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Measurement of Gas-Surface Accommodation in a Parallel-Plate Geometry

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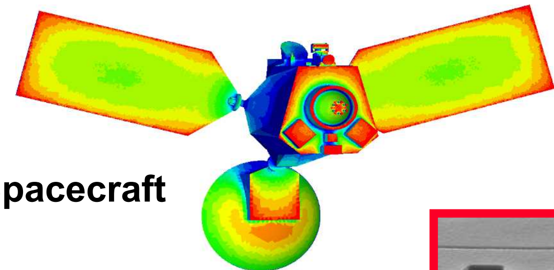
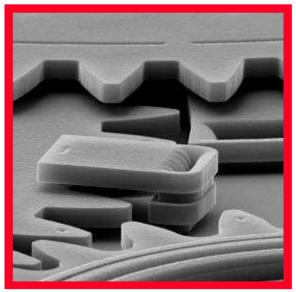
Presentation Outline

- Motivation and Background
- Experimental Capability and Data Analysis
  - Discuss DSMC-Based Analysis Methods
  - Review System Design and Important System Improvements
- Discussion of Experimental Results
- Comparison with DSMC Simulations
- Summary

Gas-Surface Interactions



Spacecraft



MEMS Devices

Problem

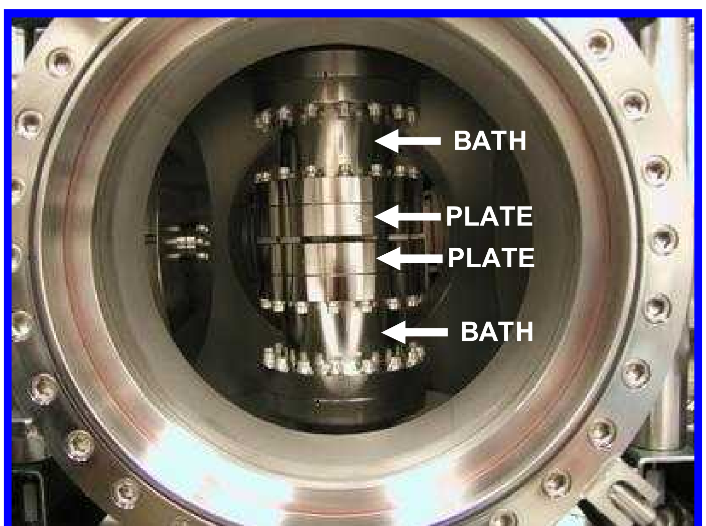
- No-slip, no-jump boundary models break down for rarefied or microscale flows
- Details of gas-surface interaction crucial

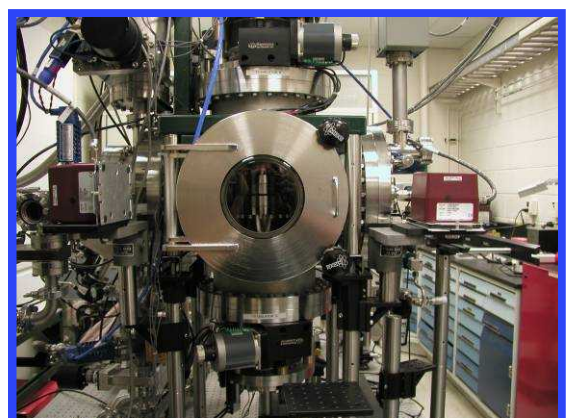
Applications

- Aerodynamic heating of spacecraft
- Heat management in MEMS devices
- DSMC *always* needs surface model

Technical Approach

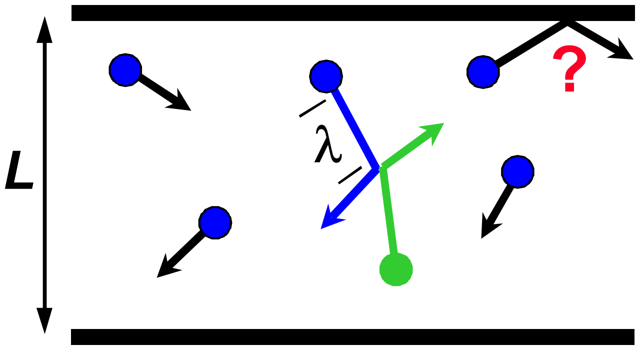
- Complex physics requires experiments
- Measure heat flux and gas density between parallel plates (*primary emphasis on heat flux measurements*)
- Infer gas-surface energy accommodation





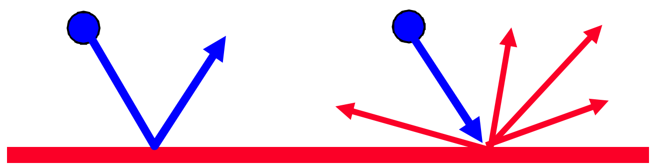
Thermal Accommodation Test Chamber

Noncontinuum Gas Behavior



Molecular and Wall Collisions

Specular reflection **Diffuse reflection**



Maxwell Wall Model

α	= diffuse fraction
$1 - \alpha$	= specular fraction

Continuum flow assumptions break down as mean free path approaches system length scale: $\lambda \sim L$

Noncontinuum flow encountered in widely different regimes

- **Low pressure, large scale (*spacecraft*)**
- **Ambient pressure, micro scale (*MEMS*)**

Gas-gas collisions *well* understood

Gas-surface collisions *not* understood

- **Simple *ad hoc* models (e.g., Maxwell, 1890)**
- **MD simulations limited to atomic scale - requires surface characterization**

DSMC Perspective

- **Probabilistic description of microscopic gas-surface interaction**
- **DSMC simulations with gas-surface model must reproduce *heat flux* data**

Surface Accommodation and Noncontinuum Heat Transfer

- **Accommodation depends on surface material, gas composition, gas pressure, surface roughness**
- **Maxwell model is successful in reproducing experimental data, allows for closed-form solutions to the Boltzmann Equation**
- **Maxwell model does not take into account internal degrees of freedom**
- **Liu and Lees (1961) approximate four-moment solution (with later extensions) reproduces noncontinuum heat transfer**
- **Teagan and Springer (1968) experiment measured accommodation coefficients but cannot be reproduced by solutions to the Boltzmann Equation (Ohwada, 1996)**
- **To resolve this, *precise heat transfer measurements* are needed**

Accommodation Coefficient Values in Literature Differ Widely

Consider one example from the compilation of Saxena and Joshi (1989):

Aluminum/Argon System

Author	Method	T (K)	P (Torr)	α
Faust, Jr. (1954)	Hot Wire	418-483	0.02	0.334-0.343
Mustacchi (1964)	Concentric-Cylinder (Al/Al)	500-800	0.005-0.1	0.75
Mustacchi (1964)	Concentric-Cylinder (Al/Uranium Carbide)	500-800	0.005-0.1	0.45
Teagan & Springer (1968)	Parallel-Plate	295	0.0026-5.0	0.795-0.832
Devienne (1965)	Molecular Beam	(500-3000 eV) ~energy of incident atoms	10^{-6}	0.38-0.45

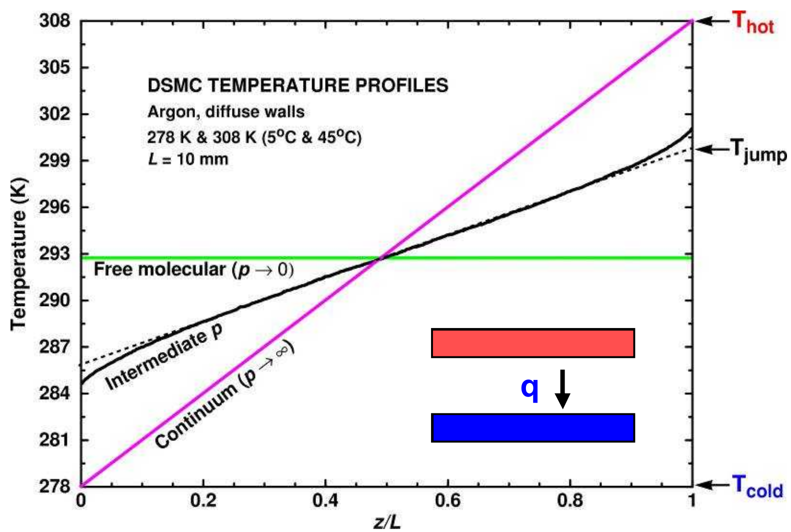
S. C. Saxena and R. K. Joshi, *Thermal Accommodation and Adsorption Coefficients of Gases*, (Hemisphere, New York, 1989)

