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# *Experimental Determination of Thermal Accommodation Coefficients for Microscale Gas-Phase Heat Transfer*

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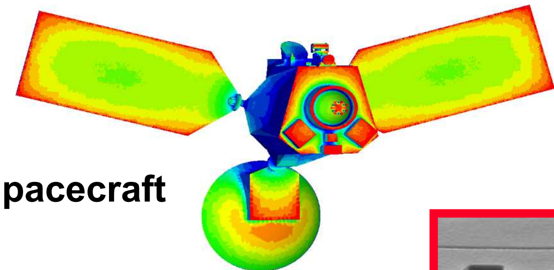
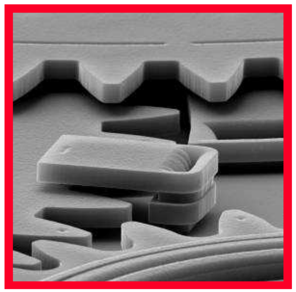
# *Presentation Outline*

- Motivation
- Experimental Capability and Data Analysis
  - Review Original System Design and Early Results
  - Discuss System Improvements
  - Discuss Improvements in Analysis
    (DSMC-based formula to determine thermal
    accommodation coefficients)
- Recent Results for Different Gases (Single-Species)
- Helium/Argon Mixture Experiments and Modeling
- Summary and Future Work

# Gas-Surface Interactions



Spacecraft



MEMS Devices

## Problem

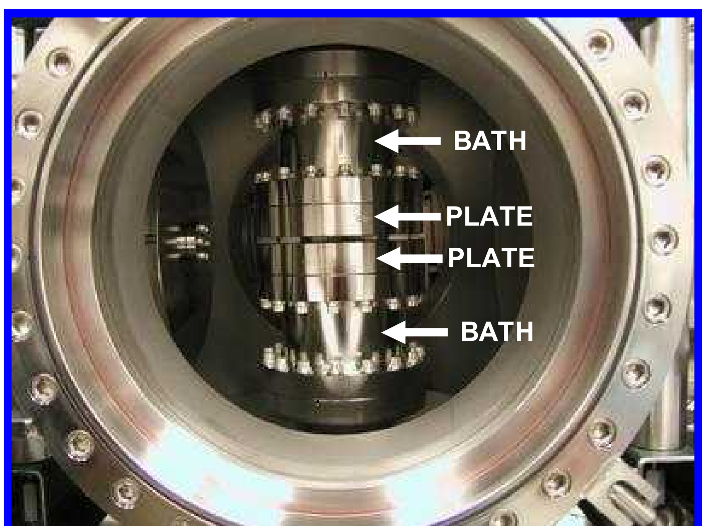
- No-slip, no-jump boundary models break down for rarefied or microscale flows
- Details of gas-surface interaction crucial

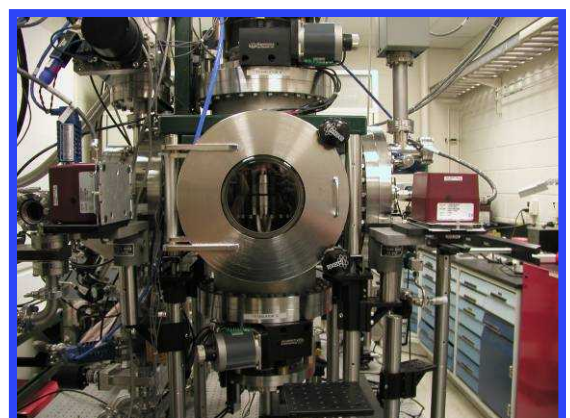
## Applications

- 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

# *Surface Accommodation and Noncontinuum Heat Transfer*

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

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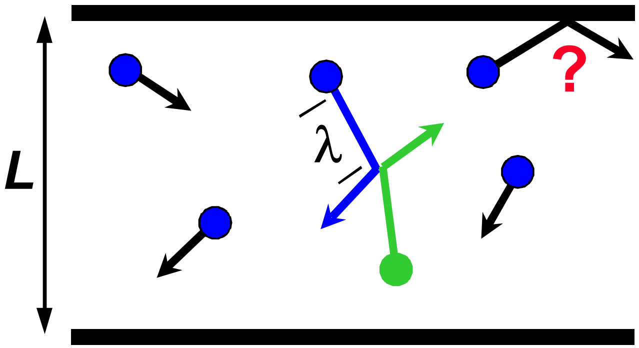
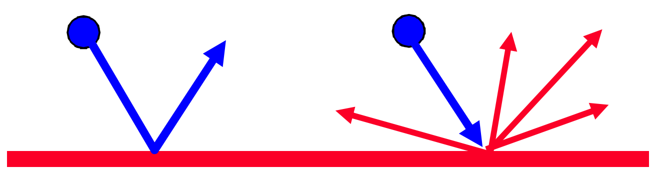
# *Noncontinuum Gas Behavior*






**Molecular and Wall Collisions**

**Specular reflection** **Diffuse reflection**



**Maxwell Wall Model**

| | |
|---|---|
| $\alpha$ | **= 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**

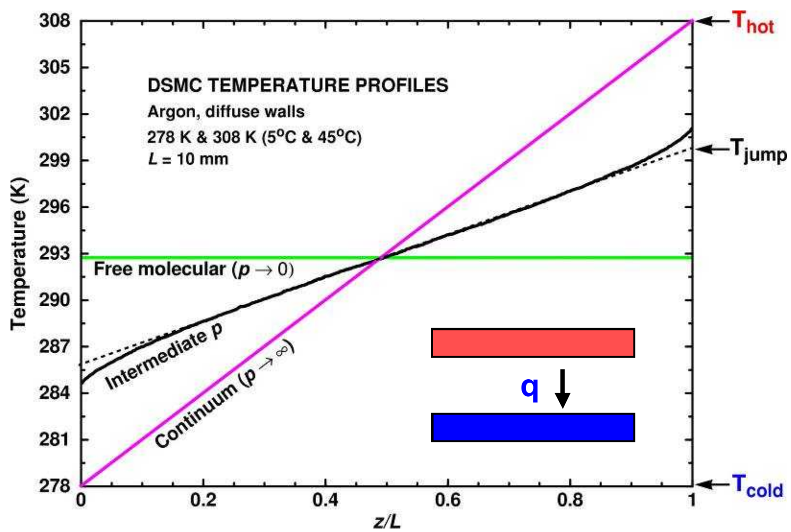
**Gas-surface collisions *not* understood**

