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Thermal Accommodation Coefficients from DSMC-Based Analysis of Parallel-Plate Heat-Transfer Experiments

Wayne M. Trott, Daniel J. Rader, John R. Torczynski, Michael A. Gallis, and Jaime N. Castañeda

Engineering Sciences Center
Sandia National Laboratories
Albuquerque, New Mexico, USA

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Presentation Outline

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

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Gas-Surface Interactions

Problem

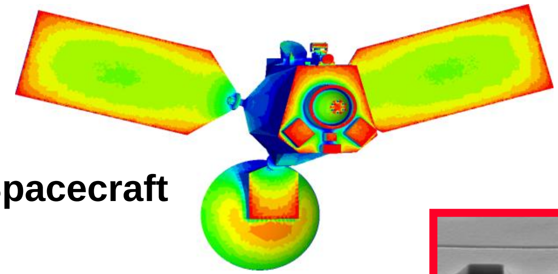
- No-slip, no-jump boundary models break down for rarefied or microscale flows
- Details of gas-surface interaction crucial

Applications

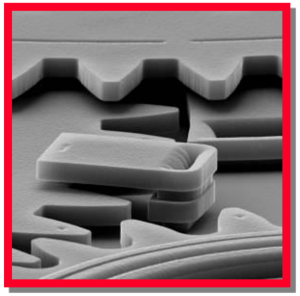
- Aerodynamic heating of spacecraft
- Heat management in MEMS devices
- DSMC *always* needs surface model

Technical Approach

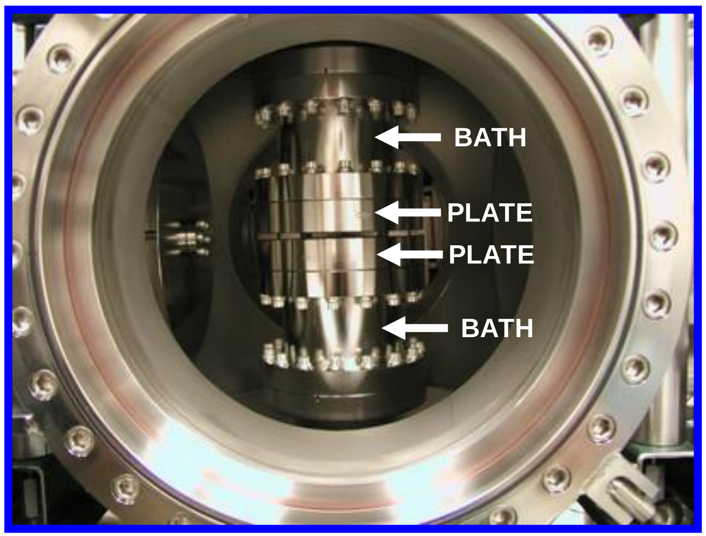
- Complex physics requires experiments
- Measure heat flux and gas density between parallel plates (*primary emphasis on heat flux measurements*)
- Infer gas-surface energy accommodation

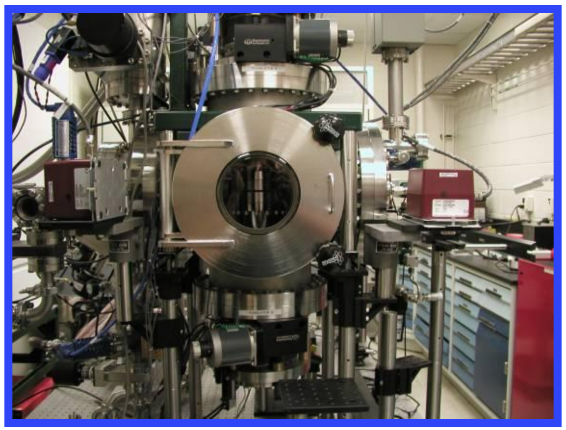


Spacecraft



MEMS Devices





Thermal Accommodation Test Chamber

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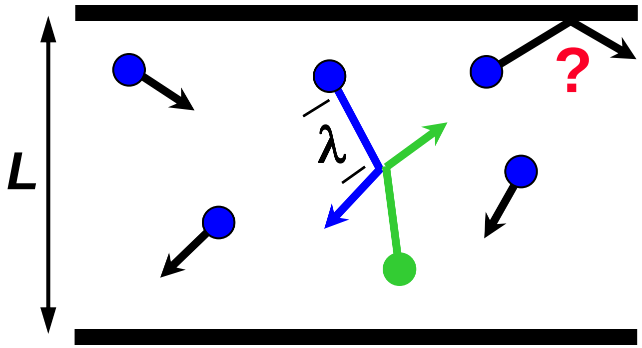
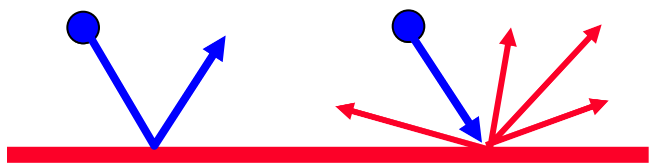
Noncontinuum Gas Behavior



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

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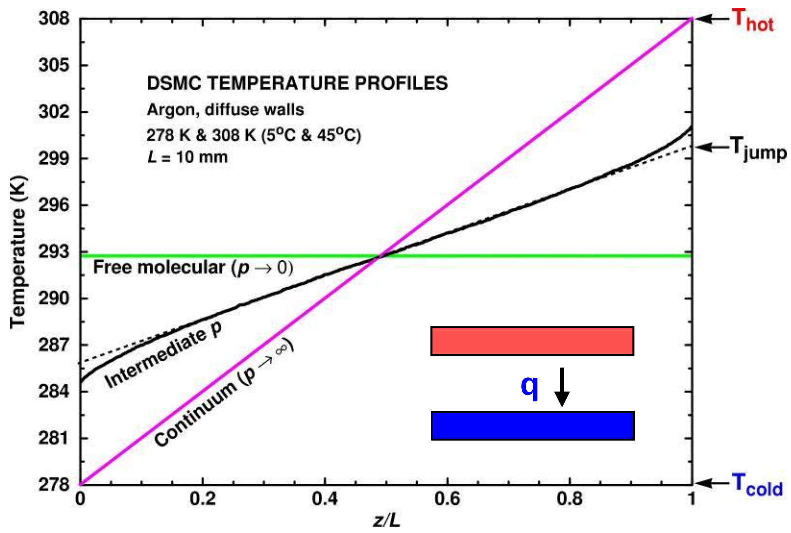
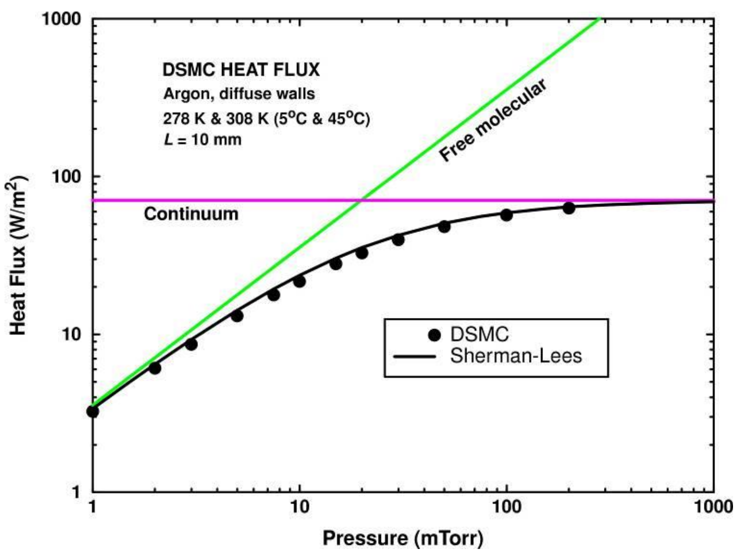
Noncontinuum Heat Flux