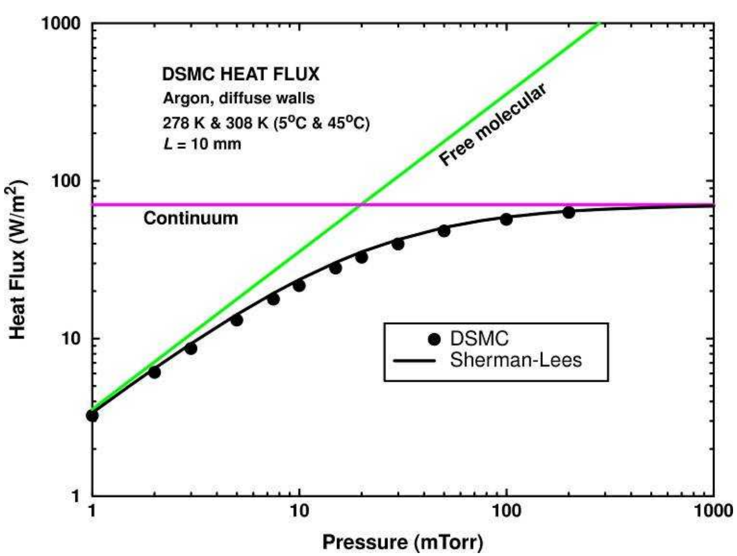
More recently…

Selden et al. (2009)	Radiometric Forces On Heated Vane	396-419	~ 10^{-4} – 10^{-2}	0.81

Results reflect a wide range of experimental methods and conditions
Many factors (e.g., surface purity) are not well characterized or specified

Noncontinuum Heat Flux





Molecular reflection at walls controls heat flux and temperature profile

- Near-wall Knudsen layers
- Temperature jumps at walls
- Pressure-dependent heat flux

Approach

- Perform precise experiments
- Parallel plates of unequal temperature maintained by temperature-controlled water bath
- Use measurement of heat flux vs. pressure to determine accommodation
- Infer heat flux by temperature drop measurement across each plate (both hot and cold)

Gas-Surface Combinations

- Gases (monatomic, diatomic, polyatomic, mixtures)
- Materials (stainless steel, gold, silicon, …)
- Surface finish (machined, polished, …)

Assess gas-surface models in DSMC

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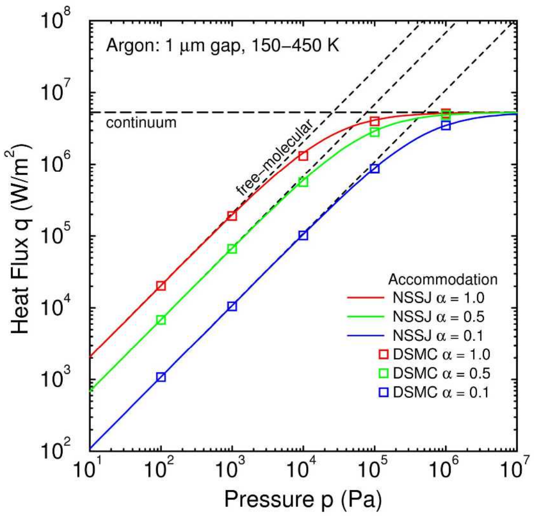
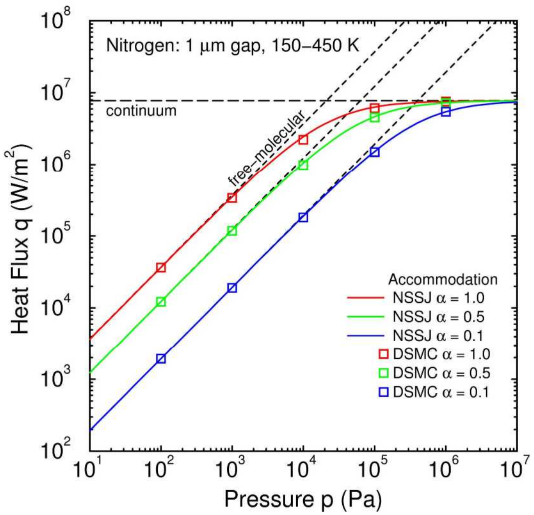
General Closed-Form Expression for Heat Flux Provided by Navier-Stokes Slip-Jump and DSMC Analyses of Microgap Heat Transfer





Gallis et al., *Sensors and Actuators A*, 134, 57 (2007).

$$h = \left(1+\frac{\zeta}{4}\right)\left(\frac{\alpha}{2-\alpha}\right)\left(\frac{p\bar{c}}{T}\right)\Bigg/\left(1+\left\{\frac{c_1\alpha}{1+c_2\left(\lambda/G\right)}\right\}\right)$$

Use DSMC to Compute Accurate Heat-Flux Values

- **Geometry: 1D with fixed wall temperatures**
- **Two gases: argon and nitrogen**
  - **Pressures: free-molecular to continuum**
- **Accommodation coefficient: 1.0, 0.5, 0.1**
  - **Same at both walls**

Perform Corresponding NSSJ Simulations

- **Fourier heat conduction in bulk gas**
- **Heat transfer coefficient *h* at each wall**
- **Adjust parameters so NSSJ matches DSMC**

Parameter Values Are Similar for Both Gases

- **Argon: c_1 = 0.176, c_2 = 0.647**
- **Nitrogen: c_1 = 0.167, c_2 = 0.599**

Applicable to temperature drop measurement method described below

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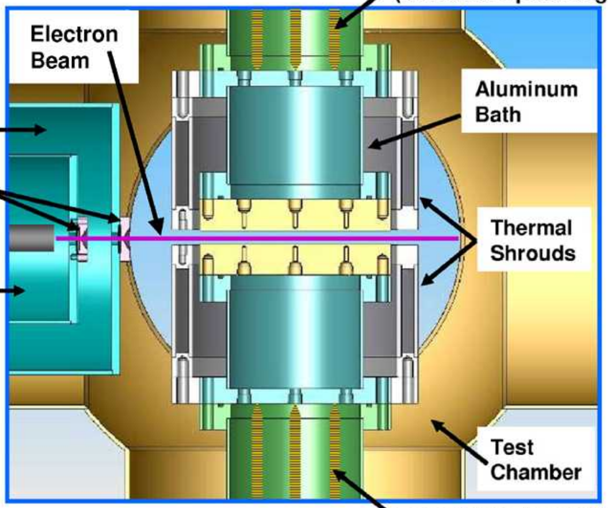
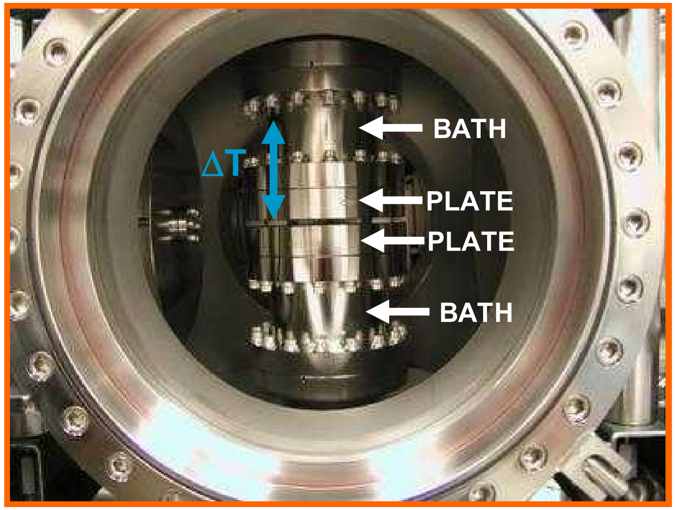
Experimental Heat-Flux Measurement



