



**EXPERIMENTAL AND COMPUTATIONAL
ANALYSIS OF THE INTERACTION OF
CARBON AND SILICON ABLATION
PRODUCTS IN EXPANDING HYPERSONIC
FLOWS**

DISSERTATION

Brian E. Donegan, Major, USAF
AFIT-ENY-DS-18-D-035

**DEPARTMENT OF THE AIR FORCE
AIR UNIVERSITY**

AIR FORCE INSTITUTE OF TECHNOLOGY

Wright-Patterson Air Force Base, Ohio

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DISSERTATION

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Air Education and Training Command
in Partial Fulfillment of the Requirements for the
Degree of Doctor of Philosophy

Brian E. Donegan, B.S., M.E.
Major, USAF

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Brian E. Donegan, B.S., M.E.
Major, USAF

Committee Membership:

Robert B. Greendyke, Ph.D.
Chairman

Kevin C. Gross, Ph.D.
Member

Maj Brook I. Bentley, Ph.D.
Member

Lt Col Darrell S. Crowe, Ph.D.
Member

Adedeji B. Badiru, Ph.D.
Dean, Graduate School of Engineering and Management

In memory of my beloved cat-who-thought-he-was-a-dog, Scooby, who passed away just days before the completion of this dissertation. He was well-traveled after three PCSs, wanted to be everyone's best friend, and could turn anyone into a cat-person.

I'll miss you, buddy.

Abstract

Thermal protection is required for vehicles entering planetary atmospheres to protect against the severe heating loads experienced. Characterization of candidate materials is often done utilizing plasma or arc-jet facilities, which provide steady-state testing of the thermal environments experienced during hypersonic flight, but do not correctly simulate hypersonic flowfields. Conversely, impulse facilities can reproduce flight velocities and enthalpies but have extremely short test times, prohibiting testing of thermal response. Modeling ablation and heating rates, particularly in the wake region, remains a significant challenge due to the complexity of the flowfield. To better understand this complex phenomenon and provide data to validate current computational models, experiments were conducted at the X2 expansion tunnel at the University of Queensland. Preheated strips of C-C and SiC-coated C-C were mounted in a two-dimensional compression wedge and tested in Earth entry flow. Calibrated spectral measurements were obtained in the near-stagnation and expansion regions targeting atomic Si, CN violet, C₂ Swan, atomic N, atomic O, CO, and CO₂ emissions for surface temperatures from approximately 1500 K to 2700 K. Emissions for C-C and SiC appeared similar in the near-stagnation region, increasing near the wall, while emissions for SiC-coated C-C displayed a distinct rise downstream of the shock, which suggests a higher concentration of ablative species. Comparisons were made to simulated results, which were conducted using the LAURA and HARA simulation codes following the process developed for this work. There was generally good agreement for CN emissions, which were most dominant, while the agreement was not as good for the other radiative phenomena investigated. It is believed that the underprediction of the ablation rate of the equilibrium-char model is a key factor.

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There are many people who made this dissertation possible. First, I am grateful for my wife for providing support and encouragement for the past three years while working on this degree. I am thankful for my research advisor, Dr. Robert Greendyke, and his guidance and wisdom throughout my time at AFIT. He enabled me to make this research my own, but redirected me when needed. The counsel and advice of my doctoral committee members, Maj Brook Bentley, Lt Col Darrell Crowe, and Dr. Kevin Gross, also played a significant role in the completion of this research.

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Brian E. Donegan

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List of Acronyms

A2/AD	Anti-Access/Area Denial
AEDC	Arnold Engineering Development Center
AFRL	Air Force Research Laboratory
AHW	Advanced Hypersonic Weapon
AOTV	Aeroassisted Orbital Transfer Vehicle
C₂	Dicarbon
C-C	Carbon-Carbon
C-CAT	Carbon-Carbon Advanced Technologies
CFD	Computational Fluid Dynamics
CHAR	CHarring Ablator Response
CMA	Charring Material Thermal Response and Ablation
CN	Cyanogen
CPS	Conventional Prompt Strike
DARPA	Defense Advanced Research Projects Agency
DoD	Department of Defense
DPLR	Data Parallel Line Relaxation
DSTO	Defence Science and Technology Organisation
EAST	Electric Arc Shock Tube

