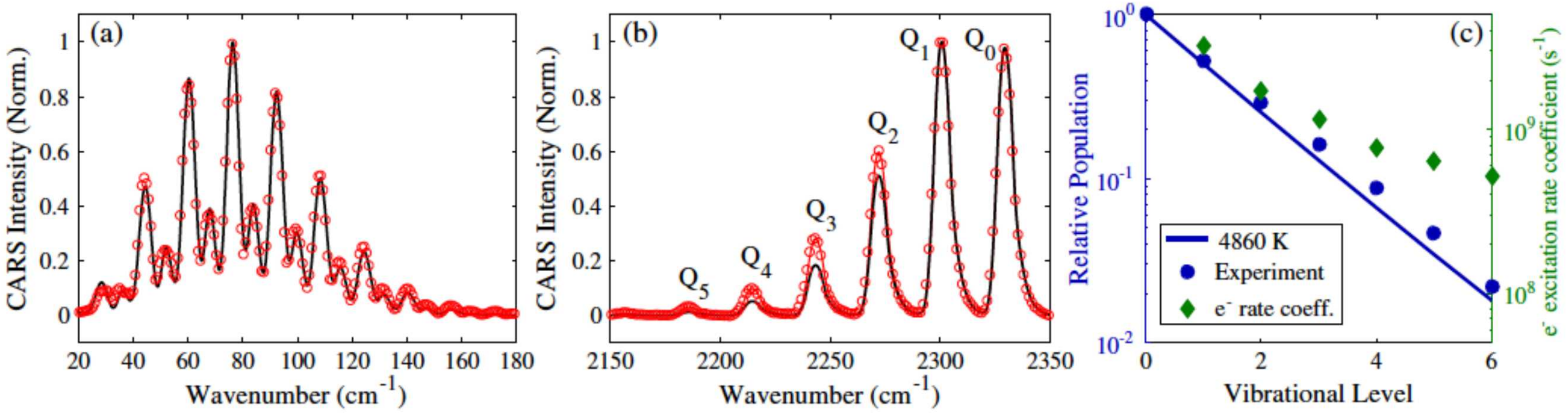
Dedic, Meyer, and Michael, "Single-shot ultrafast coherent anti-Stokes Raman scattering of vibrational/rotational nonequilibrium," *Optica* **4**, 563-569 (2017).

- Simultaneous pure-rotational and vibrational Raman spectra
- Direct measurement of distribution functions
- Signal scales with $N_{v,J}^2$
- Single-shot detection limits?

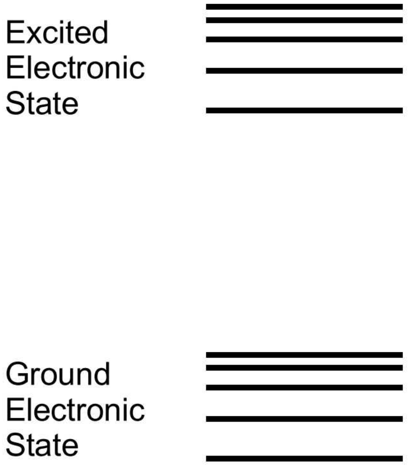


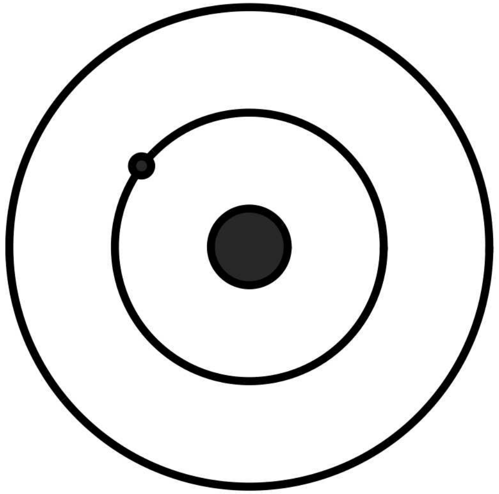
Vib. CARS pair Rot CARS pair





High-speed diagnostics II: LIF





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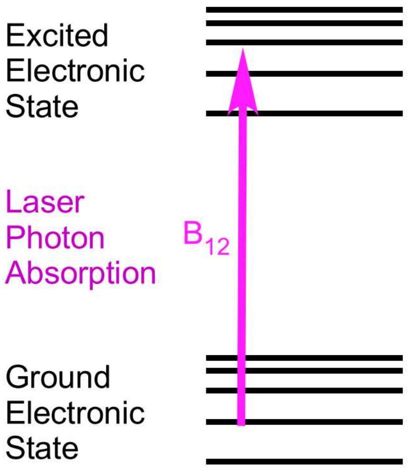

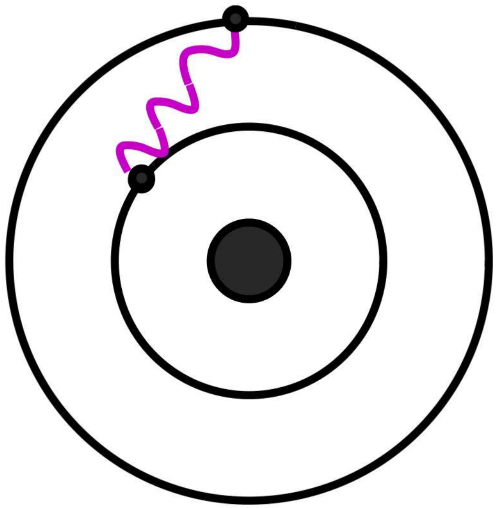

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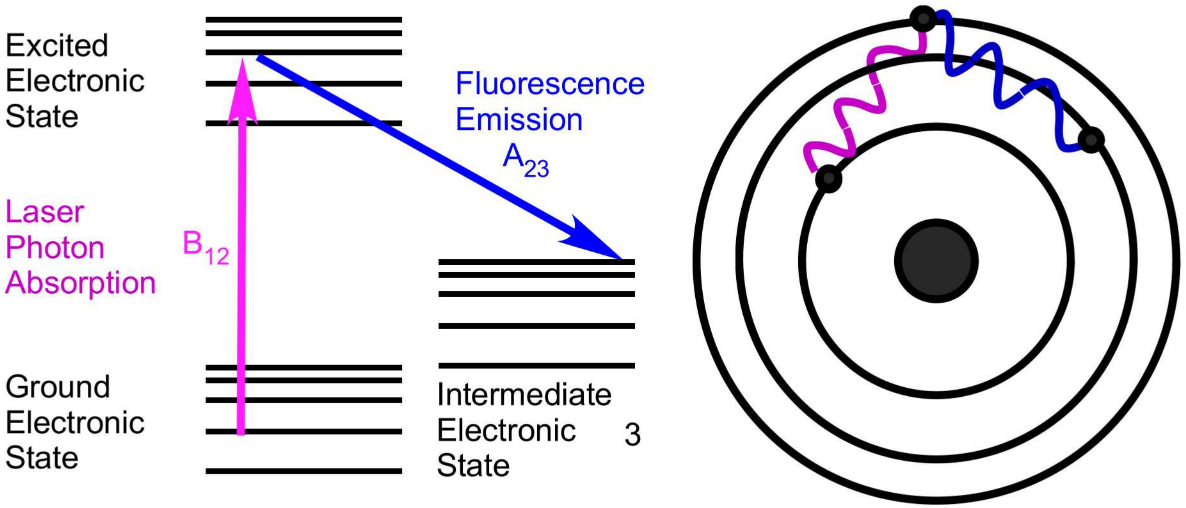