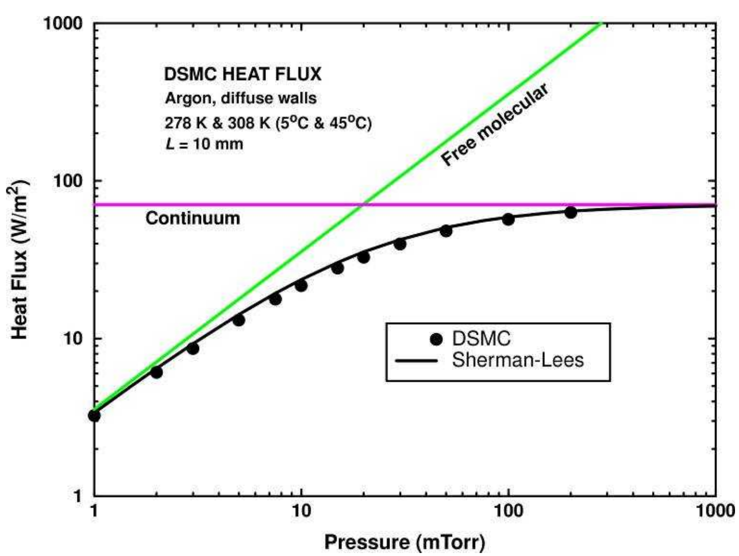
- **Simple *ad hoc* models (e.g., Maxwell, 1890)**
- **MD simulations limited to atomic scale - requires surface characterization**

**DSMC Perspective**

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

# *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
- Use measurement of heat flux vs. pressure to determine accommodation

## Gas-Surface Combinations

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

***Assess gas-surface models in DSMC***

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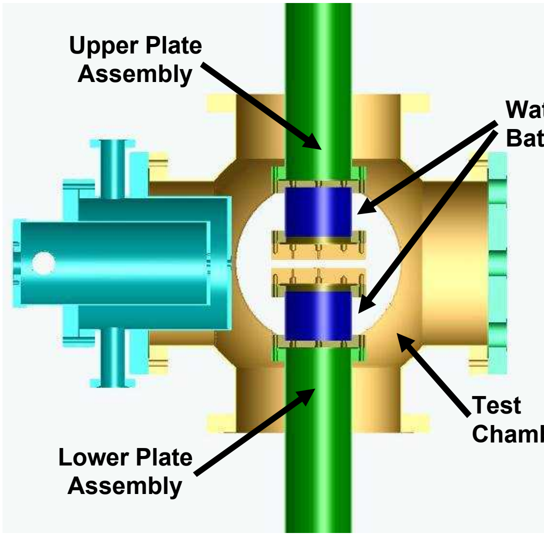
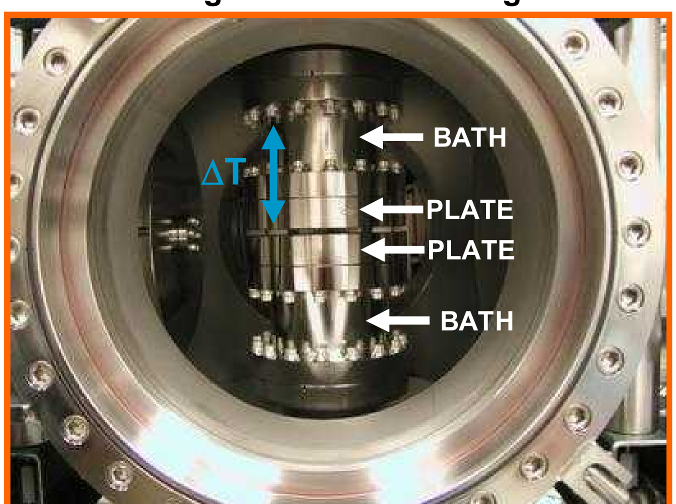
# *Experimental Heat-Flux Measurement*




Original Chamber Design




***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, proportional to ΔT

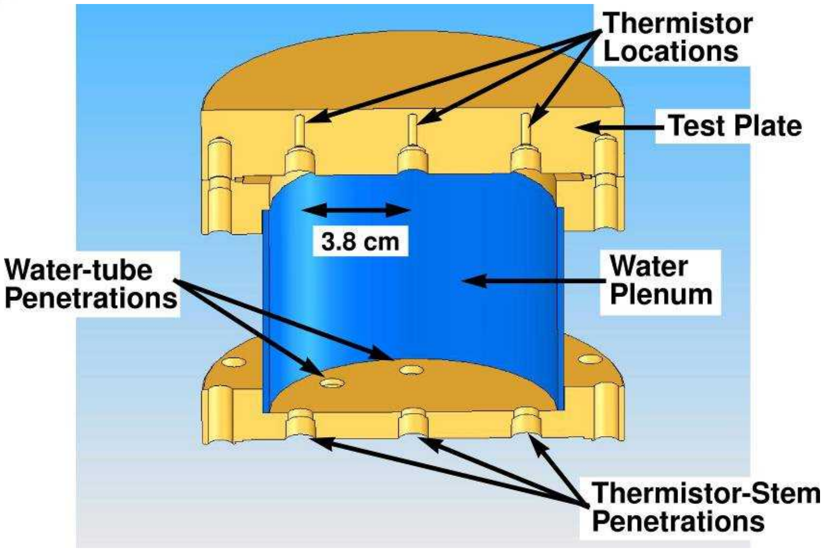
## Challenges:

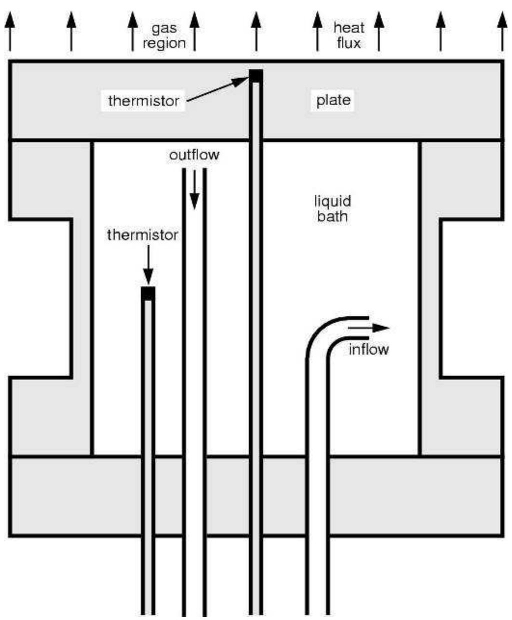
- Very low heat fluxes ⇨ small ΔT
- Need high accuracy measurement of ΔT
- Need high accuracy control of gap (requires precise, reproducible translation of high thermal-mass components)
- Need high accuracy, stable pressure