Bath/Plate Assemblies with Shrouds Removed



Infer Heat Flux from Temperature Drop Across Each Plate (Both Hot and Cold)

Principle of Operation

- **Two temperature-controlled water baths**
- **Measure temperature difference ΔT between liquid in baths and surface of plates**
- **Assume heat flux q is proportional to ΔT**

Challenges:

- **Very low heat fluxes ⇨ small ΔT**
- **Need high accuracy measurement of ΔT**
- **Need high accuracy control of gap (requires precise, reproducible translation of high thermal-mass components)**
- **Need high accuracy, stable pressure**

High Accuracy Solutions:

- **Hart Scientific thermistors**
- **Robust, independent plate positioners**
- **MKS Baratron pressure transducers**
- **MKS pressure (flow) controller**

Electron-Beam Fluorescence provides independent capability for measuring gas density variation between plates

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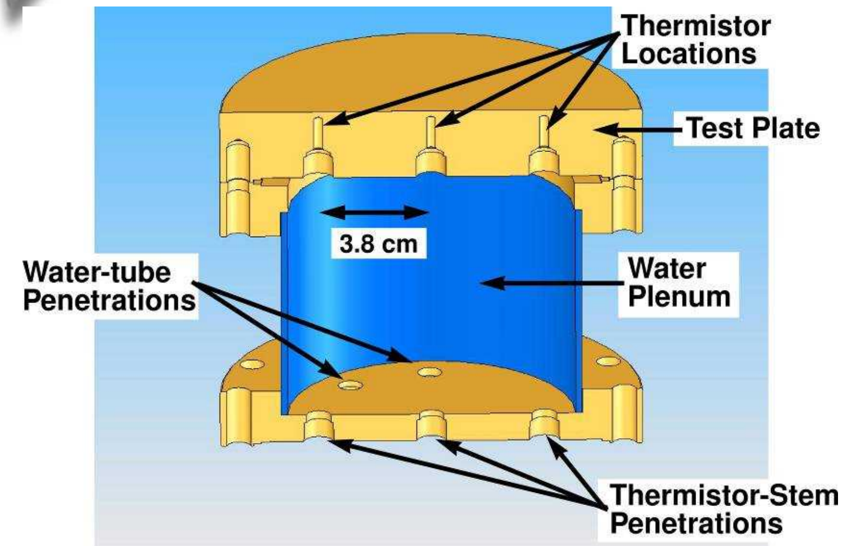
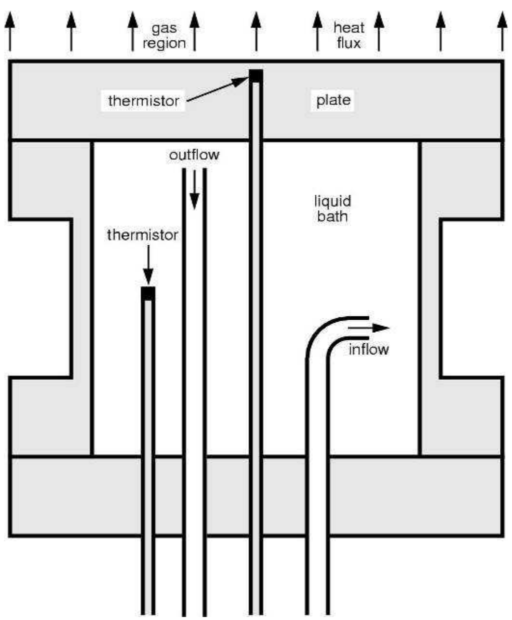
Temperature-Difference Measurement





Infer Heat Flux from Temperature Drop between Plate Surface and Bath

Assuming measured ΔT is proportional to heat flux:

$$\frac{1}{\Delta T_{gas}} = \frac{1}{\Delta T_C} + \frac{1}{\Delta T_C} \cdot \frac{2KT}{L\left(\frac{\alpha}{2-\alpha}\right)\left(1+\frac{\zeta}{4}\right)\bar{c}} \cdot \left(1+\frac{c_1 \alpha L}{L + c_2 \lambda}\right) \cdot \frac{1}{P}$$

--adjust α until model and experiment match ("GTR Formula")

Test Plates:

- Based on 6-inch conflat flange
- Stainless steel provides low conductivity
- Coat working surface with other materials
- Interchangeable relatively quickly

Bath Temperature

- Thermistor immersed in water
- Water stirred by constant flow
- Simulations of bath show some temperature drop across fluid/wall boundary layers

Plate Temperature

- Three thermistors embedded ~1.6 mm from plate working surface
- Central thermistor used for measurement
- Side thermistors test for uniformity

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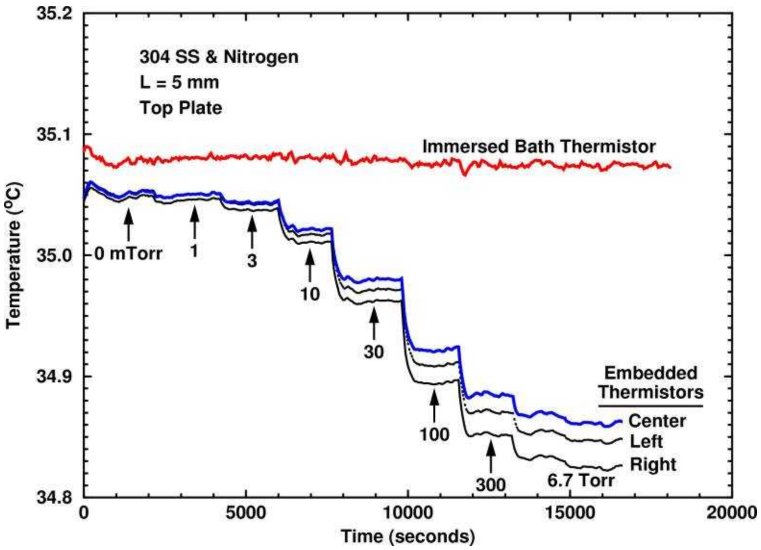
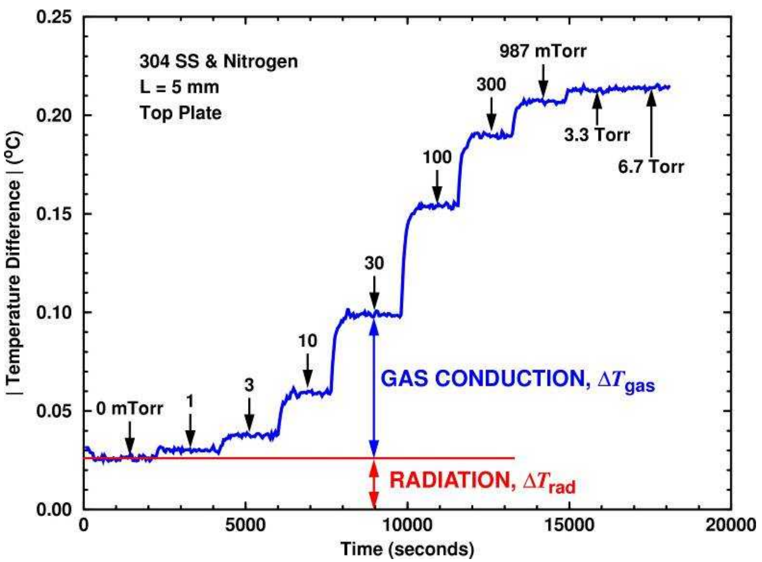
Analysis of Temperature Data