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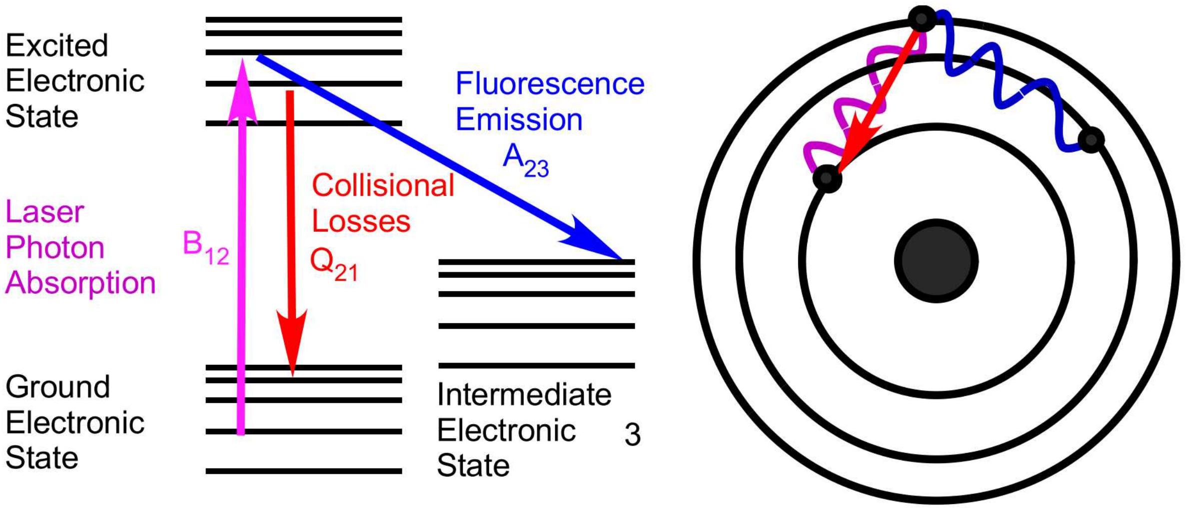

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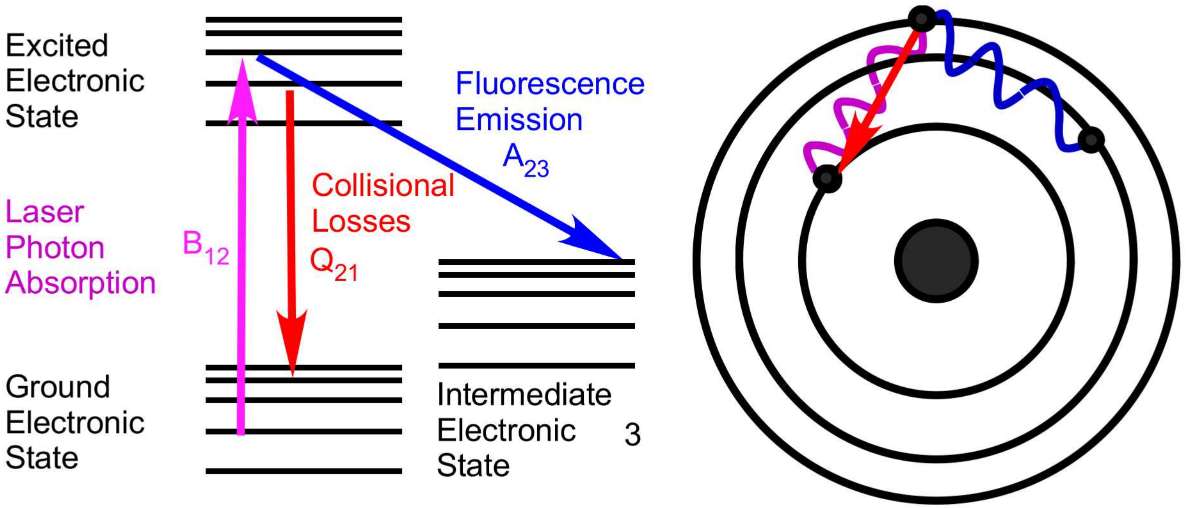
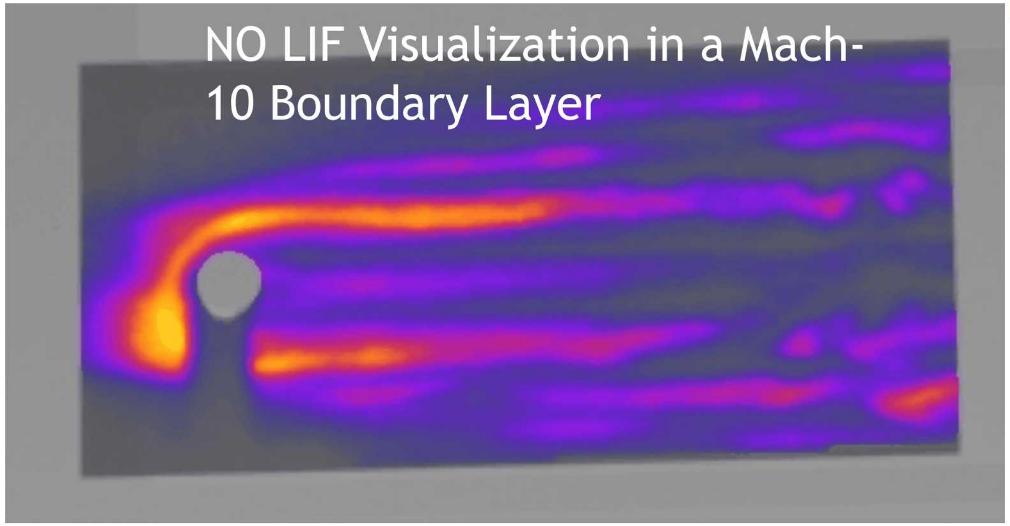
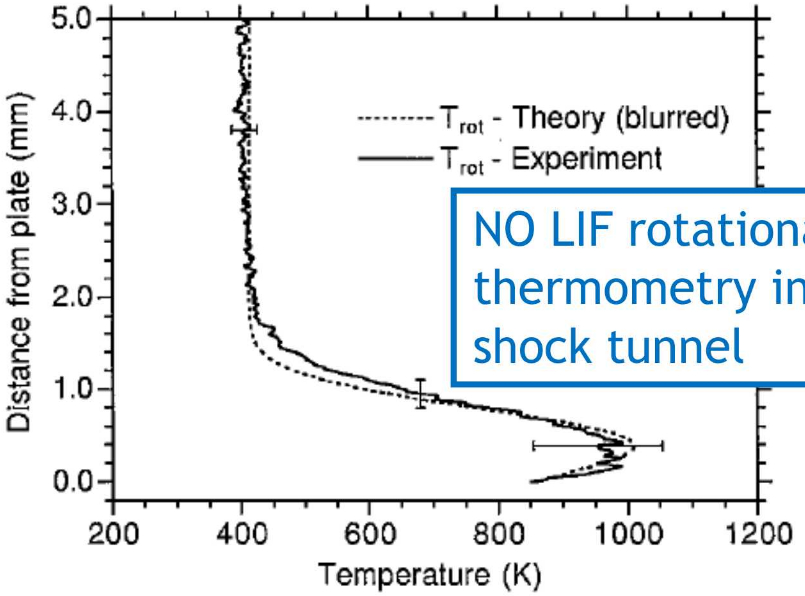