EDM	Electrical Discharge Machining
EDS	Energy-dispersive X-ray Spectroscopy
FIAT	Fully Implicit Ablation and Thermal Response Program
FUN3D	Fully Unstructured Navier Stokes 3D
FWHM	Full-Width at Half-Maximum
HARA	Hypersonic Air Radiation Algorithm
HAWC	Hypersonic Airbreathing Weapon Concept
HIFiRE	Hypersonic International Flight Research Experimentation
HSSW TM	High Speed Strike Weapon Technology Maturation
HTV	Hypersonic Technology Vehicle
HVST	Hypervelocity Shock Tube
HyFly	Hypersonic Flight Demonstration
HYMETS	Hypersonic Materials Environmental Test System
ICBM	Intercontinental Ballistic Missile
ICCD	Intensified Charge-Coupled Device
JAXA	Japan Aerospace Exploration Agency
KATS	Kentucky Aerothermodynamics and Thermal-response Solver
LAURA	Langley Aerothermodynamic Upwind Relaxation Algorithm
MDA	Missile Defense Agency

MOPAR	Modeling of Pyrolysis and Ablation Response
MWIR	Midwave Infrared
NASA	National Aeronautics and Space Administration
NDAA	National Defense Authorization Act
NEQAIR	Nonequilibrium Air Radiation
NIST	National Institute for Standards and Technology
NPR	Nuclear Posture Review
ONR	Office of Naval Research
PGS	Prompt Global Strike
PHAROS	Parallel Hypersonic Aerothermodynamics and Radiation Optimized Solver
PICA	Phenolic Impregnated Carbon Ablator
QSS	Quasi-Steady State
SAB	Scientific Advisory Board
SEM	Scanning Electron Microscope
SiC	Silicon Carbide
SPARTA	Stochastic PARallel Rarefied-gas Time-accurate Analyzer
SRB	Smeared Rotational Band
TBG	Tactical Boost Glide

TCRP	Two Color Ratio Pyrometry
TITAN	Two-dimensional Implicit Thermal Ablation
TPS	Thermal Protection System
TRL	Technology Readiness Level
TVD	Total Variation Diminishing
UQ	University of Queensland
US	United States
USAF	United States Air Force
UV	Ultraviolet
vis/nIR	Visible/Near Infrared

List of Symbols

$A_{f,r}$	pre-exponential term used in evaluating the forward reaction rate coefficient
A_{sj}	constant used in determining μ_{sj}
a_{sr}	nondimensional parameter for collision of species s and r used in defining thermal conductivity
b_ν	line-shape function
C_p^s	specific heat at constant pressure for species s , $\text{J kg}^{-1} \text{K}^{-1}$
C_v^s	specific heat at constant volume for species s , $\text{J kg}^{-1} \text{K}^{-1}$
$C_{v,rot}^s$	specific heat at constant volume for species s for rotational energy, $\text{J kg}^{-1} \text{K}^{-1}$
$C_{v,tr}^s$	specific heat at constant volume for species s for translational energy, $\text{J kg}^{-1} \text{K}^{-1}$
$C_{v,vib}$	specific heat at constant volume for vibrational energy, $\text{J kg}^{-1} \text{K}^{-1}$
$C_{v,vib}^s$	specific heat at constant volume for species s for vibrational energy, $\text{J kg}^{-1} \text{K}^{-1}$
c	velocity of light, $2.997925 \times 10^{10} \text{ cm s}^{-1}$
$c_{c,k}$	mass fraction of species k in the char gas
$c_{g,k}$	mass fraction of species k in the pyrolysis gas
c_k	mass fraction of species k
$\bar{c}_s$	average molecular velocity of molecule s , m s^{-1}
$c_{s,k}$	mass fraction of species k at the gas-solid interface
$c_{w,C}$	mass fraction of atomic carbon at the wall
$c_{w,k}$	mass fraction of species s at the wall
D_k	effective diffusion coefficient of species k , $\text{m}^2 \text{s}^{-1}$
D_s	effective diffusion coefficient, $\text{m}^2 \text{s}^{-1}$
D_s^a	effective diffusion coefficient for ions, $\text{m}^2 \text{s}^{-1}$
D_{sr}	binary diffusion coefficient for species s and r , $\text{m}^2 \text{s}^{-1}$
E	total energy per unit mass of the mixture, J kg^{-1}
$E_{f,r}$	activation energy for forward reaction r , J