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, …)
- Surface purity

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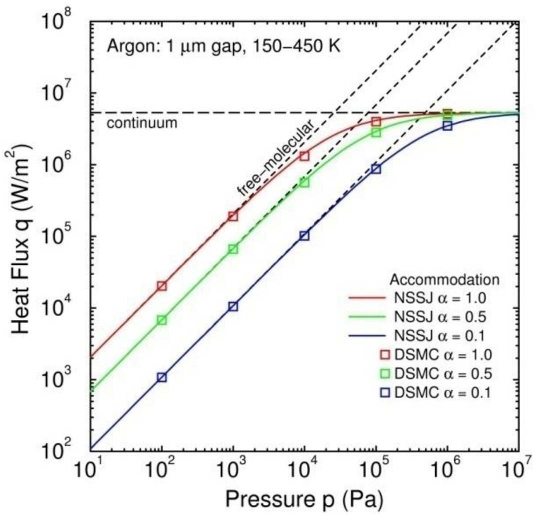
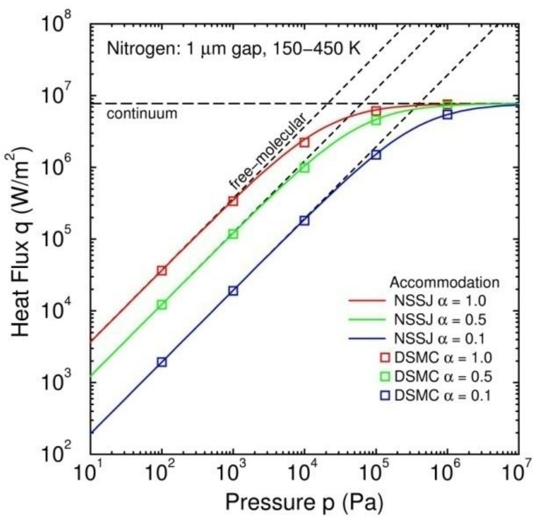
Closed-Form Expression for Heat Flux





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

Provided by Navier-Stokes Slip-Jump and DSMC Analyses of Microgap Heat Transfer

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

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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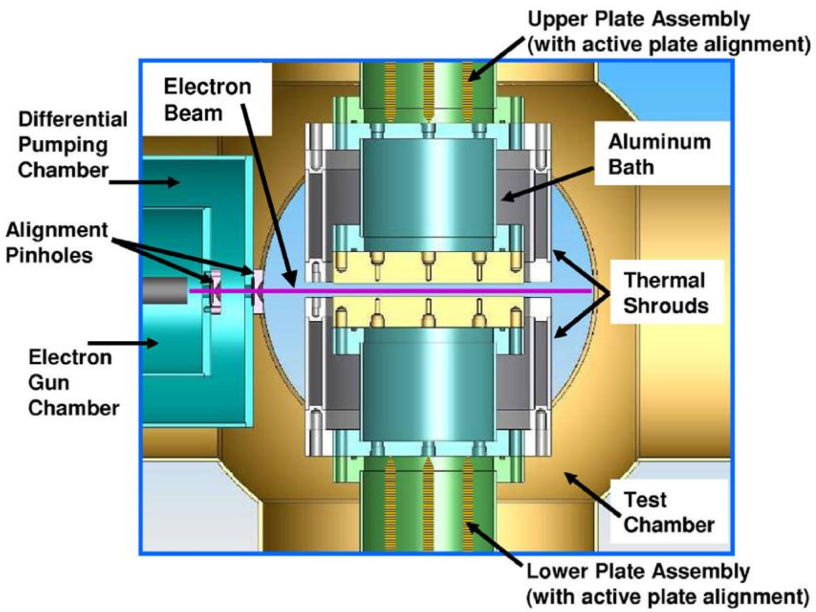
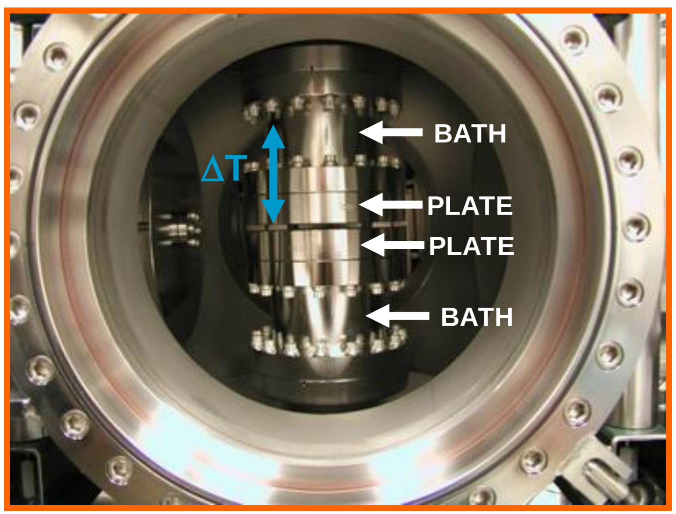
Experimental Heat-Flux Measurement



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:

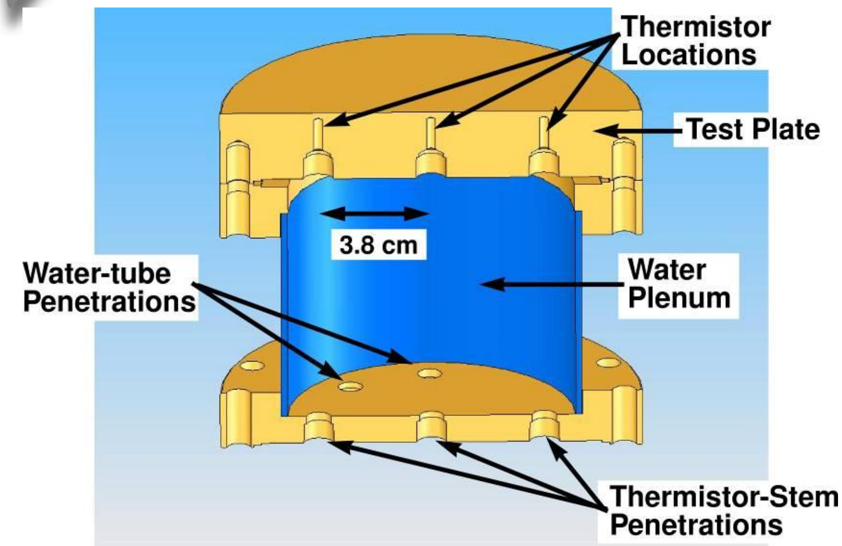
- **Very low heat fluxes ⇨ small ΔT**
- **Need high accuracy measurement of ΔT**
- **Need high accuracy control of gap (requires precise, reproducible translation of high thermal-mass components)**
- **Need high accuracy, stable pressure**

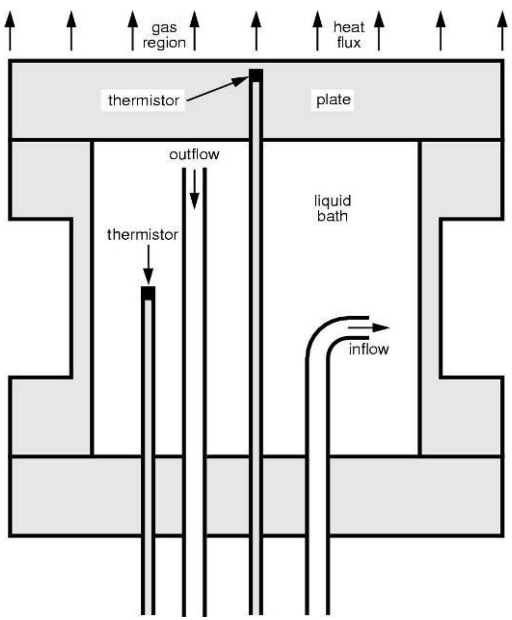
High Accuracy Solutions:

- **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

Temperature-Difference Measurement





Infer Heat Flux from Temperature Drop between Plate Surface and Bath

Assume measured ΔT is proportional to heat flux

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

Adjust α until model and experiment match

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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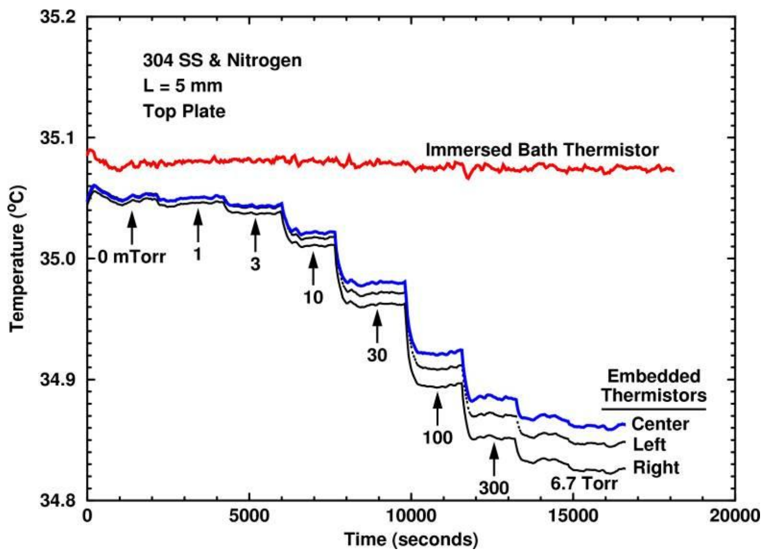
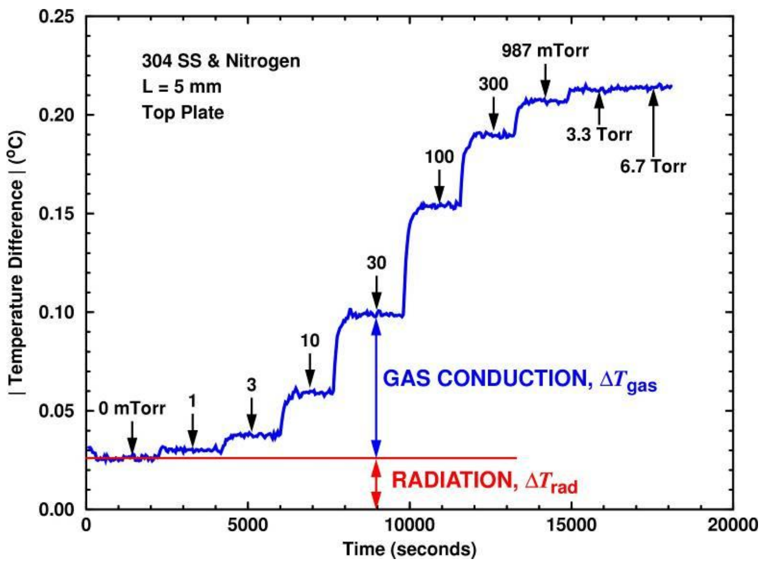
Analysis of Temperature Data





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

Initial system design used SS baths and did not include thermal shrouds—significant non-ideal system behaviors observed

New Design With Thermal Shields

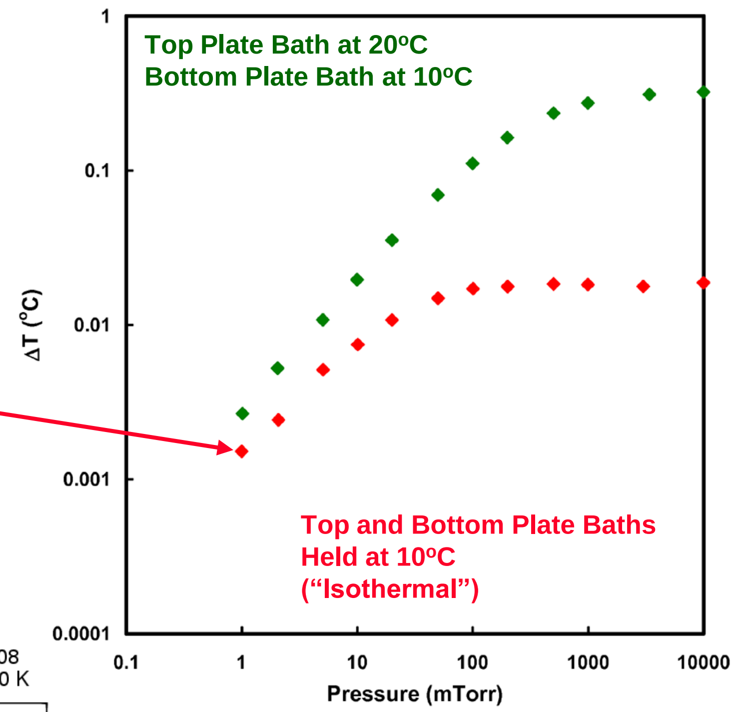
Initial Results Demonstrated Need for New Design With Thermal Shields for Bath/Plate Assemblies