## High Accuracy Solutions:

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

# Temperature-Difference Measurement




***Infer Heat Flux from Temperature Drop between Plate Surface and Bath***

## 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

# Analysis of Temperature Data

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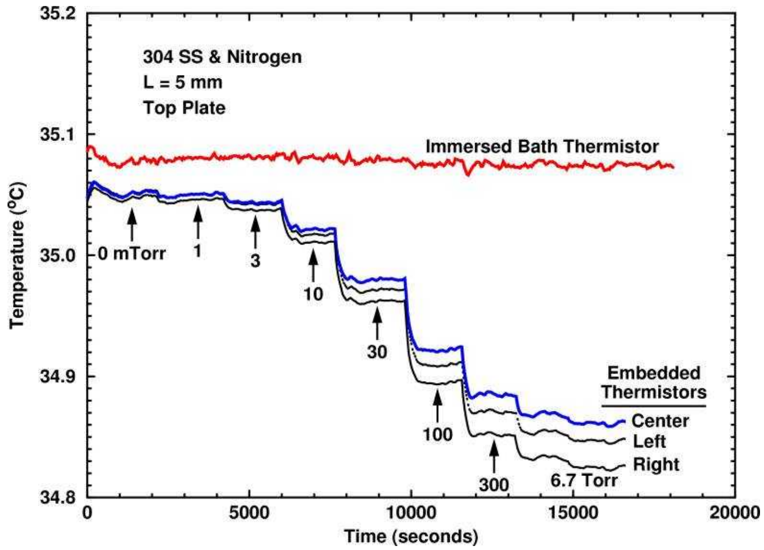


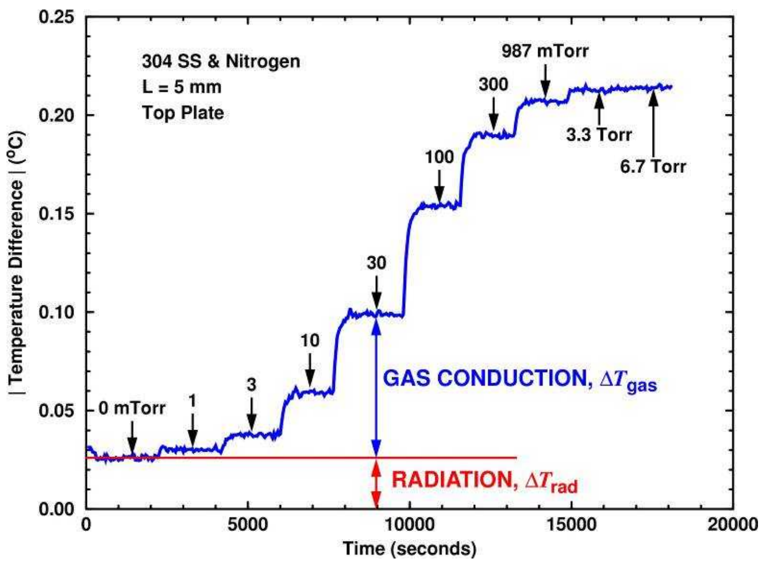


## *Infer Heat Flux from Temperature Drop Across Each Plate*

## 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, $\Delta T$
- Vanishing-pressure limit gives radiation contribution, $\Delta T_{rad}$ *(other parasitic losses may also contribute slightly)*
- Gas-phase heat flux: $\Delta T_{gas} = \Delta T - \Delta T_{rad}$

## Pressure effect clearly evident

## Continuum limit clearly observed

## Some nonideal system behaviors

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

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# Noncontinuum Modeling of Heat Conduction

## Navier-Stokes Slip-Jump (NSSJ)

- Continuum equations plus velocity slip and temperature jump
- Computationally less expensive, approximate for noncontinuum

$$\text{Bulk gas: } \mathbf{q} = -K\nabla T, \quad \rho C_p \left(\partial T / \partial t\right) = \nabla \cdot \left(K \nabla T\right) + S$$

$$\text{Jump BC: } q = h\Delta T, \qquad h = \left(1 + \frac{\varsigma}{4}\right)\left(\frac{\alpha}{2-\alpha}\right)\left(\frac{p\bar{c}}{T}\right)$$

## Direct Simulation Monte Carlo (DSMC)

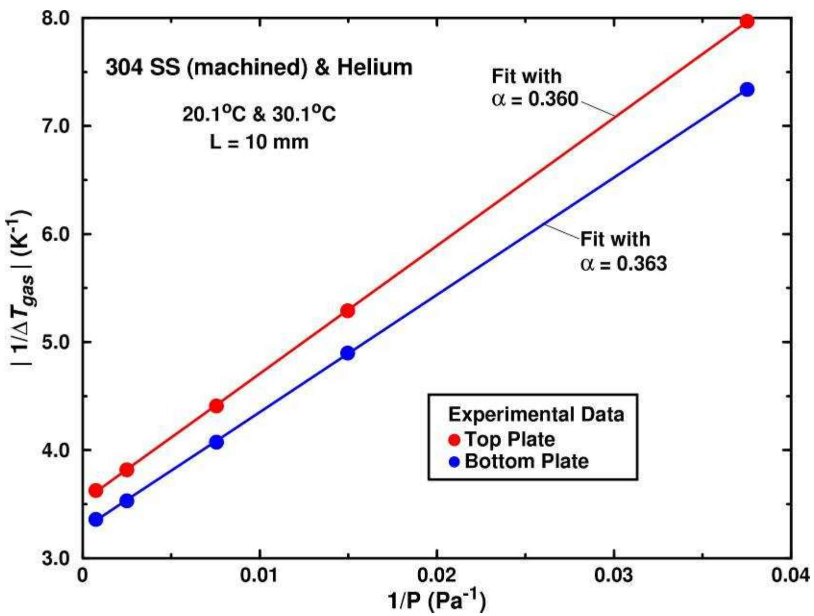
- Molecular statistical simulation of Boltzmann equation
- Computationally more expensive, accurate for noncontinuum

$$\partial\left(nf\right)/\partial t + \mathbf{c} \cdot \nabla\left(nf\right) = C\left[nf\right]$$

# Accommodation Coefficient - Kennard

$$T_g - T_{wall} = \frac{2\gamma}{\gamma+1}\frac{2-\alpha}{\alpha}\frac{\lambda}{\Pr}\frac{dT}{dx}$$

$$\frac{1}{q} = \frac{1}{q_C} + \frac{1}{q_C}\frac{2KT}{L\left(\frac{\alpha}{2-\alpha}\right)\left(1+\frac{\zeta}{4}\right)\overline{c}}\cdot\frac{1}{P}$$




*Approach of Kennard (1938)*

**Use Maxwell Wall Model**

- Fraction $\alpha$ reflected diffusely
- Remainder (1-$\alpha$) reflected specularly
- Assume equal accommodation at walls