- Quantitative species measurements with knowledge of Q_{21}
- NO, O, N have all been demonstrated
- Successful single-shot applications in shock tunnels
- 2D or 1D line imaging capability
- Temperature imaging in NO also possible (risk mitigation)



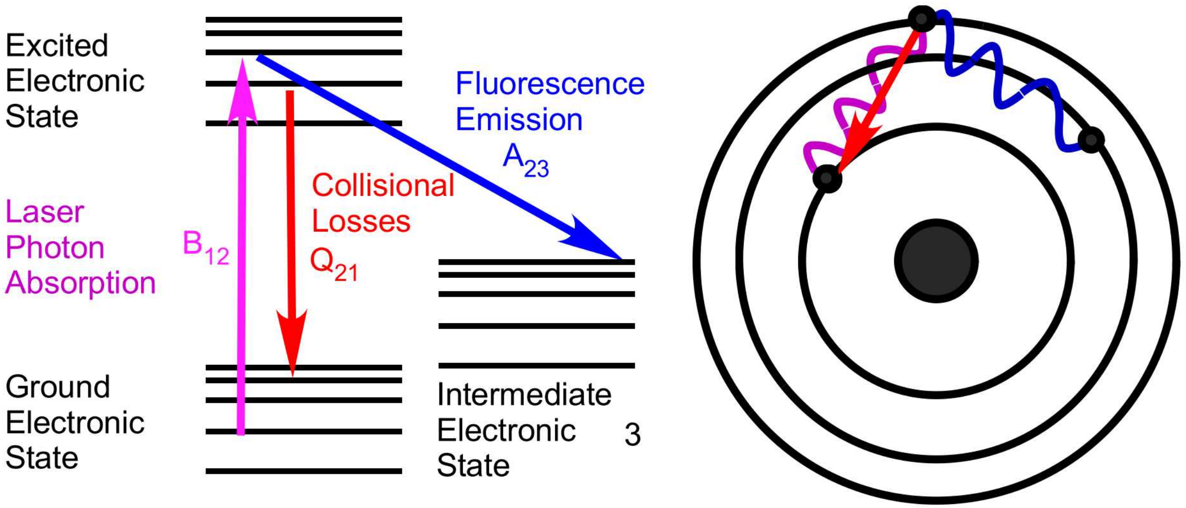
P.M. Danehy, NASA Langley Research Center



NO LIF rotational thermometry in a free-piston shock tunnel

Palma *et al.*, *AIAA J.* (1999)

High-speed diagnostics II: LIF



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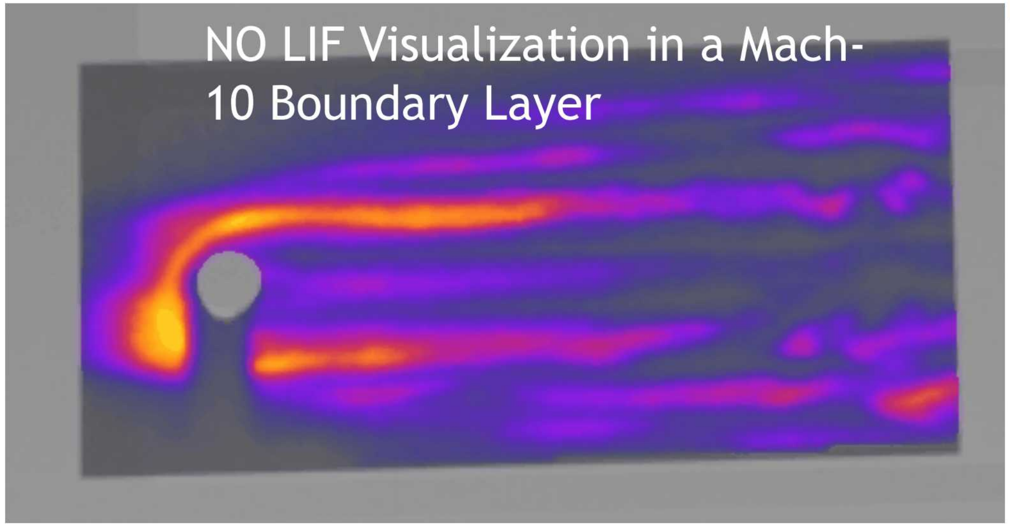

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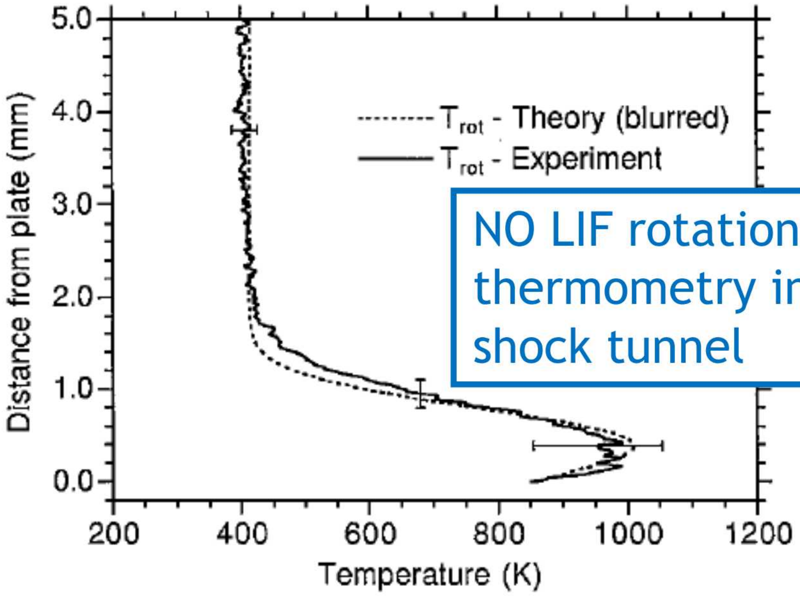