Significant Non-Ideal System Behaviors Include:

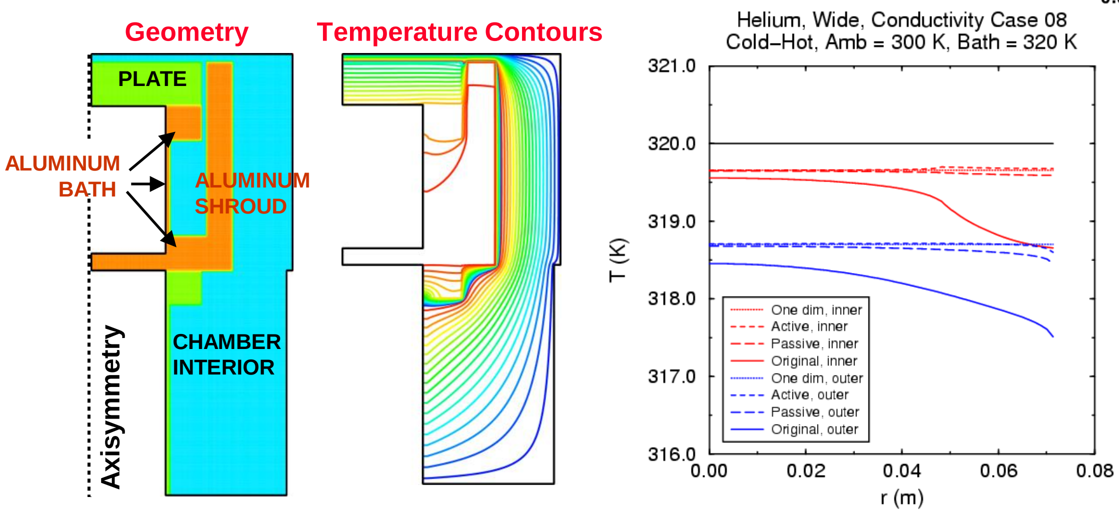
- **Temperature Variations and Side-to-Side Asymmetry Across Plates**
- **Evidence of Environmental Effects Compromising Temperature Data**
- **Observed "Background" due to Conduction to Chamber Walls in "Isothermal" Test**

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



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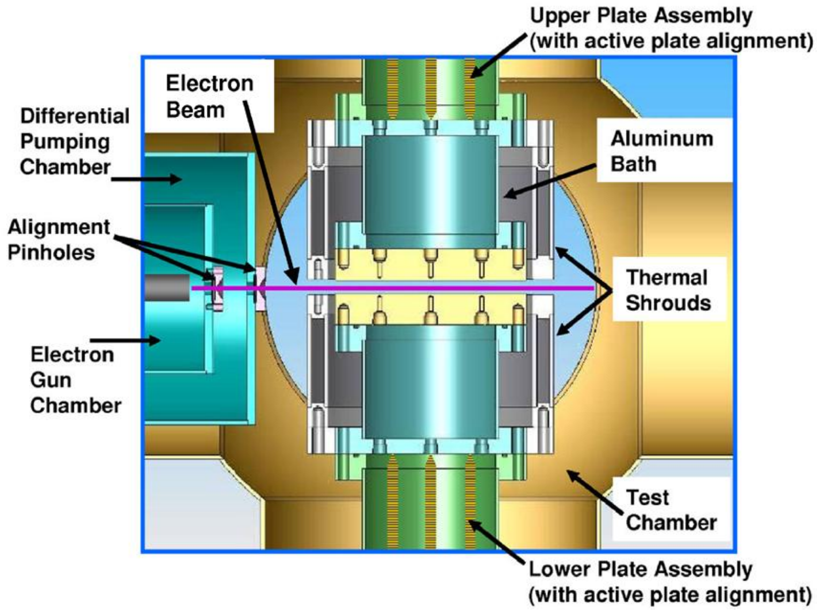
Performance Enhanced by Modifications



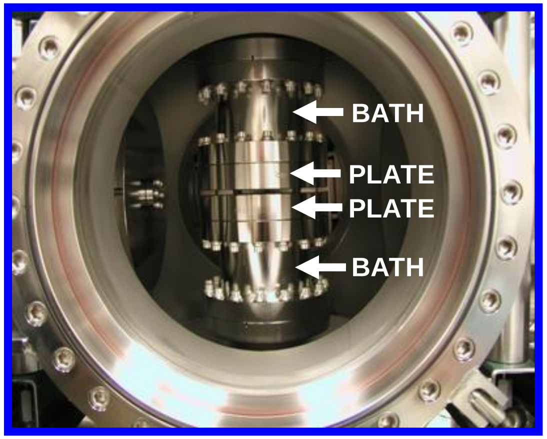
New Chamber Design with Thermal Shrouds and Active Plate Alignment System

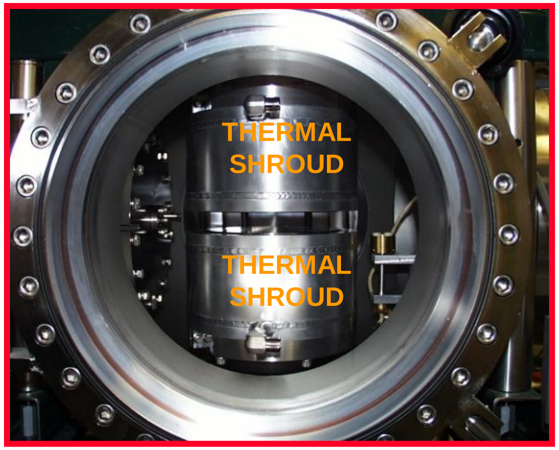
Thermal Shrouds

- Independent shroud-temperature control
- Conduction to chamber walls minimized
- 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