**Consider Near-Continuum Regime**

- Small temperature jumps
- Jump proportional to gas mean free path, $\lambda$, and temperature gradient
- Find that 1/*q* linear in 1/*P*
- *Assume* $q \propto \Delta T_{gas}$
- *Calculate* $\alpha$ *from slope*

**Simple Analysis Generally Satisfactory**

- Data well described by linear fit
- Data from top and bottom plates agree

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# *Effects of Gas Composition, Surface Finish and Surface Contamination Explored*

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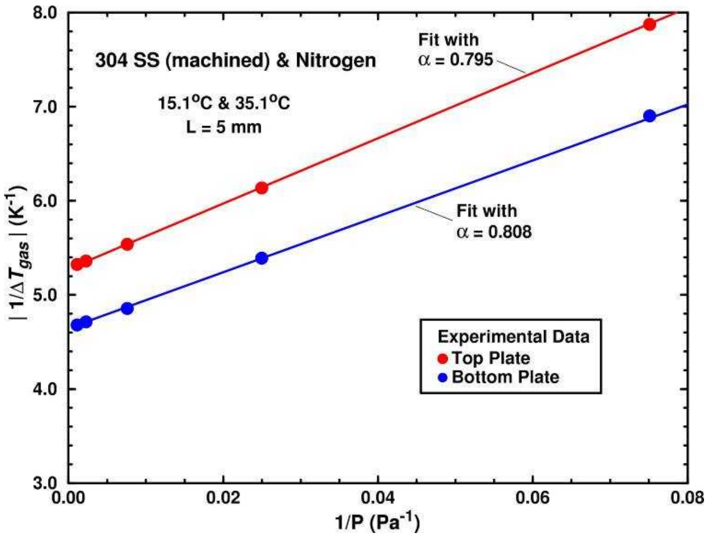


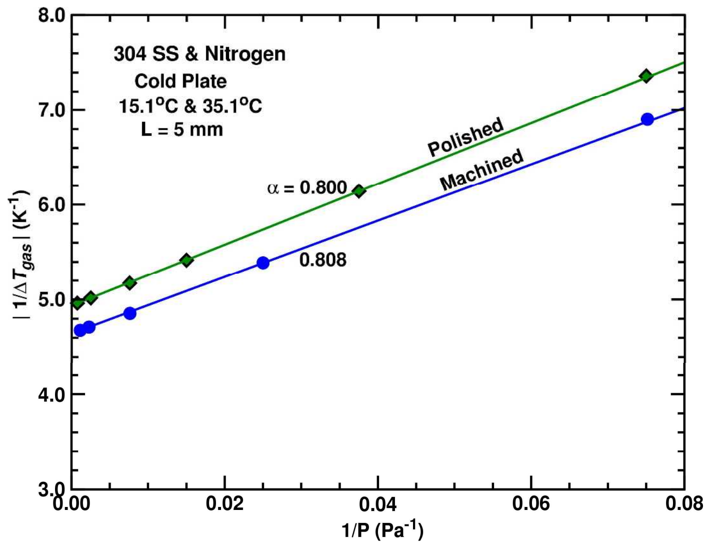


***Maxwell jump model consistent with experimental observations***

**Representative Thermal Accommodation Coefficients (α) for 304 Stainless Steel**

| Gas | α, machined (RMS roughness ~2 μm) | α, polished (RMS roughness ~20 nm) |
|---|---|---|
| Argon | 0.87 ± 0.02 | 0.88 ± 0.02 |
| Nitrogen | 0.80 ± 0.02 | 0.80 ± 0.02 |
| Helium | 0.36 ± 0.02 | 0.40 ± 0.02 |

***Surface roughness plays a minor role***

***Surface contamination identified as an important effect:***

- ***In situ*** **argon-plasma cleaning**
- **Helium and Polished SS: α ⟶ 0.32**

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# *Modifications Have Enhanced System Performance*

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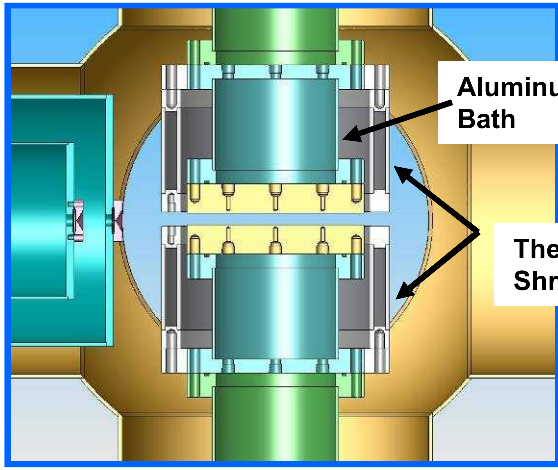
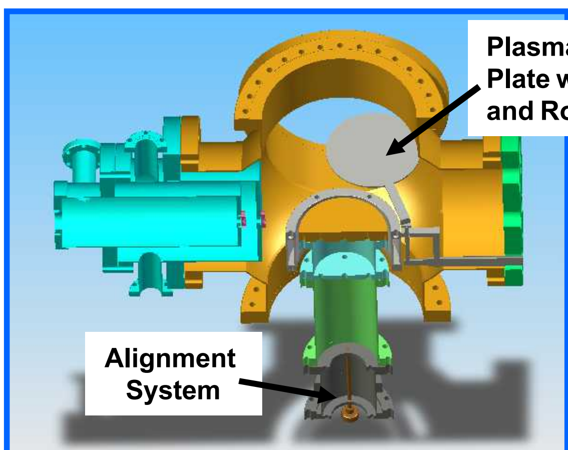



**New Chamber Design with Thermal Shrouds and Plate Alignment System**




## 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

## Inter-Plate Separation Control
- Mechanical plate alignment system
- High-precision, *in situ* plate-gap sensors

## Permanently Mounted Capability for In Situ Plasma Treatment

## Added Hardware for Precision Filling/Metering of Gas Mixtures

***Improvements in plate-temperature uniformity are significant but still less than desired***

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# *Enabling Specifications*

**Temperature Measurement and Control**

- Thermistor Precision ~0.003°C
- Accurate to 0.01°C (by in-house calibration)
- 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

**Electron-Beam Fluorescence**

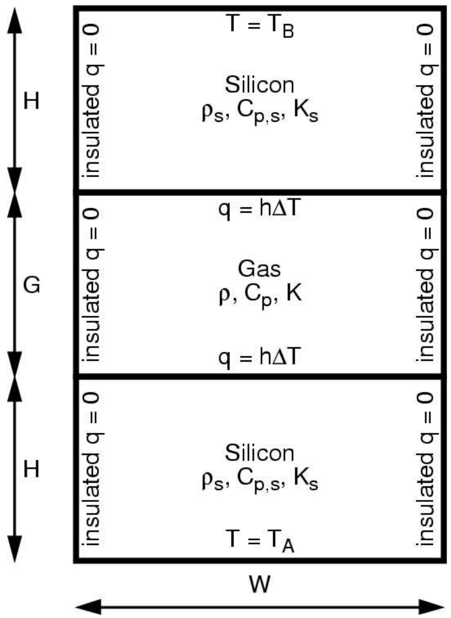
- Stable operation (~0.1% long-term drift in beam current)
- Minimum spot size ~200 μm at long working distance
- Precision gas density studies awaiting further technique improvements