NO LIF rotational thermometry in a free-piston shock tunnel

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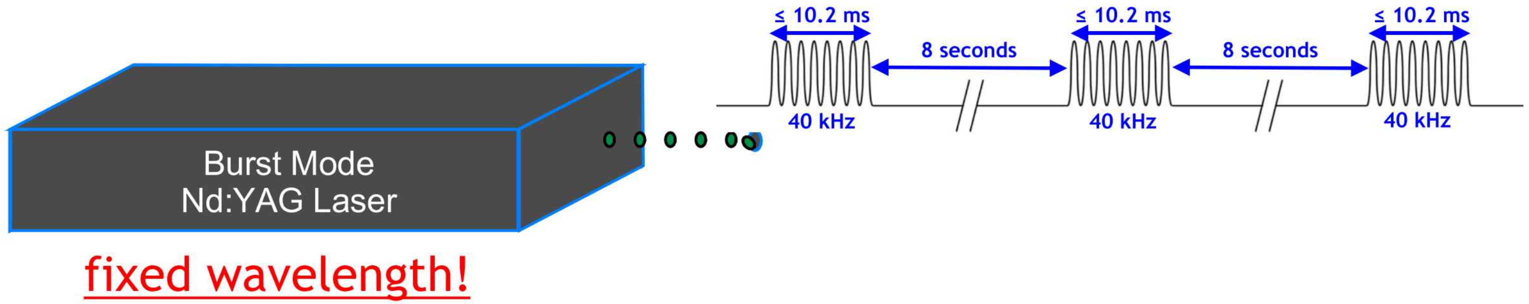
Tunable burst-mode laser development

- Burst-mode lasers have allowed experimentalists to access high-speeds (10s to 100s of kHz)
- While powerful, these systems are not wavelength tunable—this prohibits application of ***chemically specific*** imaging and spectroscopic tools



Our solution: Tunable burst-mode laser development

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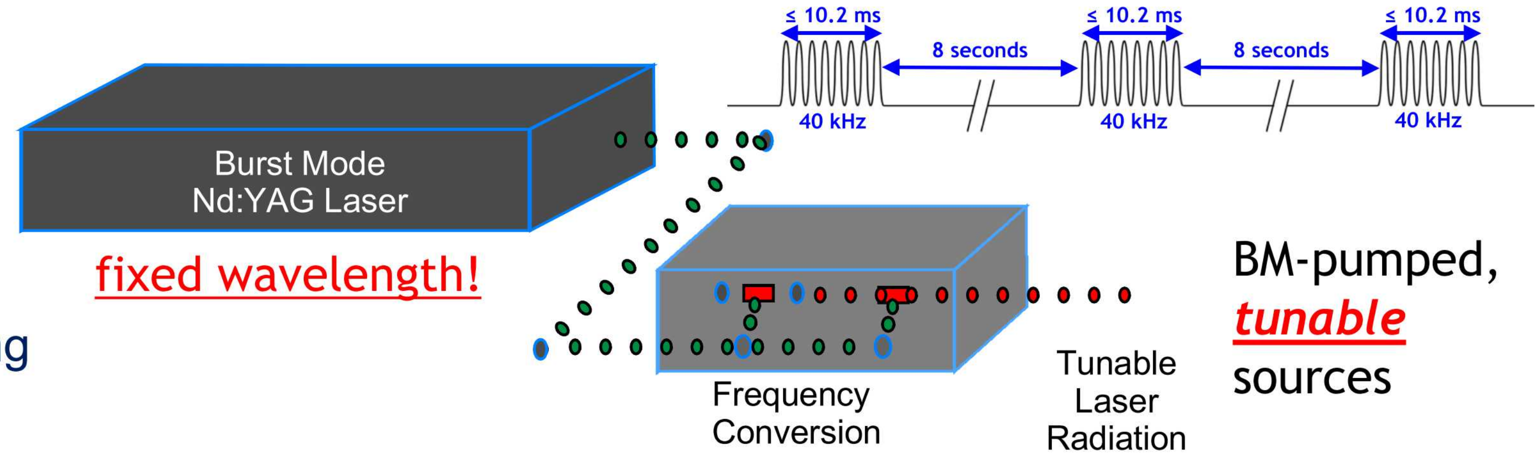


BM-pumped, ***tunable*** sources

Dye Laser Technology

- ✓ Liquid dye gain medium
- ✓ Excellent broadband performance (CARS)
- ✓ Flexible, tunable, simple to align and maintain
- ✓ Two recent demonstrations for burst-mode LIF
- ✖ More susceptible to optical damage
- ✖ Dye saturation "bleaching" and thermal degradation

Optical Parametric Oscillator (OPO)

- ✓ All solid-state design
- ✓ Multiple demonstrations for burst-mode LIF (NO, OH)
- ✓ Singe demonstration (ps) for burst-mode CARS on H_2
- ✖ Difficult to maintain and align
- ✖ Decreased flexibility

Tunable Sources: Risk Mitigation

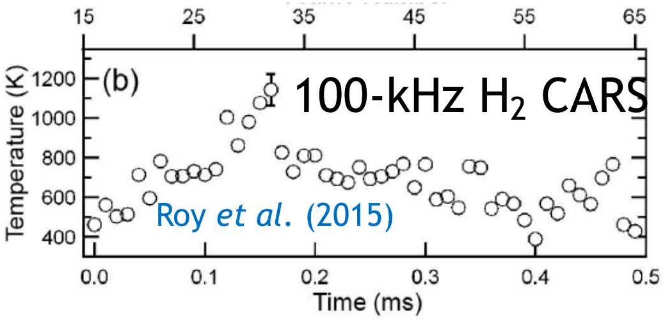
Technical Risk

NO LIF — **O-atom LIF** — **CARS**

Multiple Risk-Mitigation Pathways

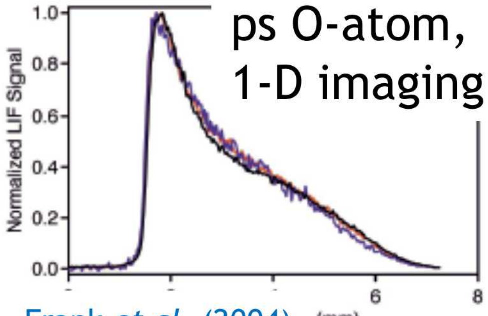
Solid-State OPO Technology

- Proven for NO, OH LIF
- Demonstrated (ps) for CARS
- Not demonstrated for atomic LIF