Infer Heat Flux from Temperature Drop Across Each Plate

Plate temperatures straddle ambient

- **Reduce parasitic losses**
- **Keep temperature differences small**
- **Use small gaps to increase heat flux**

Measure temperature differences

- **Between immersed and center-embedded thermistors, ΔT**
- **Vanishing-pressure limit gives radiation contribution, ΔT_{rad} *(other parasitic losses may also contribute slightly)***
- **Vanishing-pressure limit is material dependent: Gold < Aluminum < Stainless Steel < Silicon**
- **Gas-phase heat flux: $\Delta T_{gas} = \Delta T - \Delta T_{rad}$**

Pressure effect clearly evident

Continuum limit clearly observed

Some non-ideal system behaviors

- **Temperature varies across plates, ~0.05°C**
- **Side-to-side asymmetry**

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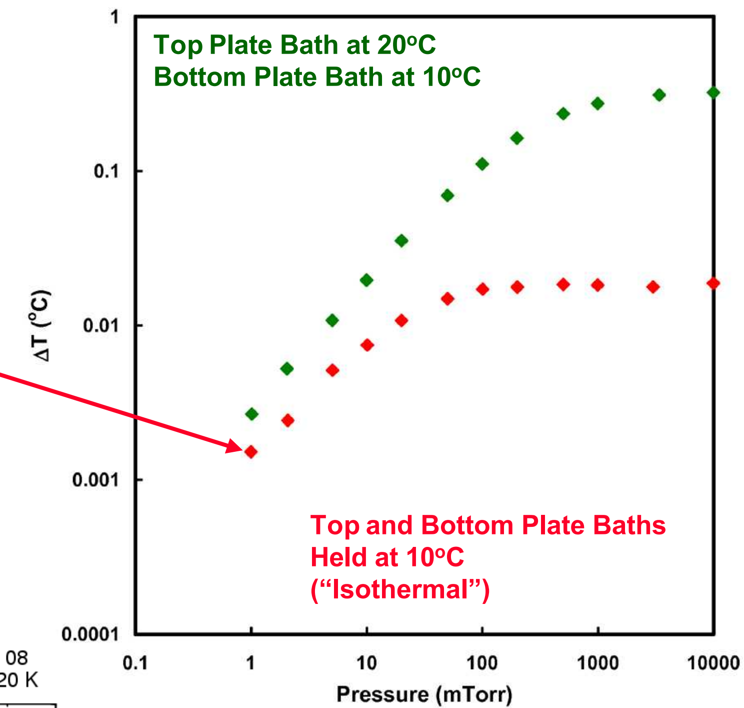
Initial Results Demonstrated Need for New Design With Thermal Shields for Bath/Plate Assemblies

Significant Non-Ideal System Behaviors Include:

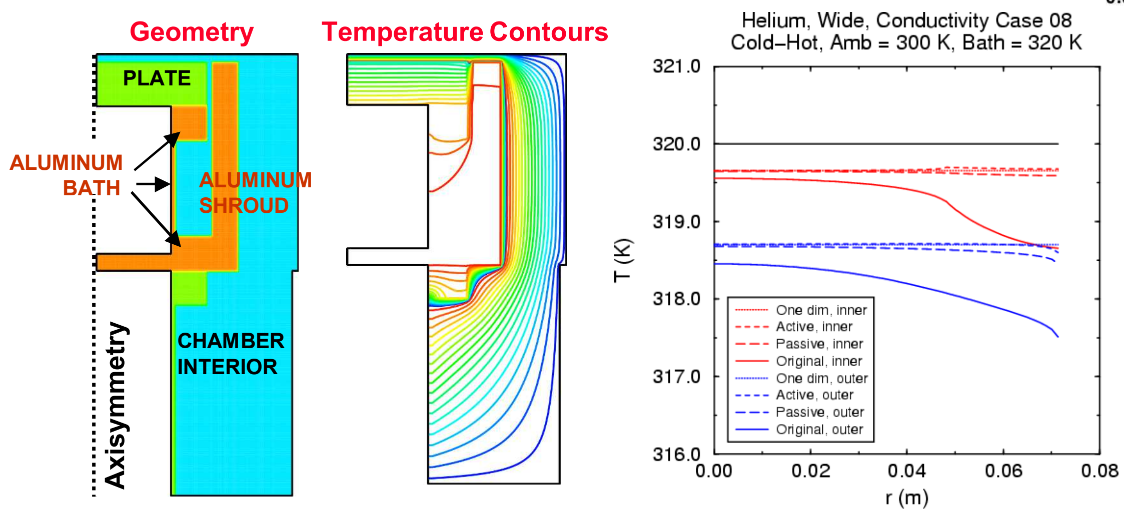
- Temperature Variations and Side-to-Side Asymmetry Across Plates
- Evidence of Environmental Effects Compromising Temperature Data
- Observed "Background" due to Conduction to Chamber Walls in "Isothermal" Test

Use simulation-based design to optimize materials and geometry of new assembly

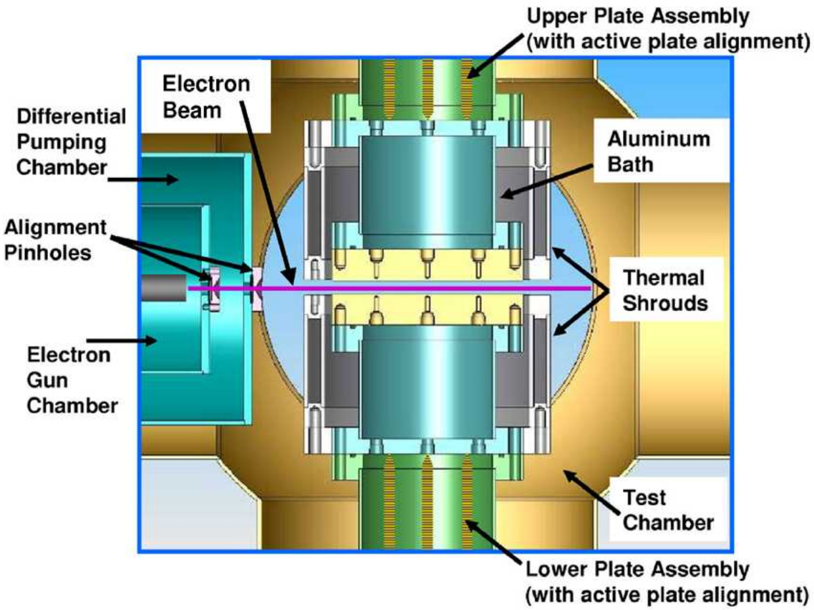
ΔT for Bottom Plate vs. Helium Pressure



NSSJ Simulation of Aluminum Bath with Aluminum Shroud



Modifications Have Enhanced System Performance



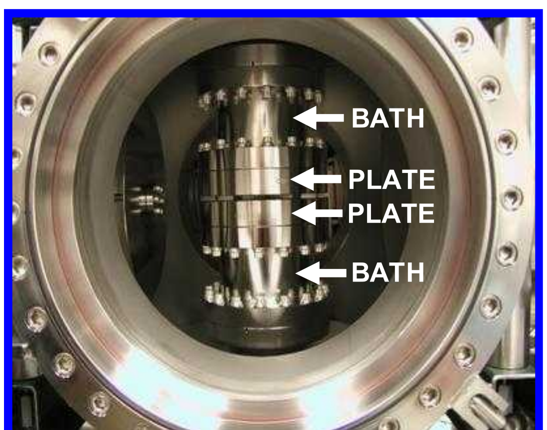
New Chamber Design with Thermal Shrouds and Active Plate Alignment System