***In Situ* Plasma Treatment**

- Mitigate surface contamination
- Maintain sample plates under vacuum
- Use electron gun to initiate plasma formation

# Computational Analysis of Microgap Heat Transfer Has Motivated New Expression for Heat-Transfer Coefficient

**Application of Navier-Stokes Slip-Jump and DSMC Methods:**




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

$$\lambda = \frac{2\mu}{\rho\bar{c}},\ \bar{c} = \sqrt{\frac{8k_BT}{\pi m}},\ \rho = \frac{mp}{k_BT}$$

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

## Maxwell Gas-Wall Interaction Model

- **Fraction $\alpha$ reflects diffusely**
- **Remainder (1-$\alpha$) reflects specularly**
- **Assume equal accommodation at both walls**

## Heat-Transfer Assumptions

- **All temperatures close to nominal**
- **Heat flux uniform across domain (1-D)**
- **Fourier heat conduction in bulk gas**
- **Temperature jumps at gas-wall boundaries**

## Temperature-Jump Expression

- **Extend Kennard (1938) expression**
- **$c_1$ ~ 0.17 corrects for Knudsen layer**
- **$c_2$ ~ 0.6 corrects for opposite plate**
- **Values vary slightly with gas**

## Heat-Flux/Pressure Relation

- **Find that $1/q$ is almost linear in $1/P$**

# *Accommodation Coefficient – Present Approach*

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$$T_{gas} - T_{wall} = \frac{2\gamma}{\gamma+1}\frac{(2-\alpha)(1+c_1\alpha)}{\alpha}\frac{\lambda}{\Pr}\frac{dT}{dx}$$

$$\frac{1}{q} = \frac{1}{q_C} + \frac{1}{q_C}\frac{2KT(1+c_1\alpha)}{L\left(\frac{\alpha}{2-\alpha}\right)\left(1+\frac{\zeta}{4}\right)\bar{c}}\cdot\frac{1}{P}$$

**Again Use Maxwell Wall Model**

**Consider Near-Continuum Regime**

- **Small temperature jumps**
- **Jump proportional to gas mean free path, $\lambda$, and temperature gradient**
- **Include $c_1$ to obtain correct Knudsen layer**
  - **$c_1$ ~ 0.167 for nitrogen, 0.176 for argon**
  - **Determined from DSMC simulations**
- **Find again that 1/*q* linear in 1/*P***

**Relation to Kennard**

- **Reduces to Kennard when $c_1$ = 0**
- **Almost identical when $\alpha$ << 1**
- **Yields slightly larger values of $\alpha$**

**"Revisit" 304 Stainless Steel Thermal Accommodation Results:**

***Accommodation Coefficient ($\alpha$)***

| Gas | Kennard | Present |
|---|---|---|
| Helium | 0.38 | 0.40 |
| Nitrogen | 0.80 | 0.87 |
| Argon | 0.87 | 0.95 |

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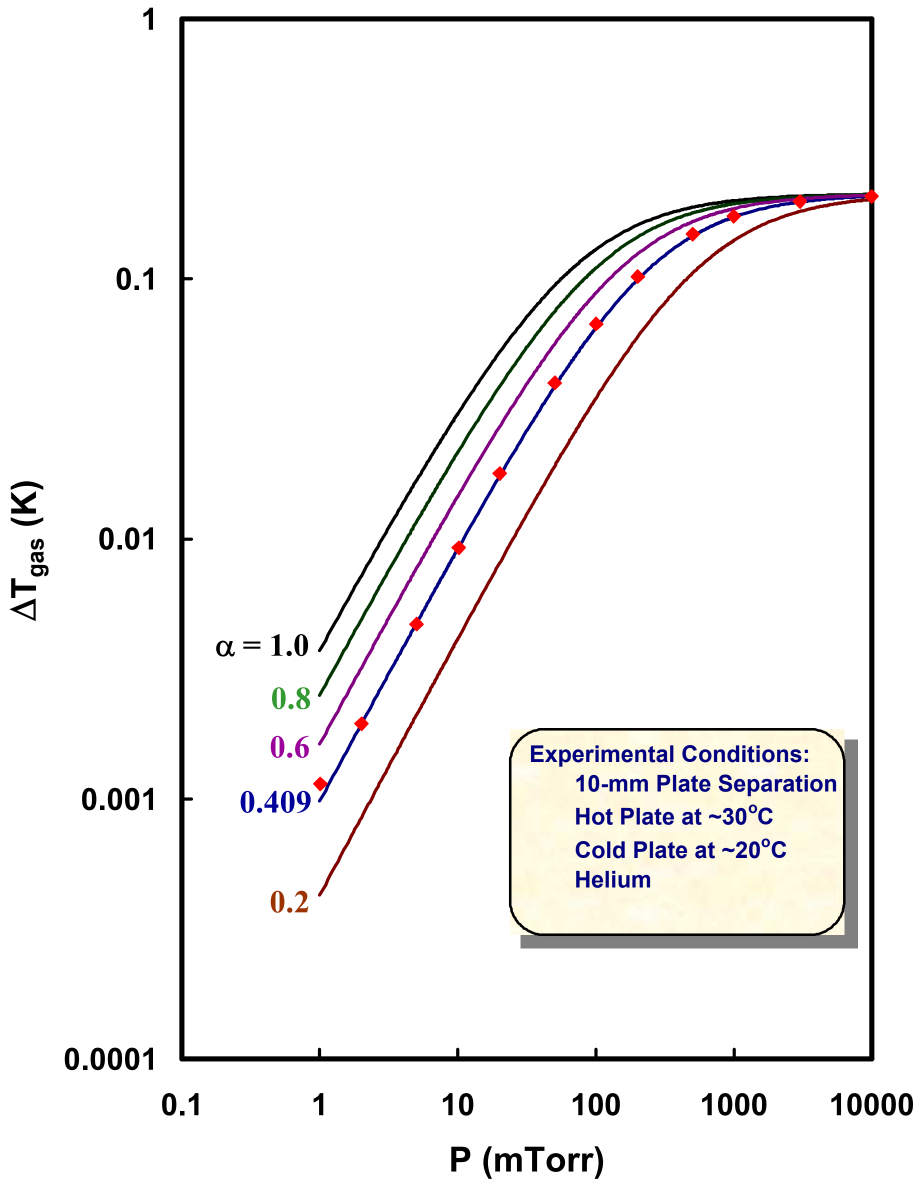
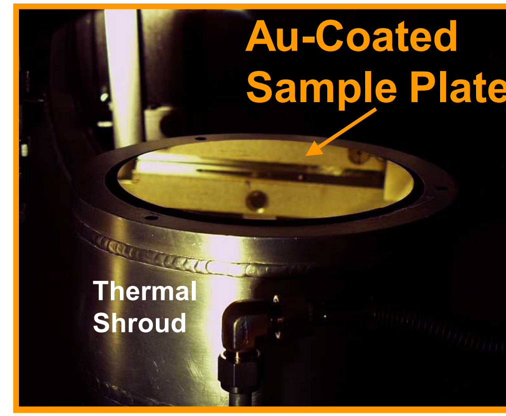
# *Improvements in Experiment and Data Analysis Applied to Gold Surface Studies*