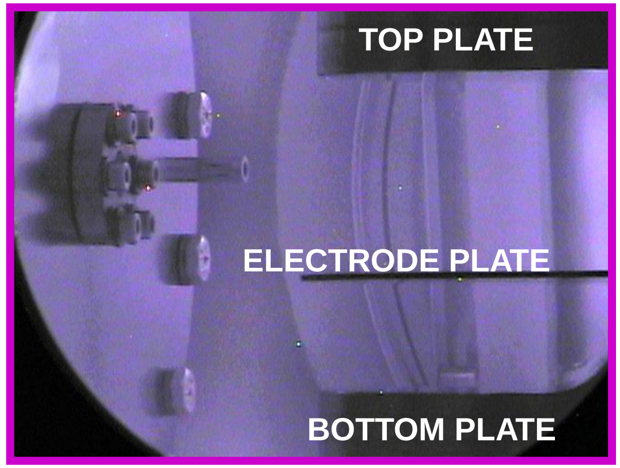
Added Oil-less Pumps and Multiple In-line Filters for Trapping Oxygen, Water, Hydrocarbons

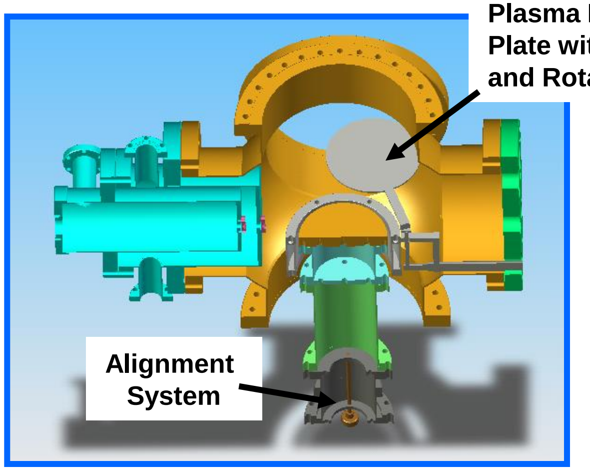
Added Hardware for Precision Filling/Metering of Gas Mixtures

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

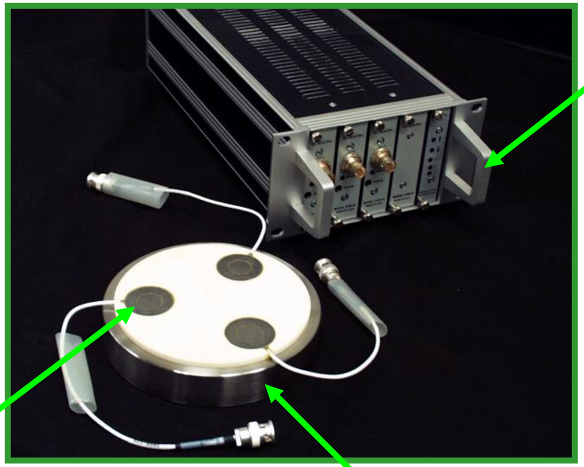


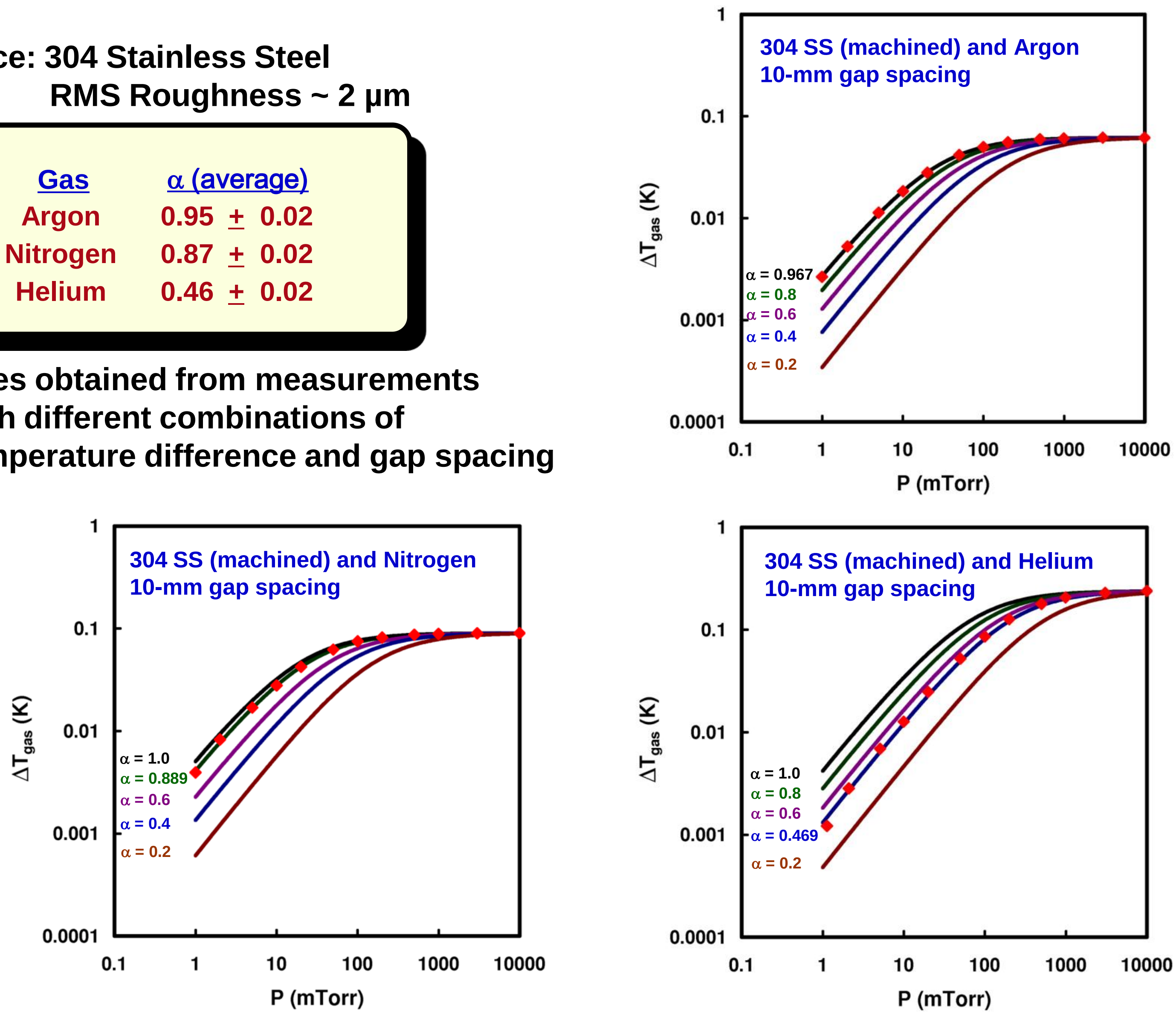
Plate Parallelism to within 20-30 μm can be achieved and maintained indefinitely