E_i	electronic energy for an atomic level i , cm^{-1}
E_{ionize}	ionization energy of an atomic level i , cm^{-1}
e	electron charge, $4.80298 \times 10^{-10} \text{ cm}^{3/2} \text{ g}^{1/2} \text{ s}^{-1}$
e_e	mixture electronic energy per unit mass, J kg^{-1}
$e_{e,s}$	electronic energy (enthalpy) per unit mass of species s , J kg^{-1}
e_s	energy per unit mass of species s , J kg^{-1}
$e_{s,o}$	energy of formation of species s , J kg^{-1}
e_V	mixture vibrational-electronic energy per unit mass, J kg^{-1}
e_v	mixture vibrational energy per unit mass, J kg^{-1}
$e_{v,s}$	vibrational energy (enthalpy) per unit mass of species s , J kg^{-1}
$e_{v,s}^*$	vibrational energy (enthalpy) per unit mass of species s evaluated at temperature T , J kg^{-1}
$f_{i'j'}$	absorption oscillator strength for a line with an upper level j' and a lower level i'
$f_{V'V''}$	band absorption oscillator strength
g_e'	degeneracy of the upper electronic state
g_e''	degeneracy of the lower electronic state
g_i	degeneracy for an atomic level i
H	total enthalpy per unit mass of the mixture, J kg^{-1}
h	Planck's constant, $6.6256 \times 10^{-34} \text{ J s}^{-1}$
h_c	enthalpy of solid char at T_w , J kg^{-1}
h_g	enthalpy of pyrolysis gas in equilibrium at T_w and P_w , J kg^{-1}
h_w	enthalpy of gas at the wall, J kg^{-1}
h_s	enthalpy per unit mass of species s , J kg^{-1}
$h_{s,o}$	enthalpy of formation of species s , J kg^{-1}
$h_{V,s}$	vibrational-electronic enthalpy per unit mass of species s , J kg^{-1}
I_ν	frequency-dependent radiative intensity, $\text{J cm}^{-2} \text{ sr}^{-1}$

J_k	diffusion mass flux of species k , $\text{kg m}^{-2} \text{s}^{-1}$
J_s	mass diffusion fluxes of species s , $\text{kg m}^{-2} \text{s}^{-1}$
j_ν	frequency-dependent emission coefficient, $\text{J s cm}^{-3} \text{sr}^{-1}$
$j_{\nu,i'j'}^{bb}$	frequency-dependent bound-bound emission coefficient, $\text{J s cm}^{-3} \text{sr}^{-1}$
$j_{\nu,i'j'}^{bf}$	frequency-dependent bound-free emission coefficient, $\text{J s cm}^{-3} \text{sr}^{-1}$
j_ν^{ff}	frequency-dependent free-free emission coefficient, $\text{J s cm}^{-3} \text{sr}^{-1}$
$j_{\nu,ul}$	frequency-dependent emission coefficient of a single rotational line resulting from a transition from u to l , cm^{-1}
$K_{eq,r}$	equilibrium constant for reaction r
$K_{s,C}$	equilibrium constant for heterogeneous reaction $\text{C(solid)} \rightarrow \text{C(gas)}$
k	Boltzmann constant, $1.380622 \times 10^{-23} \text{J K}^{-1}$
$k_{b,r}$	backward reaction rate coefficient for reaction r , units vary
$k_{f,N}$	forward reaction rate for the carbon nitridation reaction
$k_{f,O}$	forward reaction rate for the primary carbon oxidation reaction
k_{f,O_2}	forward reaction rate for the secondary carbon oxidation reaction
$k_{f,r}$	forward reaction rate coefficient for reaction r , units vary
k_ν	frequency-dependent absorption coefficient, cm^{-1}
$k_{\nu,i'j'}^{bb}$	frequency-dependent bound-bound absorption coefficient, cm^{-1}
$k_{\nu,i'j'}^{bf}$	frequency-dependent bound-free absorption coefficient, cm^{-1}
k_ν^{ff}	frequency-dependent free-free absorption coefficient, cm^{-1}
$k_{\nu,ul}$	frequency-dependent absorption coefficient of a single rotational line resulting from a transition from u to l , cm^{-1}
M_C	molecular weight of atomic carbon, $12.01 \text{ kg kmol}^{-1}$
m	electron mass, $9.1091 \times 10^{-28} \text{ g}$
$\dot{m}$	mass flux at the surface, $\text{kg m}^{-2} \text{s}^{-1}$
$\dot{m}_c$	mass flux of surface char, $\text{kg m}^{-2} \text{s}^{-1}$