Thin (~10s nm) Gold Coating Applied to 304 Stainless Steel Sample Plate

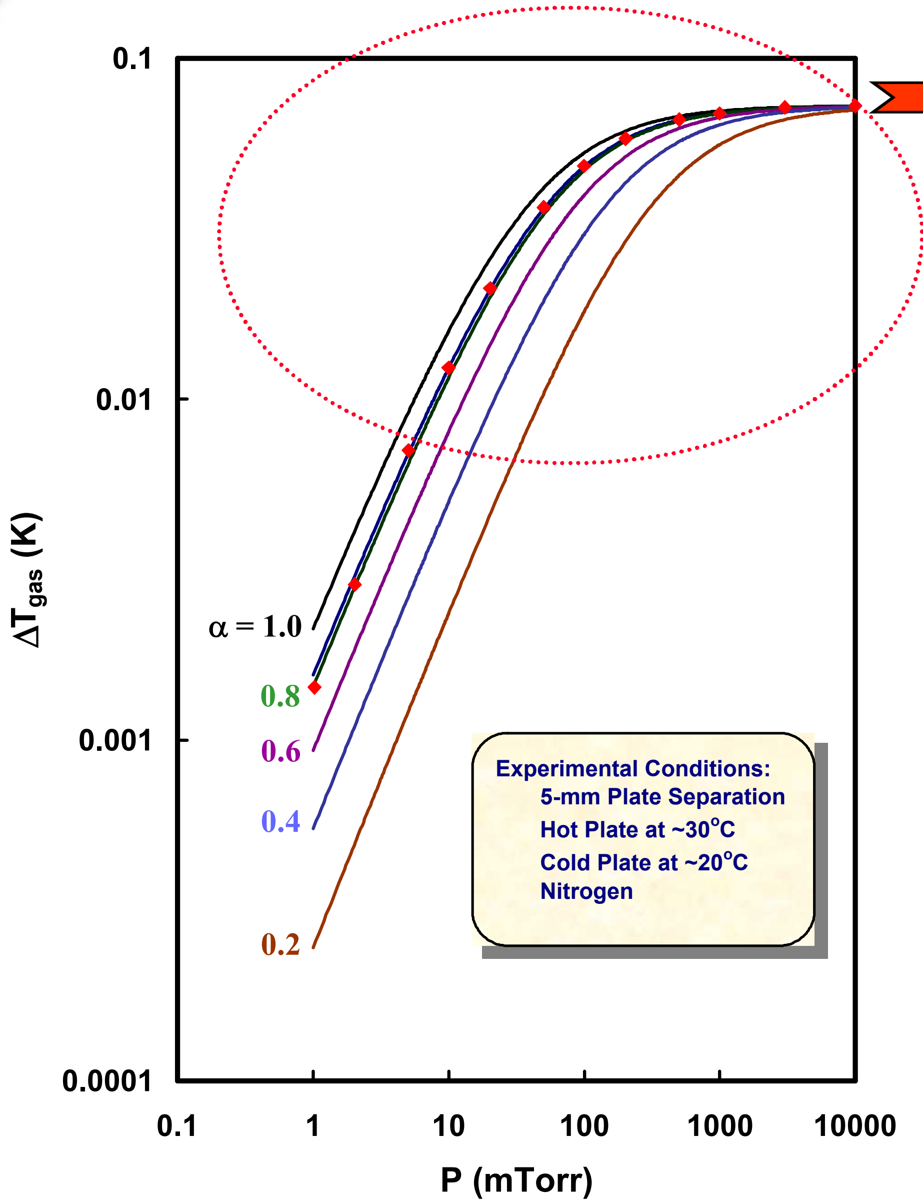
Essentially Identical Top and Bottom Plates

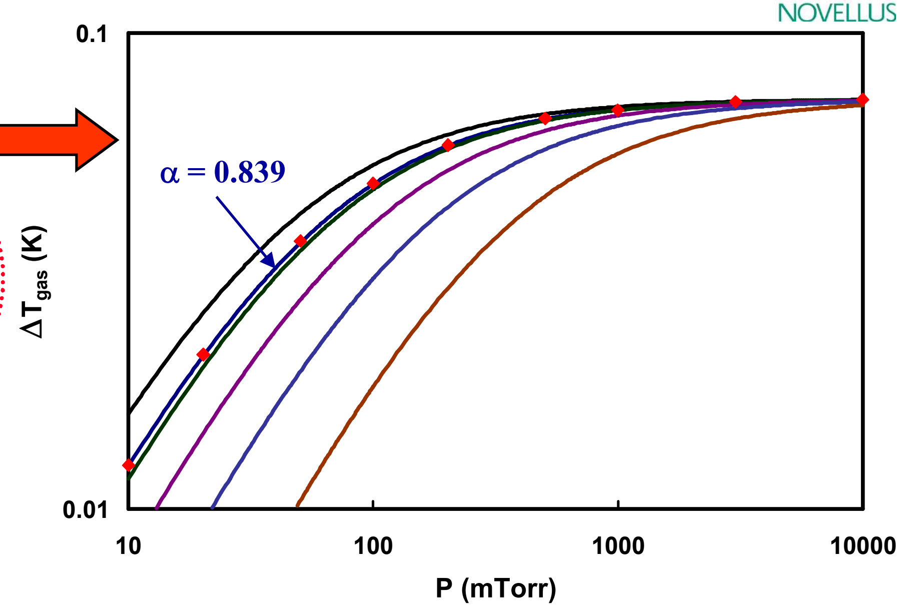
Regression Analysis Provides Optimal Fit to Experimental Data

Accommodation Coefficients Obtained with Different Plate Separations Are in Reasonable Agreement