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



Effect of Surface Roughness

304 Stainless Steel (machine finish)

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

304 Stainless Steel (polished)

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

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

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Effect of Surface Material

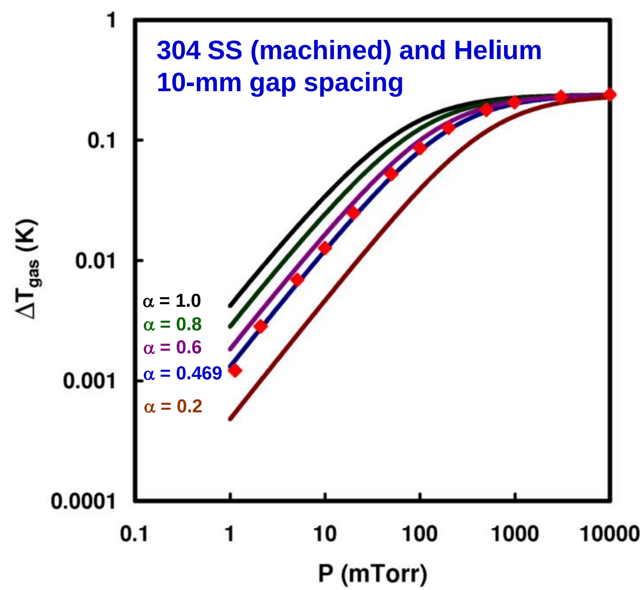
Comparison of Different Surface Materials

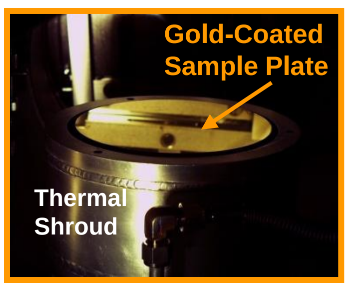
Gas	α 304 Stainless	α Gold-Coated 304 SS	α Aluminum
Argon	0.95 ± 0.02	0.92 ± 0.02	0.96 ± 0.02
Nitrogen	0.87 ± 0.02	0.83 ± 0.02	0.86 ± 0.02
Helium	0.46 ± 0.02	0.41 ± 0.02	0.47 ± 0.02

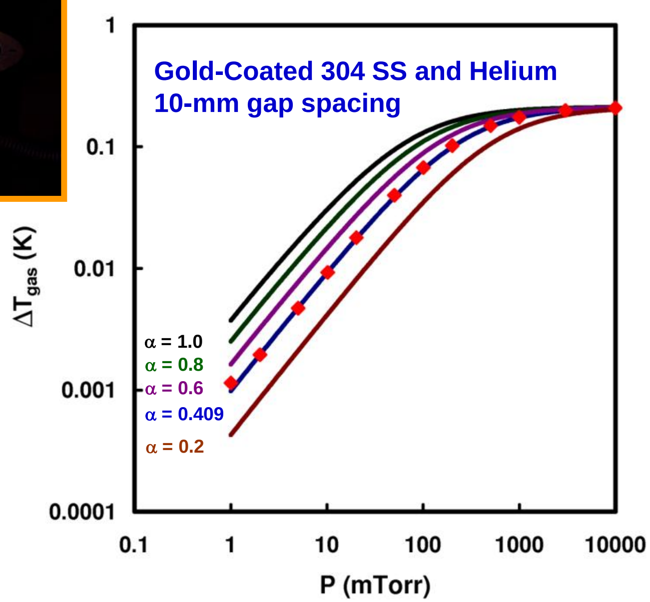
(Values correspond to average of multiple tests for each gas-surface combination)

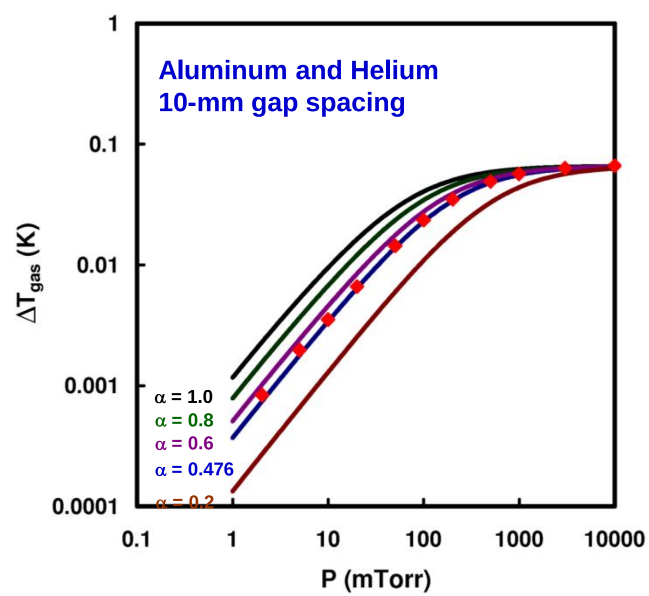
Results are quite similar for materials of widely varying molecular weight