$\dot{m}_g$	mass flux of pyrolysis gas at the surface, $\text{kg m}^{-2} \text{s}^{-1}$
m_s	mass of species s per particle, kg
N_e	electron number density, particles m^{-3}
$N_{e'}$	number density of the upper electronic state, particles m^{-3}
$N_{e''}$	number density of the lower electronic state, particles m^{-3}
N_i	number density of an atomic level i , particles m^{-3}
N_r	number of reactions in chemical kinetic model
N_+	ion number density, particles m^{-3}
$n_{f,r}$	power of temperature dependence on pre-exponential factor for forward reaction r
n_j	number density of species j , particles m^{-3}
n_s	number density of molecule s , particles m^{-3}
P	pressure, Pa
P_e	electron pressure, Pa
P_s	partial pressure of species s , Pa
P_w	pressure at the wall, Pa
$Q_{J'}$	partition function of the upper rotational state
$Q_{J''}$	partition function of the lower rotational state
$Q_{V'}$	partition function of the upper vibrational state
$Q_{V''}$	partition function of the lower vibrational state
Q_{rad}	radiative energy transfer rate, $\text{J m}^{-3} \text{s}^{-1}$
Q_+	ion partition function, non-dimensional
q_{cond}	heat flux conducted into surface, W m^{-2}
q_{conv}	convective heat flux, W m^{-2}
q_{rad}	radiative heat flux, W m^{-2}
$\bar{R}$	universal gas constant, $8314.2 \text{ J kmol}^{-1} \text{ K}^{-1}$
$R_{b,r}$	backward reaction rate for reaction r , $\text{kmol m}^{-3} \text{s}^{-1}$

$R_{f,r}$	forward reaction rate for reaction r , $\text{kmol m}^{-3} \text{s}^{-1}$
$S_{J'J''}$	line-intensity factor
s	gas species
s_s	entropy per unit mass of species s , $\text{J kg}^{-1} \text{K}^{-1}$
T	translational-rotational temperature, K
T_d	rate controlling temperature for dissociation reactions, K
T_e	electron-electronic excitation temperature, K
T_V	vibrational-electron-electronic temperature, K
T_w	wall Temperature, K
u_i	velocity in the i direction, m s^{-1}
u_j	velocity in the j direction, m s^{-1}
u_k	velocity in the k direction, m s^{-1}
v_w	velocity normal to the wall, m s^{-1}
y_s	mole fraction of species s
$\dot{w}_s$	mass rate of production of species s per unit volume, $\text{kg m}^{-3} \text{s}^{-1}$
Z	charge number of the species
α	surface absorptivity
$\alpha_{s,r}$	stoichiometric coefficient for reactants in reaction r
$\beta_{s,r}$	stoichiometric coefficient for products in reaction r
γ_s	molar concentration of species s , kmol m^{-3}
Δ_{sr}	collision integrals for species s and r , m s
δ_{ij}	Kronecker delta
ϵ	surface emissivity
η	frozen thermal conductivity for translational-rotational energy of heavy particles, $\text{J m}^{-1} \text{s}^{-1}$
η_r	frozen thermal conductivity for rotational energy, $\text{J m}^{-1} \text{s}^{-1}$

η_e	frozen thermal conductivity for electronic energy due to collisions between electrons and all particles, $\text{J m}^{-1} \text{s}^{-1}$
η_t	frozen thermal conductivity for translational energy, $\text{J m}^{-1} \text{s}^{-1}$
η_v	frozen thermal conductivity for vibrational energy due to collisions between molecules and all particles, $\text{J m}^{-1} \text{s}^{-1}$
θ_{sj}	characteristic vibrational temperature, K
λ	second coefficient of viscosity, N s m^{-2}
λ_{CL}	wavelength of the centerline in the spectrum of an atomic or molecular line, cm
μ	mixture coefficient of viscosity, N s m^{-2}
μ_{sj}	reduced molecular weight of the colliding species s and j , kg kmol^{-1}
ν_{es}	effective collision frequency for electrons and heavy particles in electronic-translational energy relaxation, s^{-1}
ρ	mixture density, kg m^{-3}
ρ_{E,C_x}	equilibrium vapor pressure, Pa
ρ_e	electron density, kg m^{-3}
ρ_s	density of species s , kg m^{-3}
ρ_w	density at the wall, kg m^{-3}
σ	Stefan-Boltzmann constant, $5.66961 \times 10^{-8} \text{ W m}^{-2} \text{ K}^{-4}$
σ_s	effective cross-section for vibrational relaxation, m^2
$\sigma_{\nu,i}^{bf}$	bound-free absorption cross-section of level i , cm^2
τ_{ij}	viscous shear stresses, Pa
$< \tau_s >$	translational-vibrational energy relaxation time for molecular species s , s
$\Omega_{s,r}$	average collision cross-section for collisions between species s and r , m^2