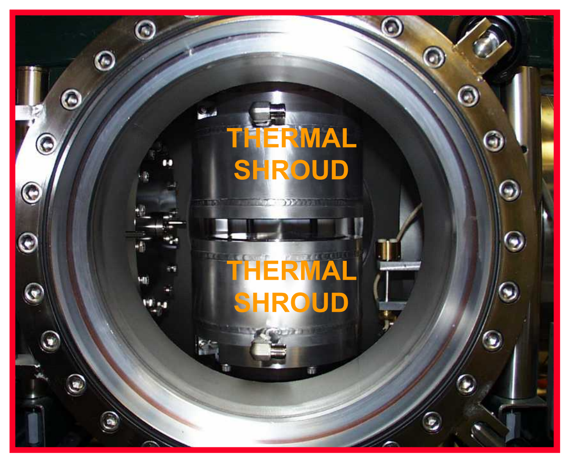
Thermal Shrouds

- Independent shroud-temperature control
- Reduce parasitic side-wall heat loss
- Improved plate-temperature uniformity

Aluminum Baths

- High thermal conductivity
- Better heat flow to plates
- Improved plate-temperature uniformity





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Additional System Modifications

Permanently Mounted Capability for
***In Situ* Plasma Treatment**

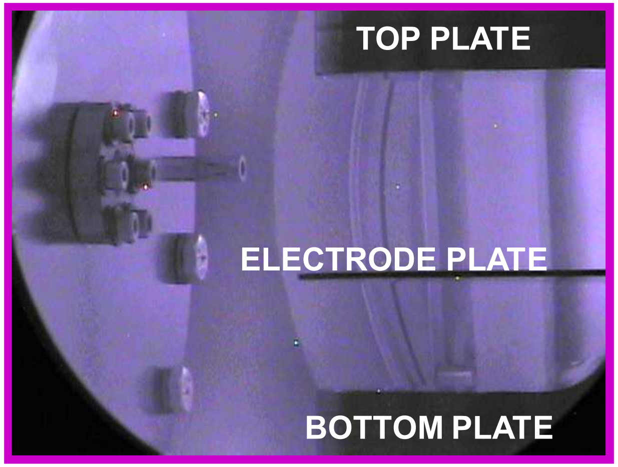
Added Oil-less Pumps and Multiple In-line Filters for Trapping Oxygen, Water, Hydrocarbons

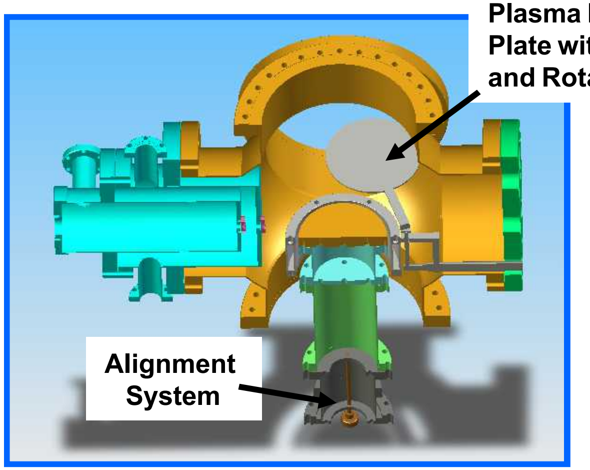
Added Hardware for Precision Filling/Metering of Gas <u>Mixtures</u>

Inter-Plate Separation Control

- Needed because of flexure when system evacuated
- Mechanical plate alignment system
- High-precision plate-gap sensors
- Measurement and alignment of plate parallelism can be performed under vacuum

Sample chamber illuminated by argon plasma used for surface treatment





Gap Measurement Hardware

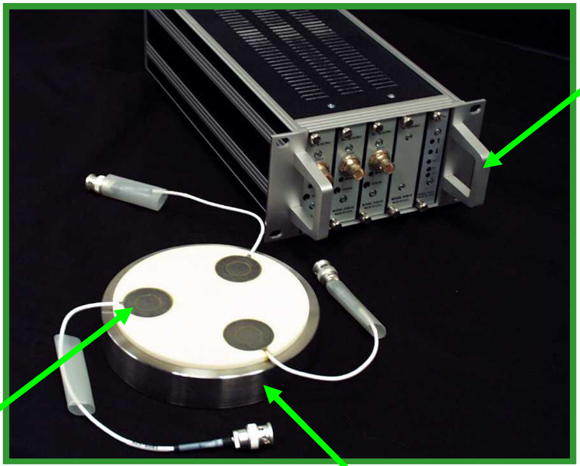


Plate Parallelism to within 20-30 μm can be achieved and maintained indefinitely

Summary of Enabling Specifications

Temperature Measurement and Control

- Thermistor Precision ~0.003°C
- Accurate to 0.01°C (by in-house calibration)
- Reproducibility in relative temperature measurements often better than 0.001°C
- Multiple measurement points
- Water-bath control of plates ±0.01 °C

Pressure Measurement and Control

- Accurate to 0.1% reading
- Redundant absolute pressure sensors, multiple ranges
- Stable pressures via automated flow control (e.g., 30 ± 0.01 mTorr)

Parallel Plate Assemblies

- Designed for facile mounting/exchange of sample plates
- Robust translators provide position accuracy ~10 μm
- Independent positioning and alignment of top and bottom plates
- Capacitive gap measurement system to ensure parallel configuration

***In Situ* Plasma Treatment**

- Mitigate surface contamination
- Maintain sample plates under vacuum
- Multiple filters in gas supply lines to maintain cleanliness
- Use electron gun to initiate plasma formation

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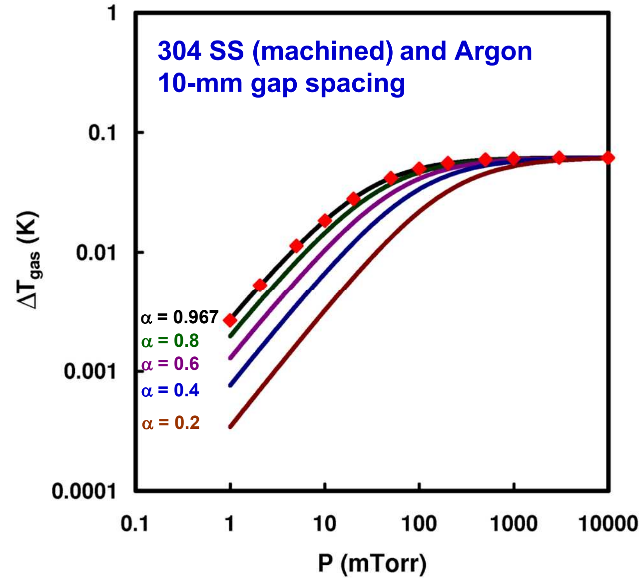
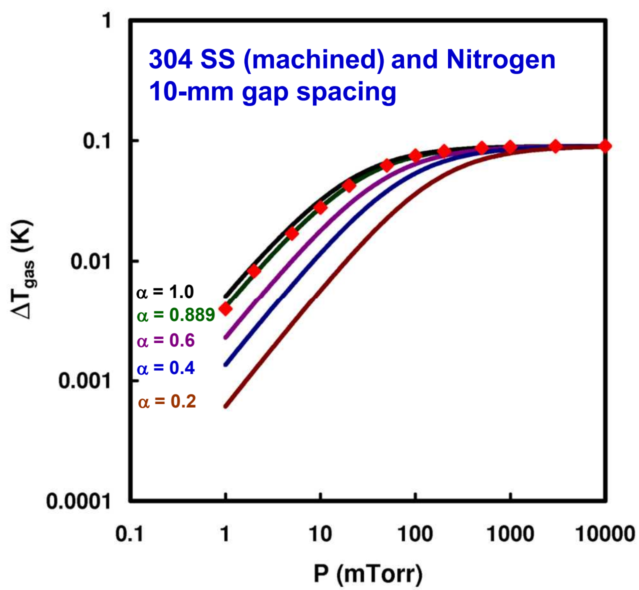
Accommodation Depends Strongly on Gas Composition