Picosecond Burst-Mode Pulses

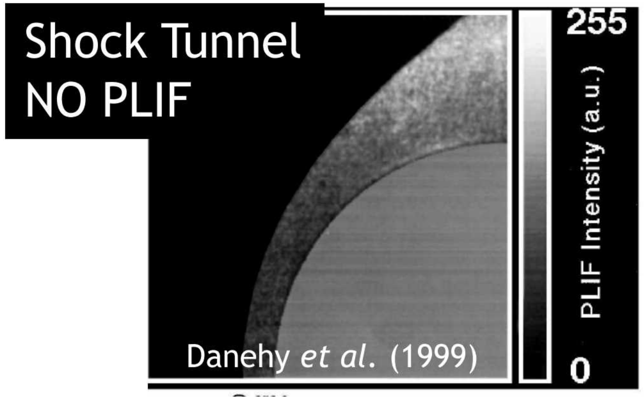
- More effective for 2-photon schemes (O-atom, CARS)
- Single demonstration for H_2 CARS in flames



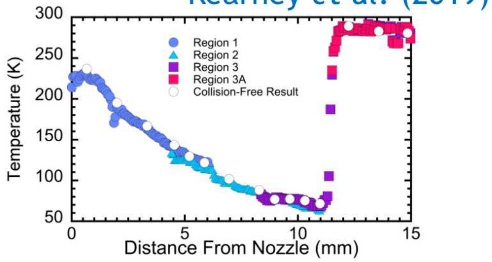
Frank *et al.* (2004)

2-D and 1-D Imaging at Reduced Rates

- High single-shot data yields
- Previous shock-tunnel LIF
- Single-shot or reduced burst-rate pump



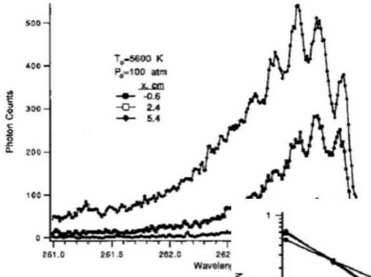
Kearney *et al.* (2019)



1-D CARS thermometry across a shock layer

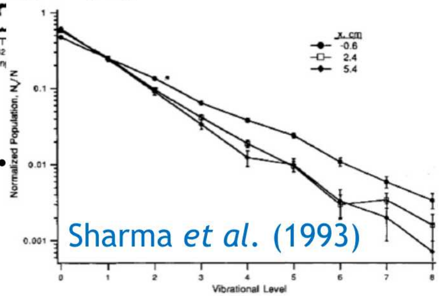
Alternative Diagnostics

- Diode laser absorption
- Spontaneous Raman scattering



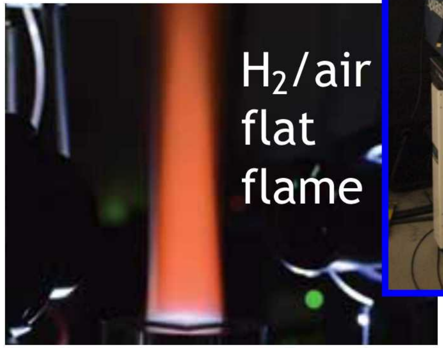
Raman Spectra
T = 5600 K

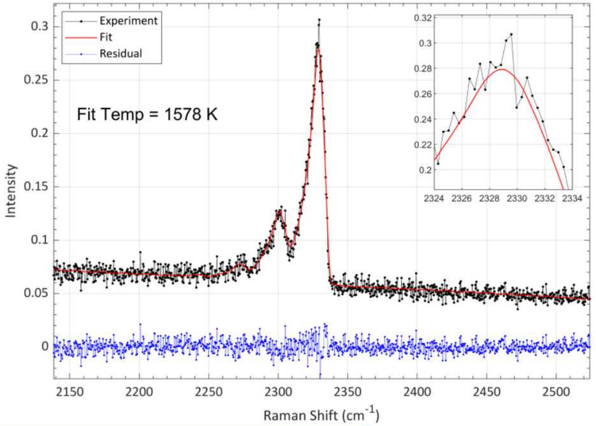
Vib. Dist. Function

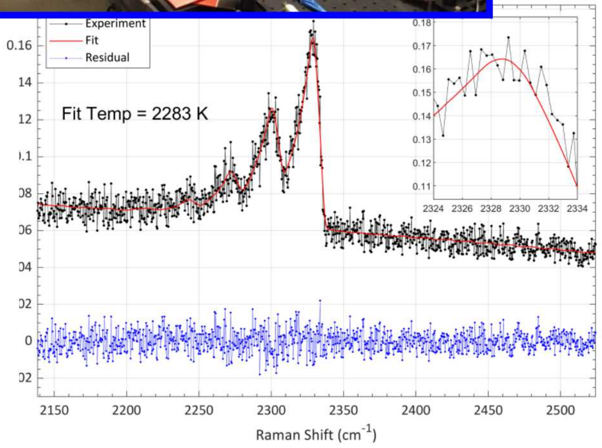


Pulse-Burst Raman Spectra: Early Results at 5 kHz

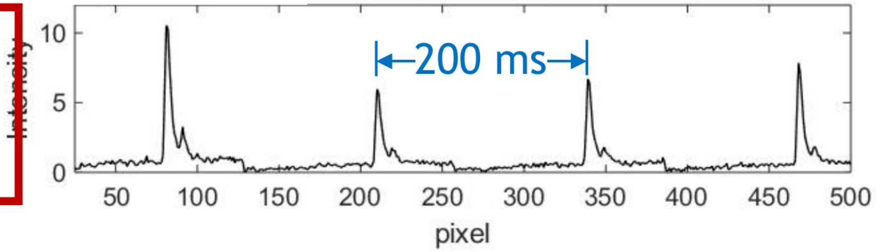
- Raman spectra at data rates
- Goal is 10-20 kHz for free-piston facility at high densities
- No tunable source required
- Spectra obtained at 5 kHz in near-adiabatic H_2/air flame
- Spontaneous Raman signals are orders of magnitude less than CARS
- Signal scales directly with $N_{v,J}$