EXPERIMENTAL AND COMPUTATIONAL ANALYSIS OF THE INTERACTION OF CARBON AND SILICON ABLATION PRODUCTS IN EXPANDING HYPERSONIC FLOWS

I. Introduction

Over the past few decades, the United States Air Force (USAF) and the Department of Defense (DoD) have had a renewed interest in hypersonics. In 2001, under the tasking of Congress, the DoD conducted a comprehensive Nuclear Posture Review (NPR). In doing so, a new Nuclear Triad was established, which integrated conventional strike capabilities with strategic nuclear weapons, broadening the range of capabilities to dissuade adversaries [1]. In 2003, the DoD identified a new mission area, Prompt Global Strike (PGS), with the goal of providing the capability to strike targets anywhere in the world with a conventional weapon in as little as an hour. The vision was to deter and defeat adversaries while providing the ability to strike high-value, time-sensitive targets. A number of systems have been considered to provide this capability including bombers, cruise missiles, ballistic missiles, and boost-glide technologies [2].

In 2008, Congress created a single, combined fund to support research and development for the PGS mission area with much of the funding allocated to hypersonic glide experiments and concept demonstration development. In April 2010, the DoD conducted the first test of the Hypersonic Technology Vehicle (HTV)-2, which failed minutes after liftoff. A second test of the HTV-2 was conducted in August 2011, which experienced an anomaly along its glide trajectory, resulting in the vehicle also failing. Both tests were considered partial successes as the boost mechanism performed as

expected, the detachment of the glide vehicle was successful, and a significant amount of data was collected [2].

While the Air Force and Defense Advanced Research Projects Agency (DARPA) were developing the HTV-2, the Army was developing a hypersonic glide vehicle with a shorter range, known as the Advanced Hypersonic Weapon (AHW). A first successful flight test was conducted in November 2011 [2, 3]. A second flight test was conducted in August 2014 [2, 4]. This test ended prematurely as controllers destroyed the vehicle due to an anomaly.

The past two decades have also seen significant development of scramjet technologies, necessary for sustained hypersonic flight. In 2005, the Air Force Research Laboratory (AFRL) awarded a contract for the development of the X-51A Waverider to demonstrate an endothermically fueled scramjet engine in flight [5]. In May 2013, the X-51A vehicle separated from its booster and accelerated to Mach 5.1, flying for 240 seconds. Other recent demonstrations, including the National Aeronautics and Space Administration (NASA)-AFRL-Australian Defence Science and Technology Organisation (DSTO)'s Hypersonic International Flight Research Experimentation (HIFiRE) program and the Office of Naval Research (ONR)-DARPA Hypersonic Flight Demonstration (HyFly) have also helped to mature hypersonic technologies [6]. These recent hypersonic technology demonstration efforts, coupled with an increasing focus on access to denied airspace, have further fueled the USAF's renewed interest in hypersonics.

In July 2014, the Air Force released its 30-year strategy, *America's Air Force: A Call To The Future* [7]. In this document, the Air Force details its core missions and lays a path to meet the needs of the United States over the next 30 years. One of the key tenets of this document is the continued pursuit of game-changing technologies including hypersonics, nanotechnology, directed energy, unmanned systems, and au-

onomous systems. The Air Force’s increased interest in hypersonics has been echoed in many other recent high-level documents including the *USAF Strategic Master Plan* (May 2015) [8], which translates the Air Force’s 30-year strategy into comprehensive guidance, goals, and objectives, *Air Force Future Operating Concept: A View Of The Air Force In 2025* (September 2015) [9], which is a complementary document to the Strategic Master Plan that broadly portrays how the Air Force will conduct its mission areas, and *Air Superiority 2030 Flight Plan: Enterprise Capability Collaboration Team* (May 2016) [10], which develops capability options to enable joint force air superiority in the highly-contested environment of 2030 and beyond.