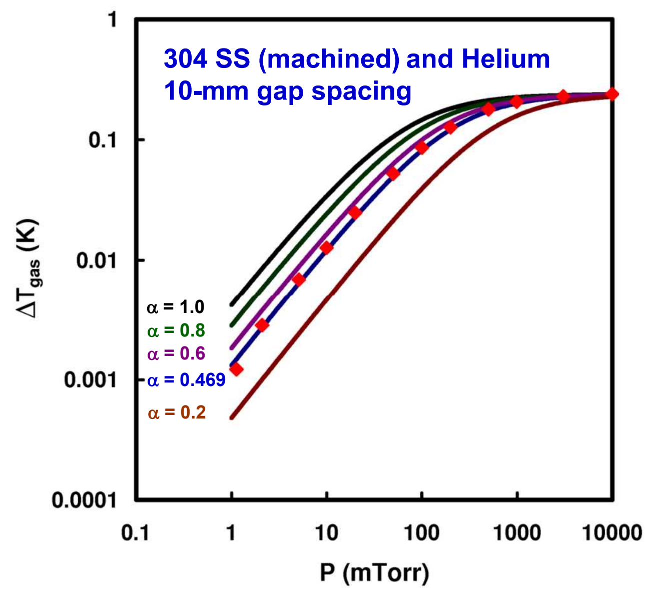
Surface: 304 Stainless Steel
RMS Roughness ~ 2 μm

Gas	α (average)
Argon	0.95 ± 0.02
Nitrogen	0.87 ± 0.02
Helium	0.46 ± 0.02

Values obtained from measurements with different combinations of temperature difference and gap spacing







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Accommodation Results Are Self-Consistent…

…Between Top and Bottom Plates

Case 1: 304 Stainless Steel
Helium
10-mm gap
Top Plate at 30°C
Bottom Plate at 20°C

α (top) = 0.469
α (bot) = 0.464

Case 2: Gold-Coated 304 SS
Nitrogen
10-mm gap
Top Plate at 30°C
Bottom Plate at 20°C

α (top) = 0.82
α (bot) = 0.84

Worst Case: 0.04 difference between hot and cold plates

…With Different Plate Separations

Case 1: Gold-Coated 304 SS
Helium
Top Plate at 30°C
Bottom Plate at 20°C

α (5-mm gap) = 0.425
α (10-mm gap) = 0.409
α (15-mm gap) = 0.410

Case 2: Gold-Coated 304 SS
Nitrogen
Top Plate at 30°C
Bottom Plate at 20°C

α (5-mm gap) = 0.839
α (10-mm gap) = 0.830
α (15-mm gap) = 0.824

Worst Case: 0.03 difference over range of 5-15 mm

…With Different ΔTs Between Plates

Case 1: 304 Stainless Steel
Argon
10-mm gap

α (20° ΔT) = 0.946
α (40° ΔT) = 0.958

Case 2: Aluminum
Helium
10-mm gap

α (10° ΔT) = 0.468
α (20° ΔT) = 0.462

Worst Case: 0.015 difference

Effect of Surface Roughness Has Been Explored

304 Stainless Steel (machine finish)

- **RMS Roughness ~ 2 μm**
- **Helium: α = 0.46 $\pm$ 0.02**
- **Nitrogen: α = 0.87 $\pm$ 0.02**
- **Argon: α = 0.95 $\pm$ 0.02**

304 Stainless Steel (polished)

- **Mirror finish**
- **RMS roughness ~ 20 nm**
- **Helium: α = 0.42 $\pm$ 0.02**
- **Nitrogen: α = 0.87 $\pm$ 0.02**
- **Argon: α = 0.96 $\pm$ 0.02**

Surface roughness plays a minor role (at least in this particular test case)

Effect of Surface Material Has Also Been Explored

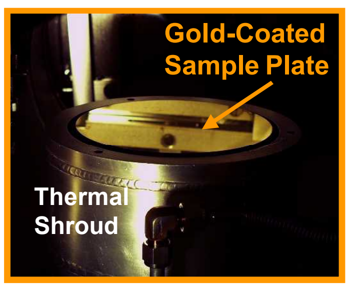
Comparison of Different Surface Materials:

Gas	α 304 Stainless	α Gold-Coated 304 SS	α Aluminum
Argon	0.95 ± 0.02	0.92 ± 0.02	0.96 ± 0.02
Nitrogen	0.87 ± 0.02	0.83 ± 0.02	0.86 ± 0.02
Helium	0.46 ± 0.02	0.41 ± 0.02	0.47 ± 0.02

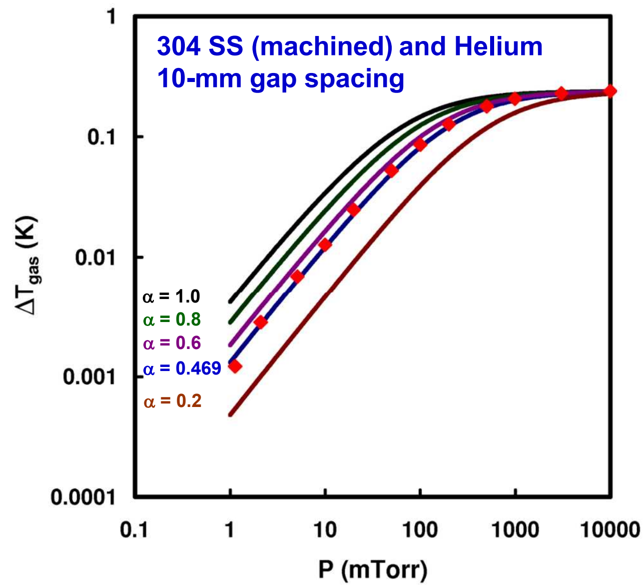
(Values correspond to average of multiple tests for each gas-surface combination)

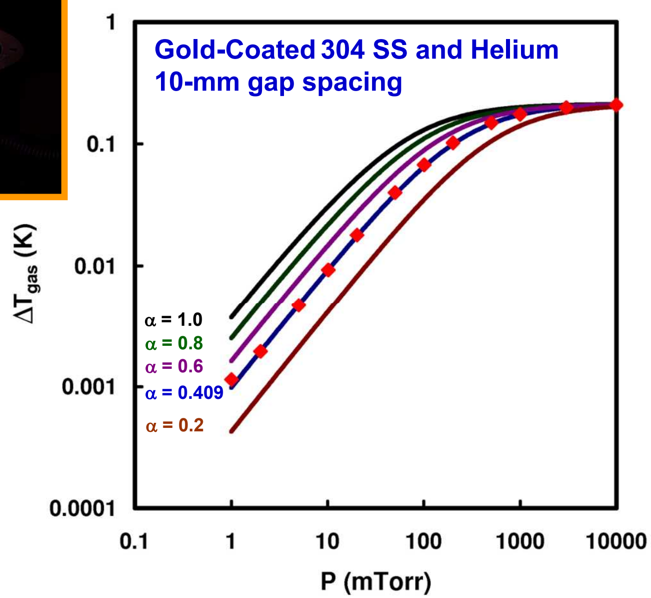
Results are quite similar for materials of widely varying molecular weight

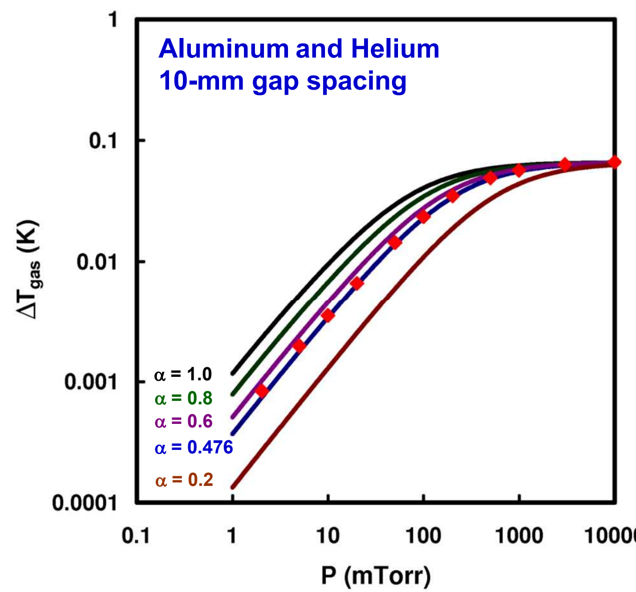
Role of Coating Thickness? Surface Contamination?