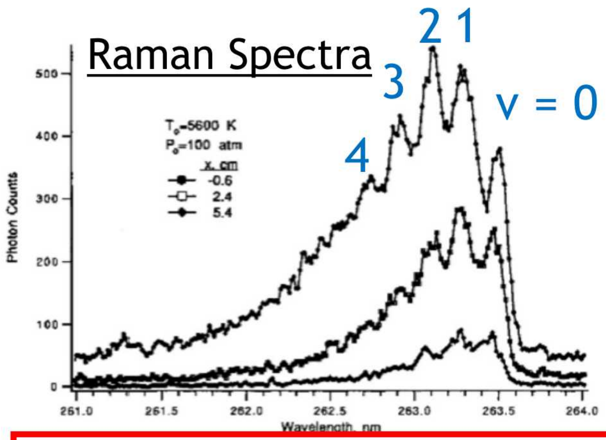


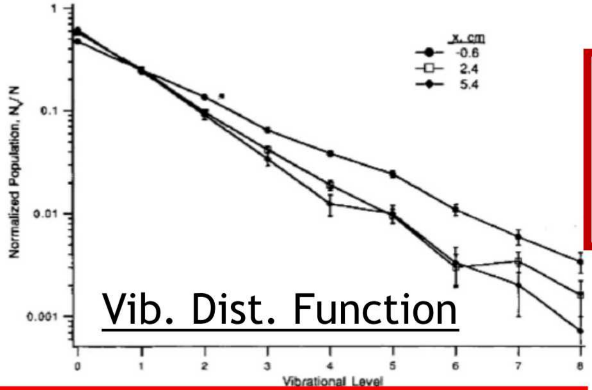


5-kHz Spectral Acquisition



with C. Winters, P. Varghese, and T. Haller





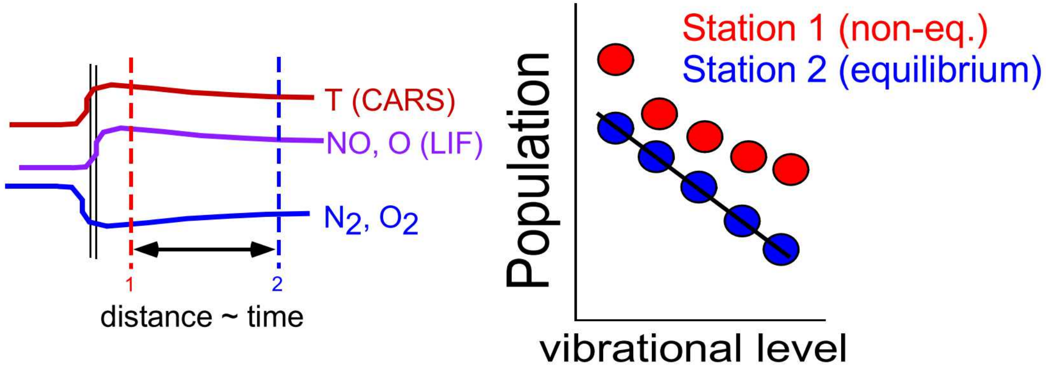
Raman measurements in NASA EAST nozzle expansion

Sharma *et al.*, *J. Thermophysics Heat Transfer* **7** (1993)

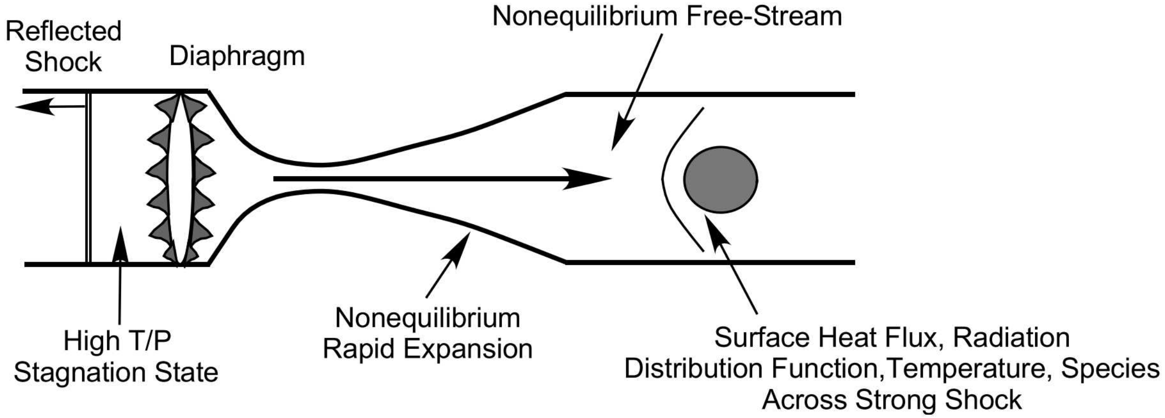
This 3-year LDRD will demonstrate quantifiable validation capabilities

Target Canonical Experiments

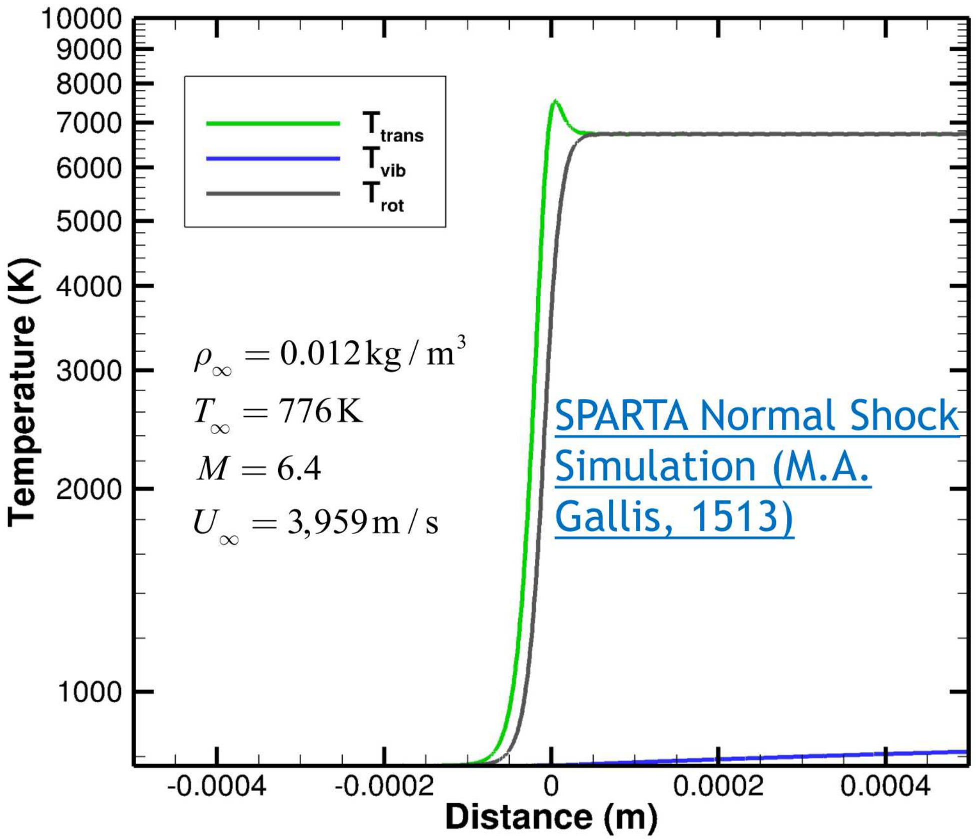
1. Canonical normal-shock experiment (SPARTA/DSMC)



2. 'Capstone' validation demonstration (SIERRA/SPARC)