Likely reflects dominant role of surface purity/contamination









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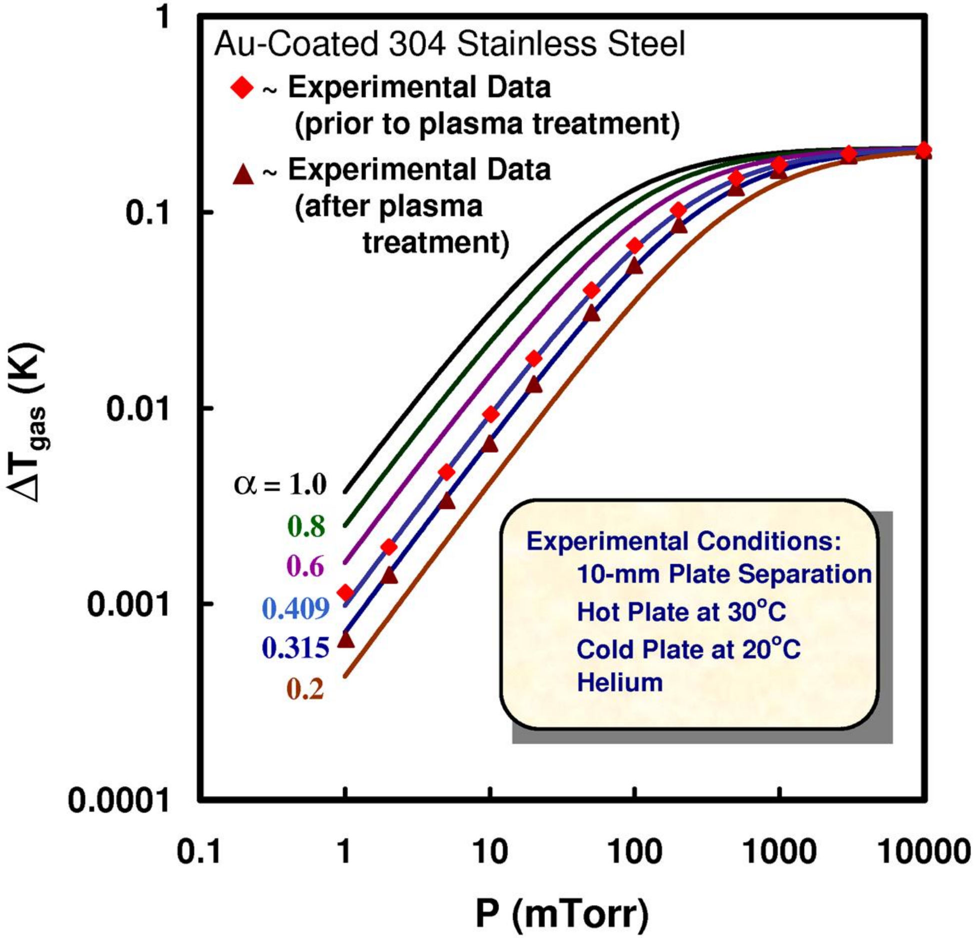
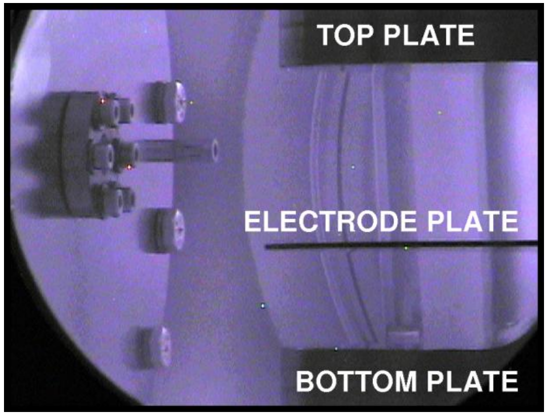
Effect of Surface Contamination for Various Surfaces and Gases





Sample chamber illuminated by argon plasma used for surface treatment

Decrease in α with plasma treatment is similar for different materials

Extent of cleaning appears limited

Compare hot-wire results of L. B. Thomas and E. B. Schofield, J. Chem. Phys. **23**, 861 (1955).

Helium on Tungsten

Untreated W: $\alpha = 0.283$

Thoroughly Cleaned W: $\alpha = 0.017$

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

→ *In situ* surface analysis would be very informative

System design/materials are not amenable to thorough thermal annealing but could accommodate incorporation of surface analysis diagnostics

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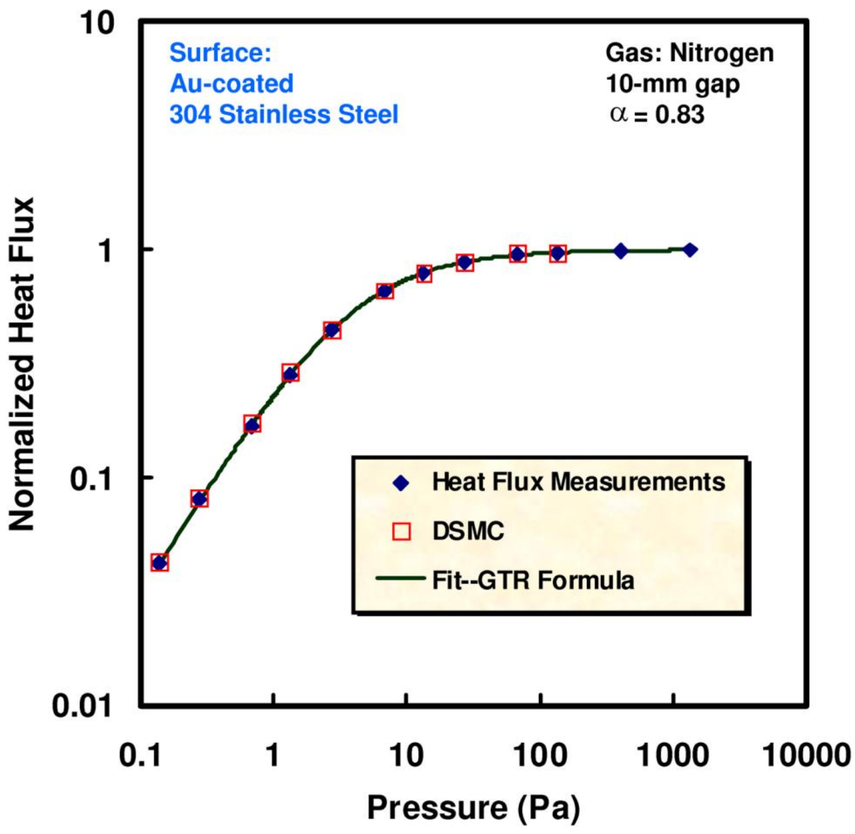
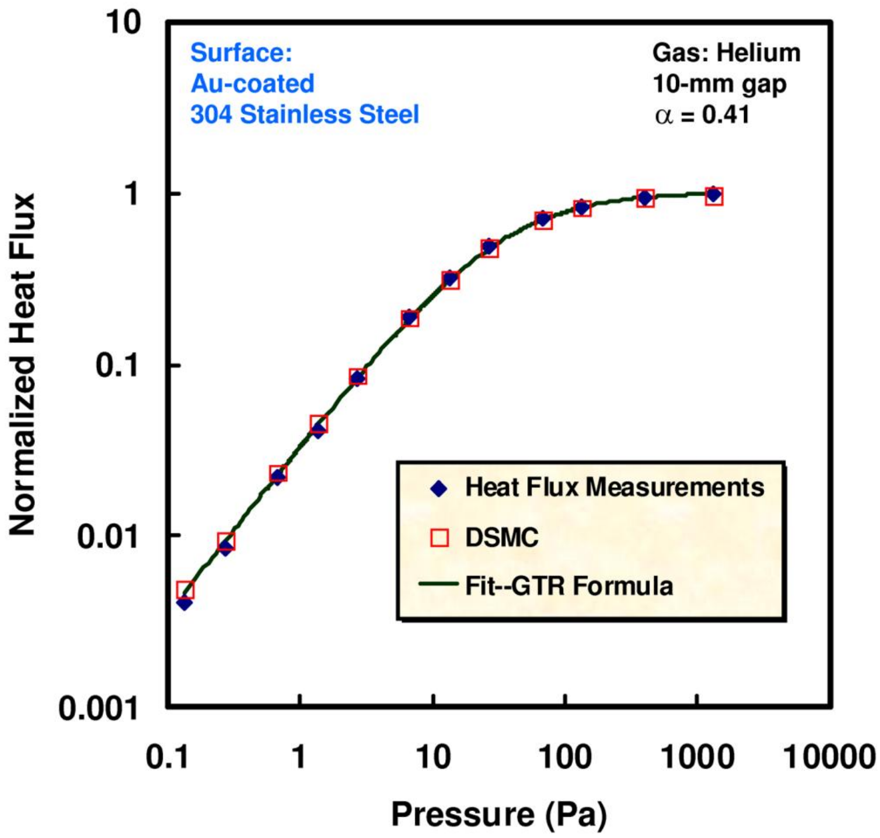
Extensive Database of Thermal Accommodation Coefficients