Gold Coating Thickness ~ 10s nm







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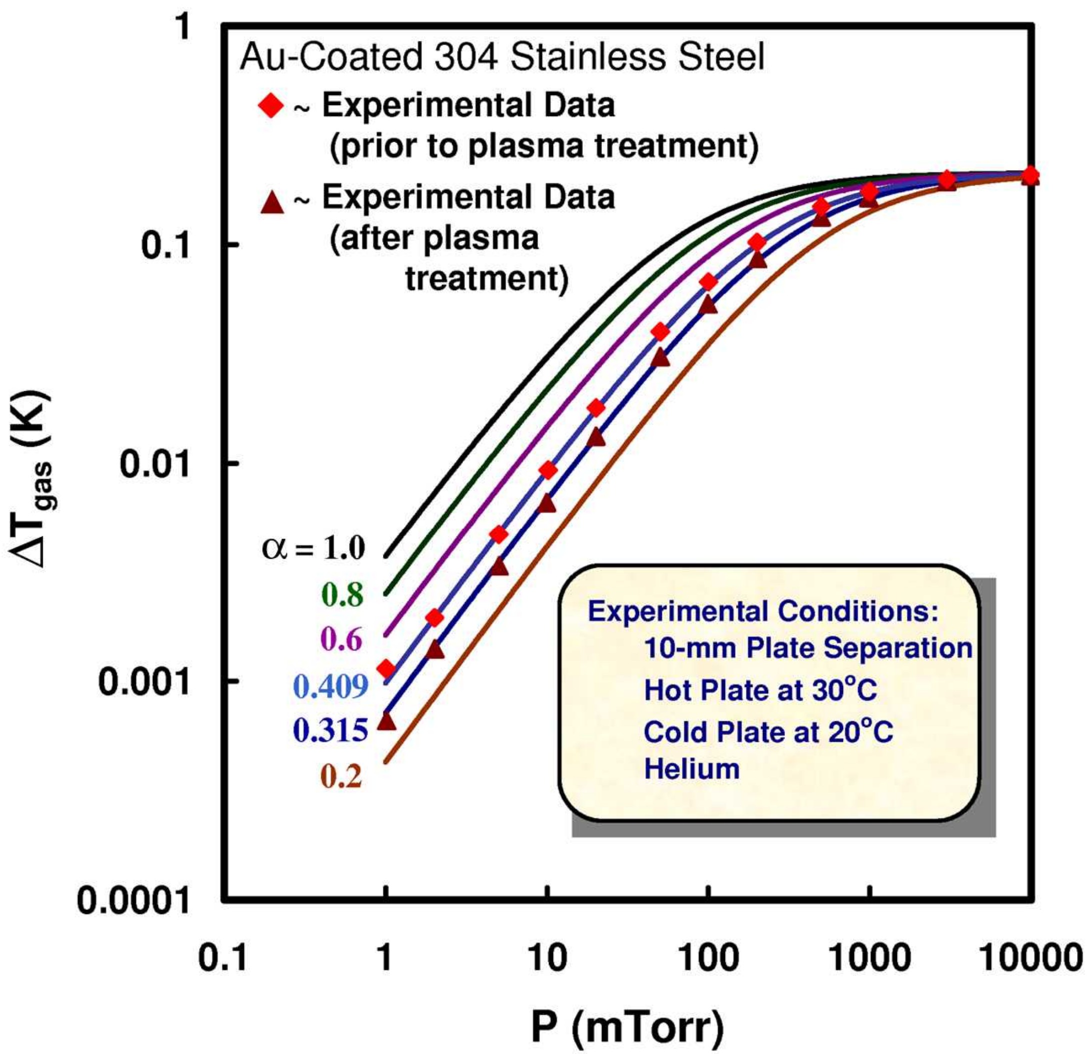
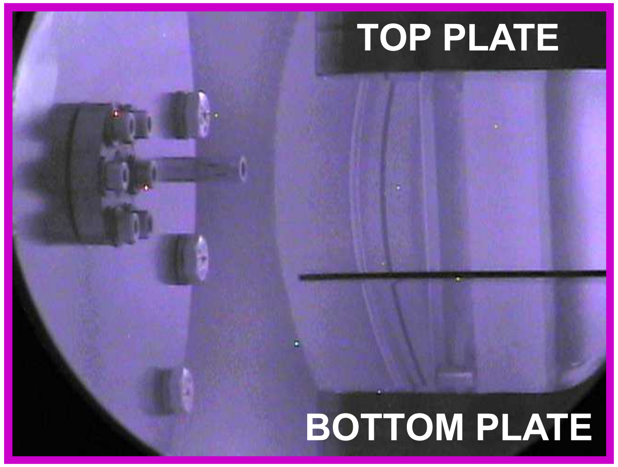
Effect of Surface Contamination Has Been Evaluated for Different Surfaces and Gases





Sample chamber illuminated by argon plasma used for surface treatment

Effect appears to be largely reversible upon returning sample plates to ambient conditions

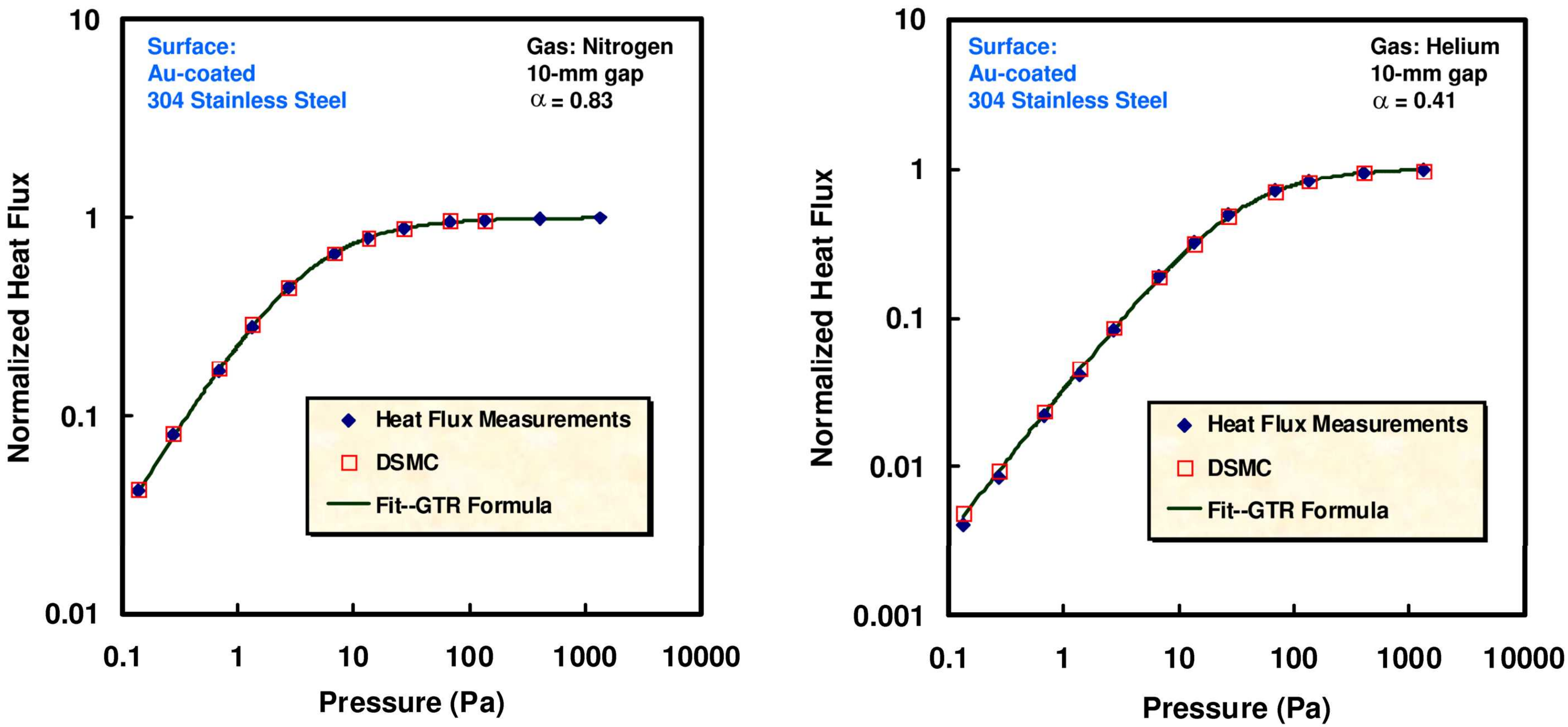
- **For many materials, adsorption of contaminants occurs quickly but desorption is difficult**
- ***In situ* surface analysis would be very informative**