In 2014, the USAF Scientific Advisory Board (SAB), which is a Federal advisory committee chartered by the Secretary of Defense to conduct studies on topics deemed critical to the Air Force, executed a study to examine the potential military utility of hypersonic technologies to the Air Force [6, 11]. In conducting this study, the SAB characterized the maturity of enabling technologies and identified system concepts. The committee collected data from across the USAF operational, research, and test communities as well as across the DoD, the Intelligence Community, and industry. The committee found that, based on the current state of hypersonic technology readiness and DoD plans for further advancement of the required capabilities, an air-launched tactical range hypersonic strike weapon could be fielded with substantial operational utility in projected Anti-Access/Area Denial (A2/AD) environments in the 2025 timeframe. The SAB, which considered both airbreathing and boost-glide technologies, found that hypersonic technology research and demonstration efforts over the past decade have advanced many of the key technologies including aerodynamics, propulsion, structures, materials, and flight controls, to a Technology Readiness Level (TRL) of 5 or higher, which is indicative of component-level testing in a relevant environment. Current technology maturation efforts and

flight demonstrations, including the High Speed Strike Weapon Technology Maturation (HSSW TM), Hypersonic Airbreathing Weapon Concept (HAWC), and Tactical Boost Glide (TBG), which combined constitute a nearly billion dollar investment, are postured to bring the remaining technologies to a TRL of 6+, indicating system or subsystem demonstration in a relevant environment, by 2020 [6].

High temperature materials have long been a critical technology area for hypersonics dating back to the 1950s and the development of the Intercontinental Ballistic Missile (ICBM) [12]. A Thermal Protection System (TPS), which is typically characterized as ablative or non-ablative, represents a single point of failure [13] and is necessary to protect crews and payloads from the severe thermal and mechanical loads experienced by a hypersonic vehicle. Ablative TPSs, which can be characterized by sacrificial loss of material, are comprised of two categories of materials: charring/pyrolyzing and non-charring/non-pyrolyzing. Charring ablators, such as Phenolic Impregnated Carbon Ablator (PICA) or Avcoat, are composites consisting of a polymer filler (or resin) with a reinforcing material, such as carbon [14]. When heated, the resin experiences chemical reactions that release gaseous products, known as pyrolysis, leaving a layer of char at the surface. Non-charring ablators, such as reinforced Carbon-Carbon (C-C), lose mass by surface ablation and mechanical erosion [14]. Although C-C is particularly well-suited for structural applications where thermal shock resistance is needed [6], oxidation is a significant concern at surface temperatures as low as 700 K [15–17]. Under these conditions, the TPS experiences significant material loss and strength degradation [15, 18], limiting its utility as a reusable TPS material [19].

Due to the oxidation concerns of C-C, several high-temperature materials have been proposed as possible material candidates for hypersonic vehicles. Silicon Carbide (SiC), for example, has been extensively studied as a potentially-reusable TPS

material, particularly for critical vehicle components including leading edges, control surfaces, and nose tips, and as a possible protective coating material for C-C [15–30]. Much of this research has been focused on characterizing the oxidation of SiC, particularly the transition from “passive” oxidation to “active” oxidation. This transition, which is a complex phenomenon that is dependent on both temperature and the partial pressure of oxygen, occurs at a temperature of approximately 1800 K and is characterized by a rapid increase in the production of Silicon Monoxide (SiO) and a sudden increase in surface temperature caused by exothermic reactions [21–23]. Under passive oxidation, a solid glassy layer of Silicon Dioxide (SiO₂), or silica, forms on the surface which acts as a protective barrier. Mass loss is significantly lower than under active oxidation, and there could even be mass gain due to the formation of the oxide layer. Active oxidation, on the other hand, does not result in the formation of a protective silica layer and may result in material degradation [22]. Mass loss is significant which will ultimately lead to reduction in the strength of the TPS [18, 22].

Other materials, including Silicon Nitride (Si₃N₄) [28, 31], Hafnium Diboride (HfB₂) [19, 22, 24], and Zirconium Diboride (ZrB₂) [19, 22, 24] have also been considered as potential high-temperature materials. Like SiC, these materials are also limited by oxidation. The oxidation process for all of these materials is similar but occurs at different temperatures based on the composition [22]. The diborides offer the advantage of extremely high melting temperatures [19, 22] but the oxide layers they produce, Zirconium Dioxide (ZrO₂) and Boron Trioxide (B₂O₃) for ZrB₂ and Hafnium Dioxide (HfO₂) and Boron Trioxide (B₂O₃) for HfB₂, do not provide adequate protection to the underlying material. Improved oxidation resistance can be achieved by combining the diboride with SiC since the silica layer provides an effective oxygen barrier [19]. The appeal of Si₃N₄ is that like SiC, a protective silica layer is formed under passive oxidation [28]. Although they offer a potential solution to the

oxidation issue of C-C, all of these materials present the possibility of weight concerns given their high density [22].