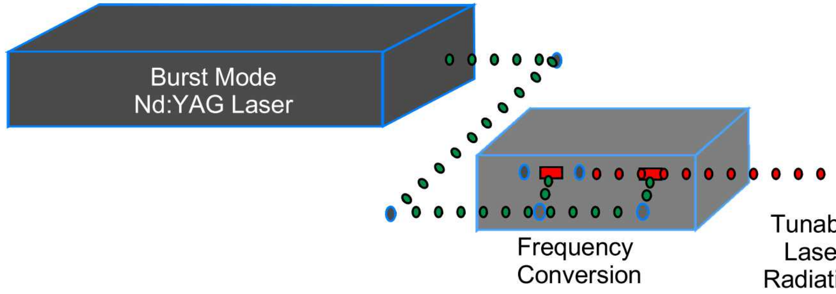


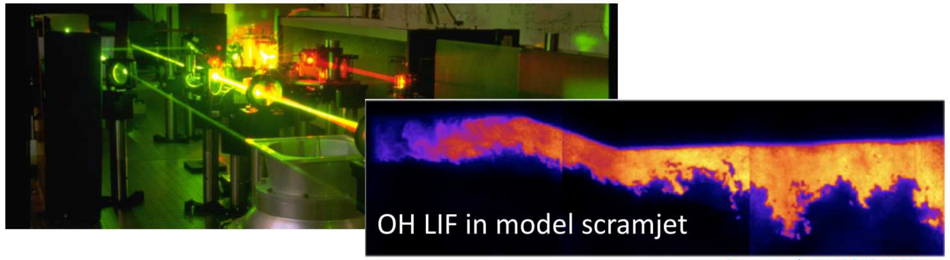
Utilize Sandia SPARTA and SPARC codes to guide experiment design



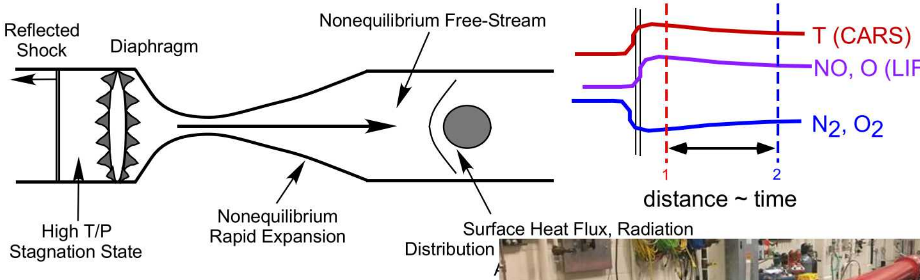
Project plan: Milestones and Objectives

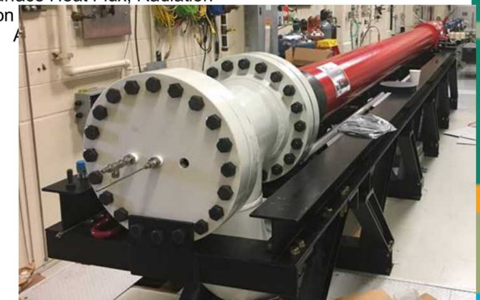
Objectives (O) and Milestones (M)		FY20	FY21	FY22
O1	**Development of flexible and tunable burst-mode sources**			
M1.1	Frequency-narrow dye laser at 30-50 kHz (LIF)			
M1.2	Broadband dye laser (CARS) at 30-50 kHz (CARS)			
M1.3	Risk mitigation option: optical parametric oscillator (OPO) development			
O2	**Integration of tunable burst-mode sources into high-speed CARS and LIF instruments**			
M2.1	N_2 CARS thermometry in lab-scale flame			
M2.2	LIF imaging in lab-scale flame			
M2.3	Assessment of collisional loss rates for quantitative LIF			
M2.4	Risk mitigation option: diode-laser, spont. Raman, e-beam diagnostics			
O3	**Diagnostic insertion into high-temperature shock-tunnel: coupling of models and experiment**			
M3.1	SPARTA DSMC simulations for normal-shock experiment design			
M3.2	Canonical normal shock experiment			
M3.3	Nonequilibrium distribution function: code-to-experiment comparison			
M3.4	NO production/consumption: code-to-experiment comparison			
M3.5	Capstone validation capability experiments			
M3.6	SPARC simulations of Capstone experiments			





Cantu *et al.* AIAA2016-1763





Sandia/U. Texas plasma torch collaboration (w/ P. Varghese)

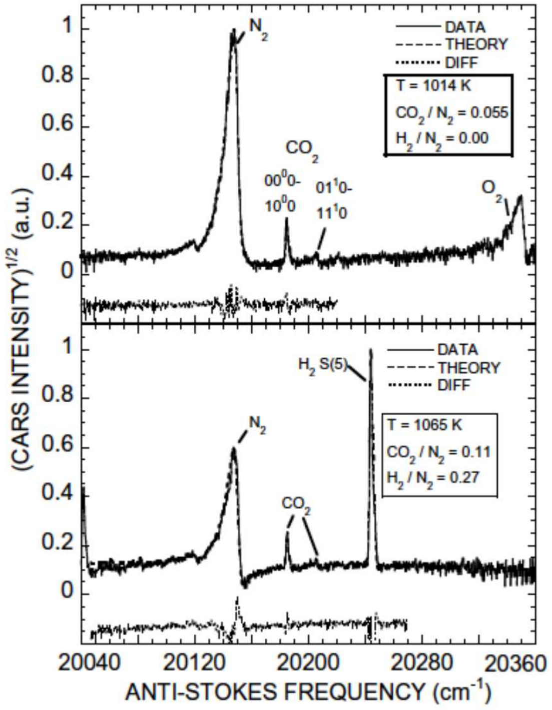
(1) Task 1: Use *existing* high-TRL Sandia experimental tools and UT-Austin plasma-torch facility to provide ablation-relevant high-temperature chemistry data for *short-term results at reasonable cost.*

(2) Task 2: take mid-TRL diagnostic methods developed for Sandia "abnormal thermal" environments and adapt them for multi-species detection in hypersonics with reduced uncertainty

UT-Austin plasma torch facility provides high-enthalpy, high-temperature environment for TPS materials testing

Target measurements:

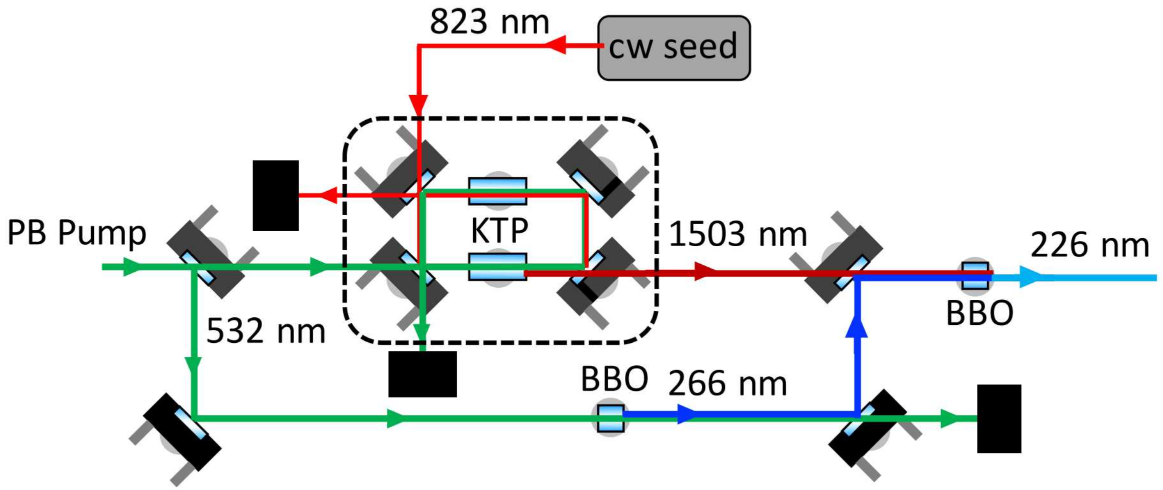
- T_r, T_v, species via ns-CARS (10 Hz)
- LIF detection of NO, atomic species
- Surface heat flux and ablation