An Extensive Database of Thermal Accommodation Coefficients Has Been Developed

Surface	Argon	Nitrogen	Helium
304 Stainless Steel (machined surface)	0.95	0.87	0.46
304 Stainless Steel (machined, plasma treated)	0.90	---	0.38
304 Stainless Steel (polished)	0.96	0.87	0.42
Gold	0.92	0.83	0.41
Gold (plasma treated)	0.85	0.77	0.31
Aluminum	0.96	0.86	0.47
Aluminum (plasma treated)	0.91	---	0.38
Silicon	0.91	0.82	0.43
Silicon (plasma treated)	---	---	0.36
Platinum	0.96	0.90	0.58
Platinum (plasma treated)	0.94	---	0.52
Silicon Nitride	0.96	0.87	0.45
Silicon Nitride (plasma treated)	0.90	0.82	0.36
Polysilicon (Poly4 Equivalent)	In progress	In progress	In progress

Comparison of Heat Flux Measurements with DSMC Simulations

DSMC simulations with gas-surface model must predict heat flux accurately



Experiment and DSMC are in good agreement (but small systematic differences)

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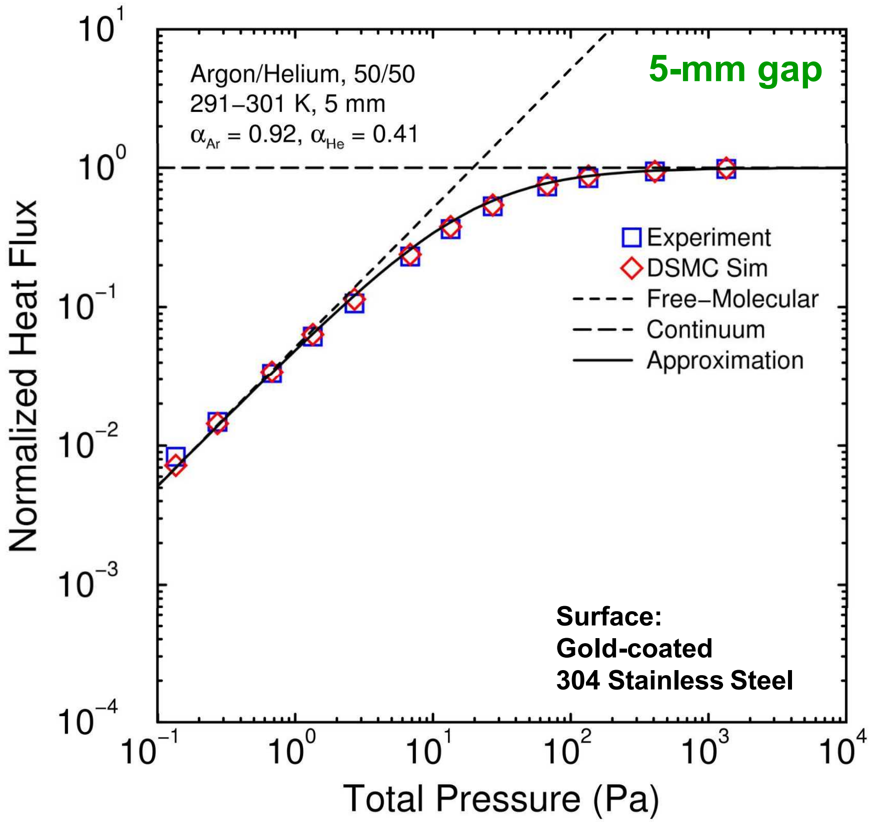
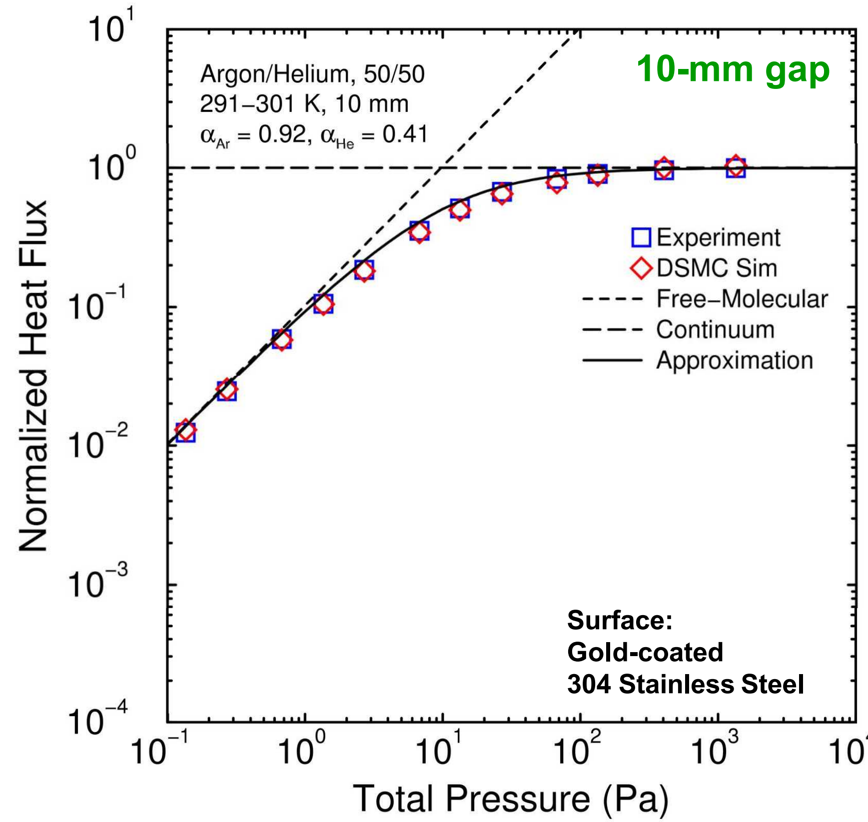
Helium/Argon Mixtures Have Also Been Evaluated

DSMC simulations with gas-surface model must predict heat flux accurately

Results provide important new validation data for DSMC optimization as well as a useful test of experimental system performance, self-consistency, etc.





Experiment and DSMC are in good agreement (but small systematic differences)

Sherman-Lees approximation overpredicts experiment and DSMC for transitional cases

Both experimental and computational issues warrant further exploration

Sandia National Laboratories

Summary

- An experimental facility for precise determination of thermal accommodation coefficients has been developed, tested, and extensively upgraded to improve performance
- Different gases, gas mixtures, and surfaces can be tested with minimal changes in setup
- Measured heat-flux results have been used with a DSMC-based formula to determine thermal accommodation coefficients
- Self-consistent results have been obtained for a variety of surfaces and gases
- Results thus far indicate that surface roughness plays a minor role in accommodation but that surface contamination is important
- Agreement of experiments and DSMC simulations is good; however, significant experimental and computational issues warrant further exploration
- Helium/argon accommodation results provide a good indicator of self-consistent experimental system performance and have generated useful new data for DSMC evaluation and optimization