Much of the research into high-temperature materials involves experimentation. Many researchers utilize plasma or arc-jet facilities [18, 20–26, 32–36] while others rely on furnaces [16, 17, 29] or torches [37, 38] to characterize these materials. While these types of facilities provide steady-state testing of the thermal environments experienced during hypersonic flight, they do not correctly simulate hypersonic flowfields [39]. Conversely, impulse facilities, such as shock or expansion tubes, can reproduce flight velocities and enthalpy conditions but have very short test times, 100 μs to 2 ms, which prohibits testing of the thermal response [40].

Often, researchers conduct experiments with the goal of characterizing materials. Williams [18] performed plasma arc-jet experiments with SiC-coated C-C to assess oxidation performance. Mass loss was measured to provide correlations and flight performance for the Space Shuttle Orbiter. Feigl [21] investigated the erosion behavior of SiC to observe the transition from passive to active oxidation and found that, based on the production of SiO, the onset of active oxidation ranged from approximately 1823 K to 2023 K and occurs at lower temperatures for lower pressure. Marschall [24] investigated $ZrB_2 - SiC$ in the Plasmatron facility at the von Karman Institute for Fluid Dynamics and observed, under certain high heat flux conditions, a rapid and spontaneous increase in surface temperature due to the transition from passive to active oxidation. Ogasawara [25] evaluated thermal response and oxidation behavior of Si-Ti-C-O fiber / Si-Ti-C-O ceramic matrix composite in an arc-jet facility and observed minimal surface recession at temperatures below 1723 K and 4 kPa in oxygen partial pressure. Yang [16] conducted a study to investigate SiC-coated carbon fibers in a thermal cycle environment. It was observed that due to their different thermal expansion coefficients, the interface of the carbon fibers and SiC coating was

partially destroyed as a result of the evolution of micro-cracks. Wakamatsu [17] performed experiments to observe oxidation and electrical impedance of SiC under high temperature conditions. Yoshinaka [29] studied oxidation of SiC and noted conditions where passive and active oxidation were observed.

At times, these experiments are being conducted to evaluate materials for further development. Glass [22] evaluated 13 different material systems fabricated into leading-edge test articles at the Arnold Engineering Development Center (AEDC) H2 arc-jet facility, including a $\text{ZrB}_2 - \text{SiC}$ composite that was considered as one of the material candidates for the nose and wing leading edge of the X-43A Mach 10 vehicle. The goal of these experiments was to assess thermal shock since the arc-jet test is a more severe thermal shock environment than flight due to the insertion into steady-state test environment whereas in flight leading edges heat up more gradually as the vehicle accelerates.

Some researchers utilize optical collection techniques to characterize materials. Of all the radiative phenomena investigated during experiments, Cyanogen (CN) violet emissions are among the most targeted. Numerous researchers at the University of Queensland (UQ), Australia have investigated ablation of carbon-based materials with emphasis on CN violet emissions [40–47]. A less-often investigated ablation-related phenomenon are the Dicarbon (C_2) Swan bands. Lewis [41], Alba [46], and Eichmann [47] targeted C_2 Swan during their experiments. Neither Lewis nor Alba observed any discernible signal during their experiments, however Lewis was able to detect C_2 emissions without flow. Eichmann observed C_2 emissions, in addition to CN violet, atomic carbon (C), atomic nitrogen (N), atomic oxygen (O), and N_2^+ , however for a simulated Mars atmosphere which is primarily carbon dioxide (CO_2). Other researchers [48–51] have targeted CO_2 emissions in the Midwave Infrared (MWIR) spectrum in Martian atmospheres.