Flexible High-Speed Optical Parametric Oscillator for Hypersonic Reacting Flow Diagnostics (Purdue AA, Slipchenko PI)

Plus-up to Proposal 20-0545

Ring cavity OPO



OPO design advances:
- Two times more efficient crystal
- Ring cavity simplifies seed coupling
- Better beam quality for mixing

Expected performance:
- Two times higher conversion efficiency
- 100 kHz operation

Mitigation of major proposal risks:
O1: aid Sandia with….
- Laser dye energy handling characterization
- Development of tunable narrowband ns OPO

O2:
- ps OPG/OPA output optimization
- Development of ns/ps quantitative NO and O atom LIF
- Development MHz-rate point fs/ps Hybrid rotational CARS

O3:
- Support Sandia measurement campaigns

Available capabilities at Purdue:
US student
BM laser
Narrowband dye laser
Broadband dye laser

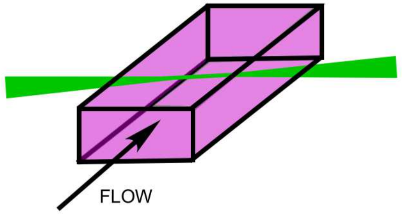
Tunable Source Development

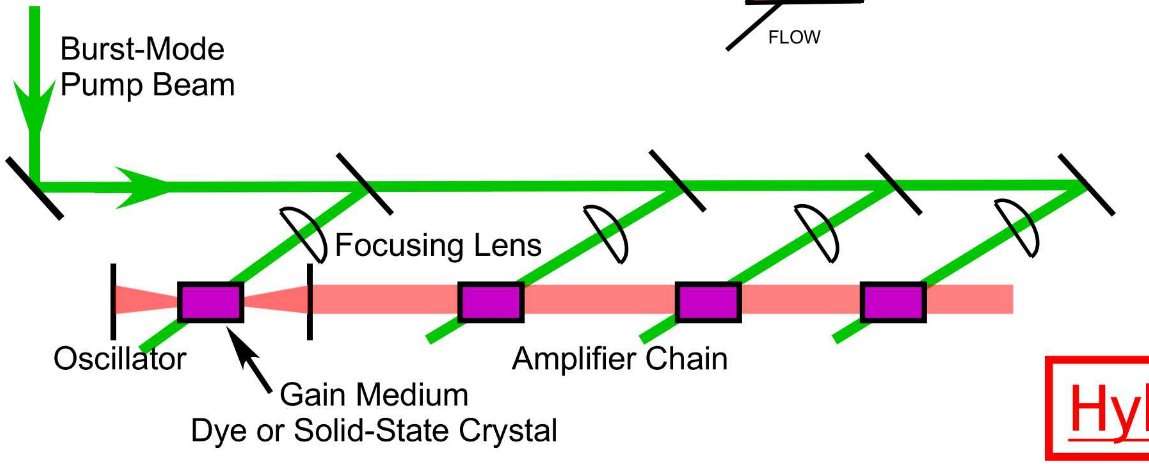
Burst-mode **dye lasers** are largely unproven technology

- ✖ Broadband dye lasers for CARS unproven
- ✓ Recent tech demonstrations promising for NO LIF at 20-30 kHz
- ✓ Commercial 10 kHz DPSS-pumped dye

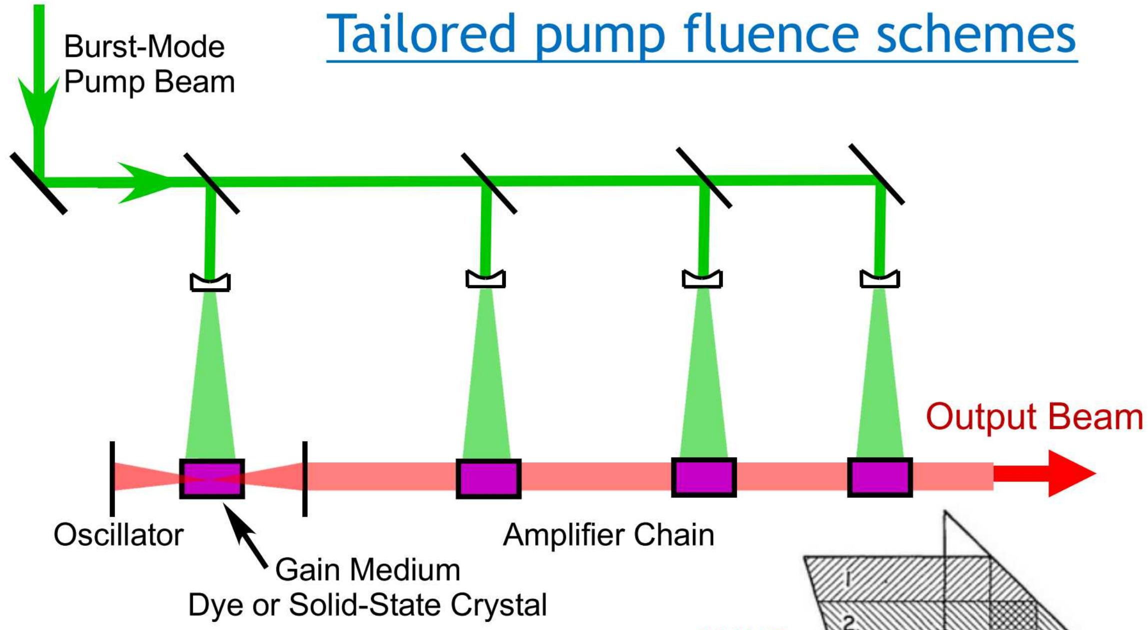
Focused pump fluence schemes

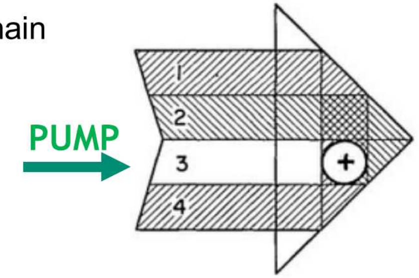
- High-speed dye pumps
- Tight pump focus
- Longitudinal pumping





Tailored pump fluence schemes





- mitigate dye saturation, heating, damage
- Staged pumping
- Multiple scalable amplifiers
- Bethune cells

Hybrid solid-state OPO/dye amplifier systems