Surface	Finish	Treatment	Argon	Nitrogen	Helium
304 Stainless Steel	Machined	None	0.95	0.87	0.46
304 Stainless Steel	Machined	Plasma	0.90	---	0.38
304 Stainless Steel	Polished	None	0.96	0.87	0.42
Gold-coated 304 SS	Deposited	None	0.92	0.83	0.41
Gold-coated 304 SS	Deposited	Plasma	0.85	0.77	0.31
Aluminum 6061-T6	Machined	None	0.96	0.86	0.47
Aluminum 6061-T6	Machined	Plasma	0.91	---	0.38
Silicon	Wafer	None	0.91	0.82	0.43
Silicon	Wafer	Plasma	---	---	0.36
Platinum	Plated	None	0.96	0.90	0.58
Platinum	Plated	Plasma	0.94	---	0.52
Silicon Nitride	Deposited	None	0.96	0.87	0.45
Silicon Nitride	Deposited	Plasma	0.90	0.82	0.36
Polysilicon (Poly4 Equivalent)	Deposited	None	0.94	0.84	0.44

Heat Flux Measurements Compared to DSMC Simulations

DSMC simulations with gas-surface model are expected to predict heat flux accurately





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

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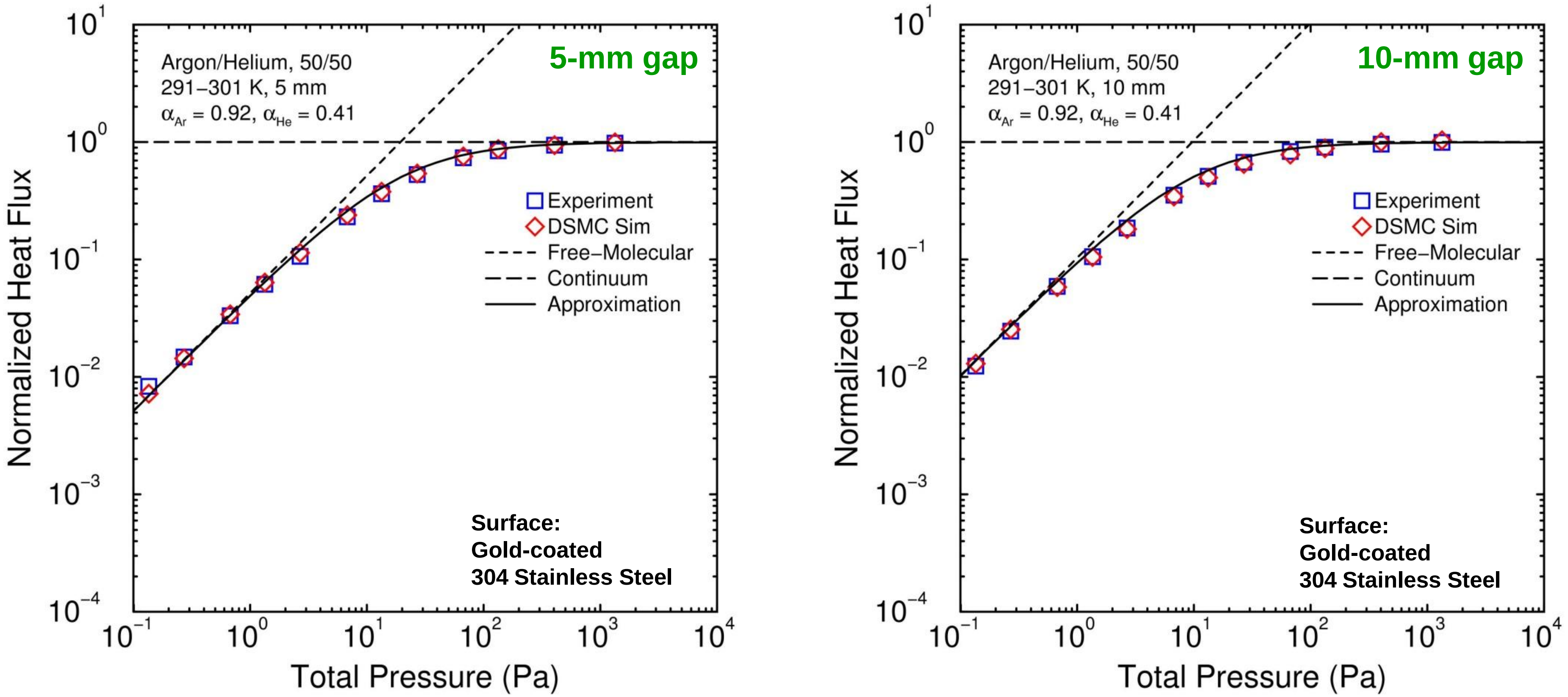
Helium/Argon Mixtures

DSMC simulations with gas-surface model are expected to 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 very good agreement (but small systematic differences)

Sherman-Lees approximation overpredicts experiment and DSMC for transitional cases

Both experimental and computational issues warrant further exploration

Summary

- An experimental facility for precise determination of thermal accommodation coefficients has been developed, tested, and refined to improve performance
- Different gases and surfaces can be tested with minimal changes in system setup
- A DSMC-based formula is used to determine thermal accommodation coefficients from measured heat-flux results
- Self-consistent results have been obtained for a variety of surfaces and gases
- Large variations are seen with different gas composition
- Surface contamination has an important role in determining thermal accommodation
- In contrast to previous parallel-plate studies, agreement between experiments and numerical simulations is very good
- Helium/argon accommodation results indicate self-consistent experimental system performance and have generated useful new data for DSMC validation

W. M. Trott, J. N. Castañeda, J. R. Torczynski, M. A. Gallis, and D. J. Rader, "An Experimental Assembly for Precise Measurement of Thermal Accommodation Coefficients," *Review of Scientific Instruments*, 82 (3), 035120, 1-12 (2011).