α (Helium) = 0.41 ± 0.02

# Effect of Gas Composition




## Thermal Accommodation Coefficients for Au-Coated 304 Stainless Steel

| Gas | α Untreated |
|---|---|
| Argon | 0.93 ± 0.02 |
| Nitrogen | 0.83 ± 0.02 |
| Helium | 0.41 ± 0.02 |

***Results are very similar to those for bare 304 Stainless Steel (!)***

***Role of Coating Thickness? Surface Contamination?***

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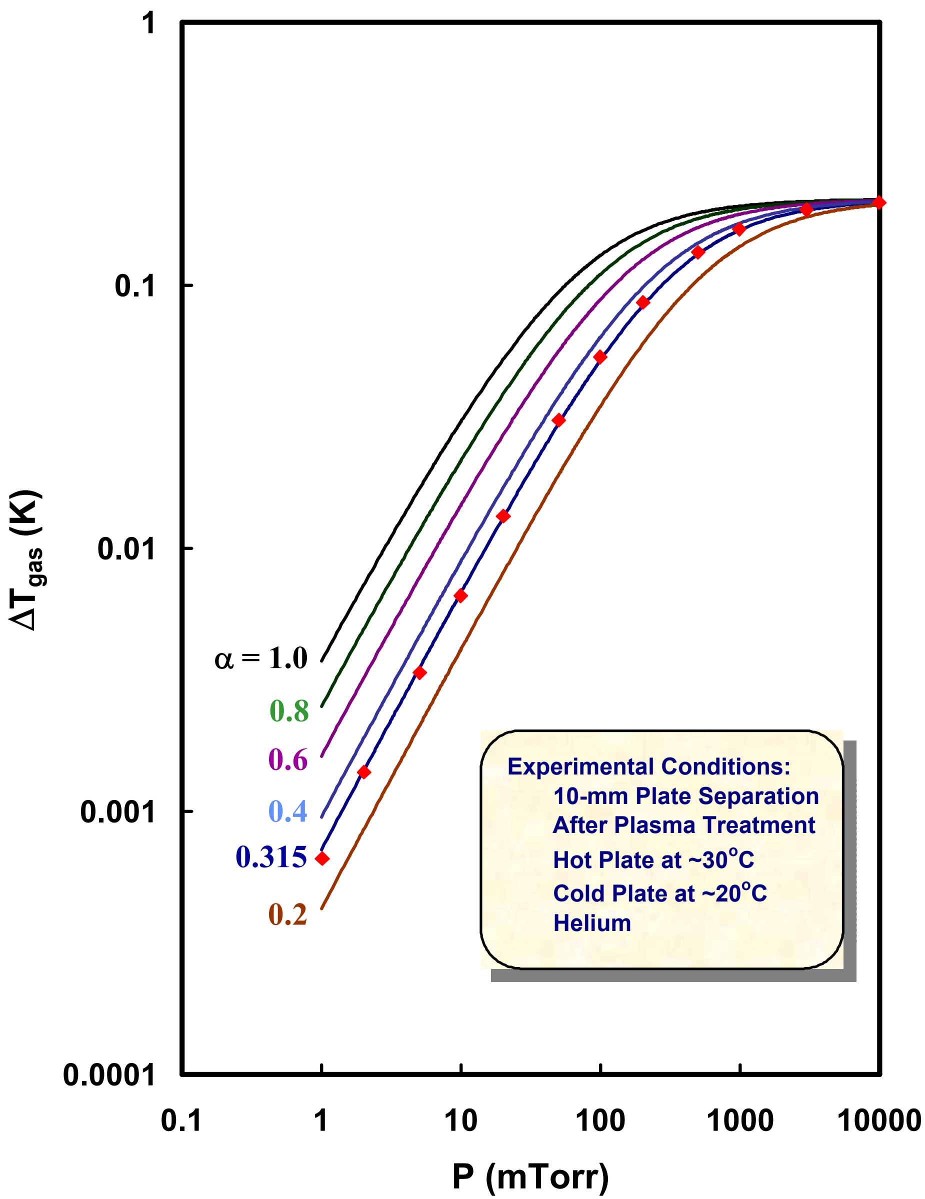
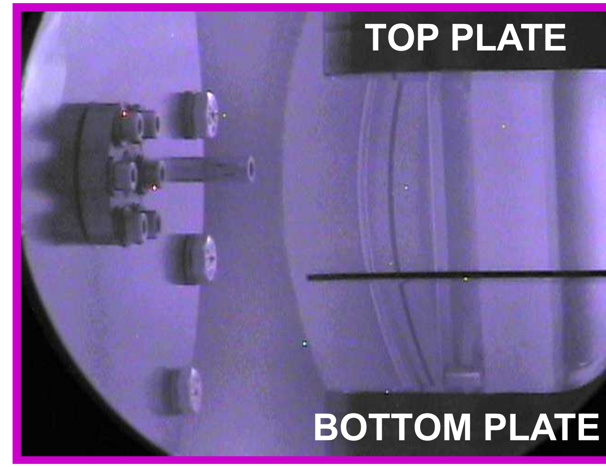
# *Effect of Surface Contamination Evaluated for Different Gases*




**Sample chamber illuminated by argon plasma used for surface treatment**

**Thermal Accommodation Coefficients for Au-Coated 304 Stainless Steel**

| Gas | α Untreated | α Plasma-Treated |
|---|---|---|
| Argon | 0.93 ± 0.02 | 0.85 ± 0.02 |
| Nitrogen | 0.83 ± 0.02 | 0.77 ± 0.02 |
| Helium | 0.41 ± 0.02 | 0.31 ± 0.02 |

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

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# Helium/Argon Mixtures Have Also Been Evaluated

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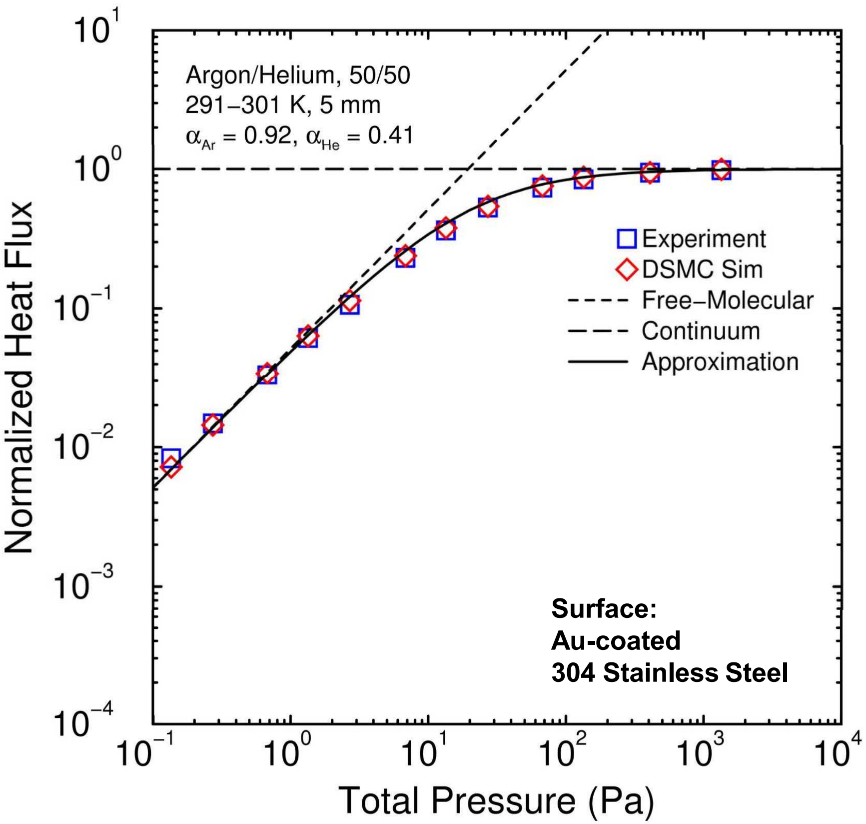
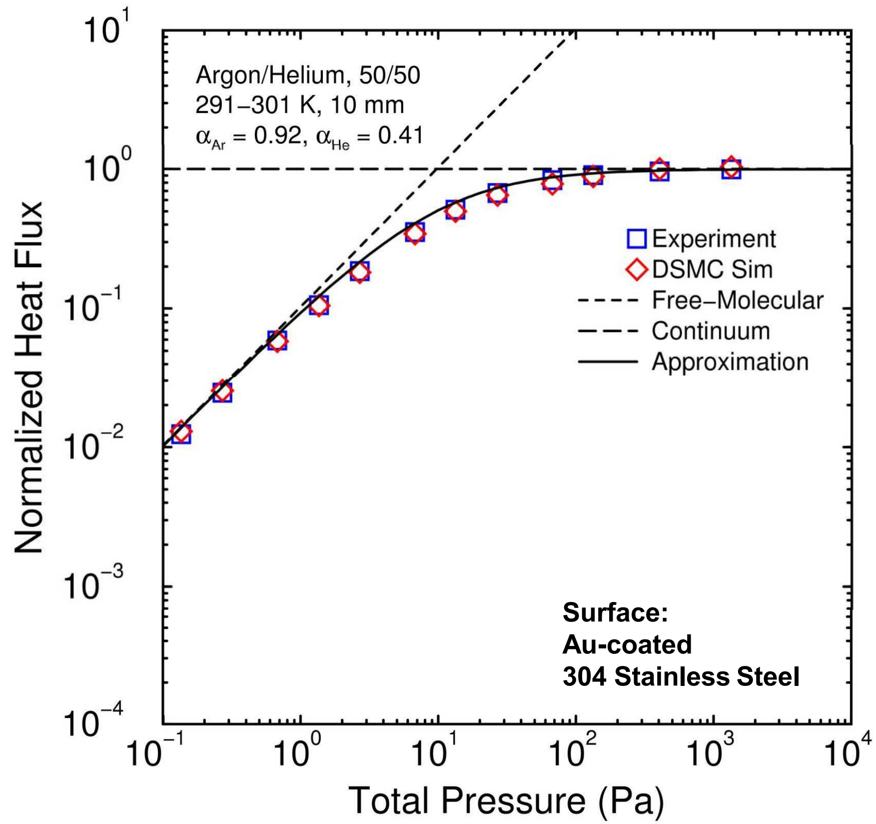
**DSMC simulations with gas-surface model must predict heat flux accurately**

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




***Agreement of experiment and DSMC simulations is good but not optimal***

***Both experimental and computational issues warrant further exploration***

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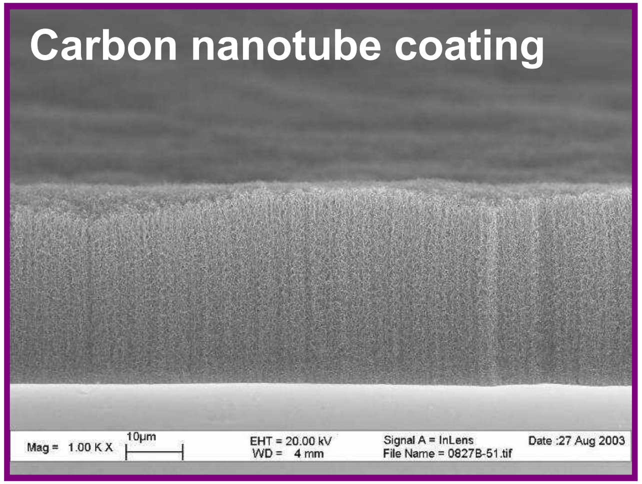
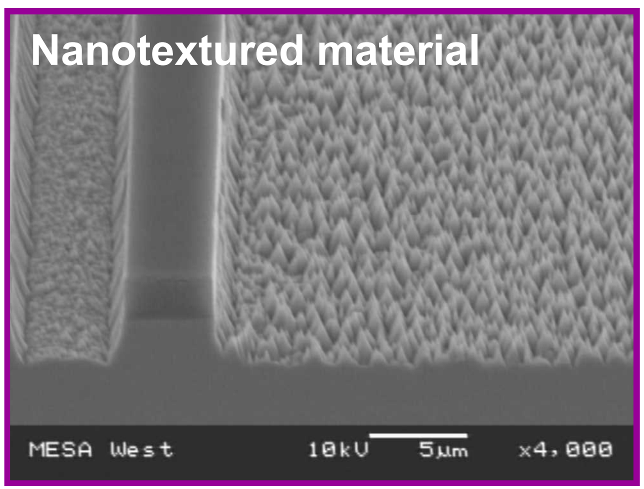
# Summary

- 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 new DSMC-based formula to determine thermal accommodation coefficients
- Self-consistent results have been obtained for a variety of surfaces and three different gas species
- Results thus far indicate that surface roughness plays a minor role in accommodation but surface contamination is important
- 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
- Agreement of experiment and DSMC simulations is good; however, significant experimental and computational issues warrant further exploration

# Future Work



Carbon nanotube coating



Nanotextured material

## Continued analysis of materials with MEMs and semiconductor applications

- Evaluate role of surface material thickness (e.g., compare gold-plating to gold-coating)
- Evaluate scope/circumstances of surface contamination effects
- Expand database to include materials such as silicon, aluminum, polysilicon, etc.

## Pursue additional improvements to experimental design

- Further mitigation of parasitic heat loss
- Develop complementary gas-density test capability

## Continued comparison with DSMC

## Apply techniques to exotic surfaces, novel materials