Panerai [26] characterized SiC in the Plasmatron facility at the von Karman Institute by investigating emissivity, catalycity, and oxidation behavior of representative specimens. Intrusive measurements for flow characterization and optical emission spectroscopy were used to characterize the materials and surrounding environment. The material showed high emissivity and low catalytic nature, making it ideal for thermal protection. A temperature jump was observed coinciding with rapid surface erosion as were strong uncalibrated spectral emission of atomic silicon (Si) and CN violet. Danehy [32] obtained calibrated spectral radiance measurements for SiC and PICA at the NASA Hypersonic Materials Environmental Test System (HYMETS) arc-jet facility in air, 95% N_2 – 5% Ar , and Martian atmospheres from 340 to 1000 nm. CN emissions were found to dominate while atomic N and atomic O lines were also observed. Grinstead [34] performed a comprehensive test series at NASA Ames Electric Arc Shock Tube (EAST) facility to validate modeling of shock radiance measurements for Mars and Venus missions. Kitagawa [35] measured spatially-resolved emission spectra from 350 to 1050 nm using an electric arc heater with the goal of understanding chemical and thermal conditions of the flow including mass flow rate, discharge current and discharge voltage of hot gas, and to obtain temperatures from emission spectra profiles. Vancrayenest [36] obtained measurements of emission spectra ahead of ablating graphite at the Plasmatron facility at the von Karman Institute and found that CN violet and N_2^+ dominate.

A smaller subset of researchers are conducting experiments to validate analytic or simulated results. Balat [20] performed analytic and experimental analysis to determine the transition from passive to active oxidation for SiC at high temperature and low partial pressures of oxygen and found good agreement between experimental and predicted results for molecular oxygen. Herdrich [23] performed a theoretical and experimental investigation of the transition from passive to active oxidation for

SiC, finding good qualitative and quantitative agreement. Additionally, a sudden temperature increase of up to 400 K was observed during the transition from passive to active oxidation. Brandis [33] presented analysis and measurements of radiation data obtained in the NASA Ames EAST facility with the goal of measuring the level of radiation encountered during atmospheric entry. While the focus was mainly on the CO 4th Positive band for Earth and Mars entry, comparisons made for CN violet for EAST, the UQ's X2 facility, and the Hypervelocity Shock Tube (HVST) at Japan Aerospace Exploration Agency (JAXA) were all in good agreement with results obtained using Nonequilibrium Air Radiation (NEQAIR), which is one of NASA's legacy radiation codes [52]. Similarly, Alba [46] used experimental results to develop a novel finite-rate surface kinetic model for determining the chemical state of an ablating boundary layer, which provided results that are in better agreement with experimental spectral measurements.

Despite decades of research, modeling of hypersonic flight conditions remains a significant challenge. Uncertainties in engineering models used to predict heating and aerodynamics can lead to large factors of safety used to determine the thickness of the TPS, which comes at the expense of the mass of the payload available [53]. As an example, the prediction of the convective heat load on the Mars Science Laboratory developed by NASA had a 60% uncertainty, resulting in a 40% increase in TPS thickness [54]. Much of this uncertainty is due to the inability to accurately predict heating rates, particularly the afterbody heating rates. Though afterbody heating rates are considerably lower than forebody heating rates, uncertainties in the prediction of these values remains significantly higher [55]. Radiative heating, which can be as high as 50% or more of the total heating rate [56], has been identified as a major contributor to afterbody heating [57].

The uncertainty in the afterbody heating rates is due to the complexity of the

flowfield in the wake region [55] which is characterized by a number of phenomena depicted in Figure 1. As the flow passes over the corner of a hypersonic vehicle, it experiences a rapid expansion causing a significant temperature drop. A hot recirculation region forms in the base region, which is separated from the outer flowfield by a turbulent shear layer that forms when the boundary layer separates from the body surface. Further downstream, the expanding flow is recompressed by an oblique shock that forms, resulting in a sudden increase in pressure, temperature, and density.

While radiative heating is a significant concern for TPS design, optical radiation in the wake region is also of interest. The military utility of detecting reentry vehicles was identified shortly after the development of ballistic missiles [59–61]. With the United States (US)’s continued development of hypersonic technologies, it is reasonable to assume that near-peer allies as well as adversaries are pursuing similar technologies. A recent study conducted by the National Academies of Sciences, Engineering, and Medicine directed by the Office of the Director of National Intelligence and the USAF highlighted the potential threat to national security that hypersonic weapons pose [62]. Recognizing this threat, the 2017 National Defense Authorization Act (NDAA) tasked the Director of the Missile Defense Agency (MDA) with developing the capability to counter hypersonic boost-glide and Conventional Prompt Strike (CPS) capabilities that may be used against the U.S. [63]. The 2018 NDAA takes this tasking a step further by providing funding for this capability [64]. In light

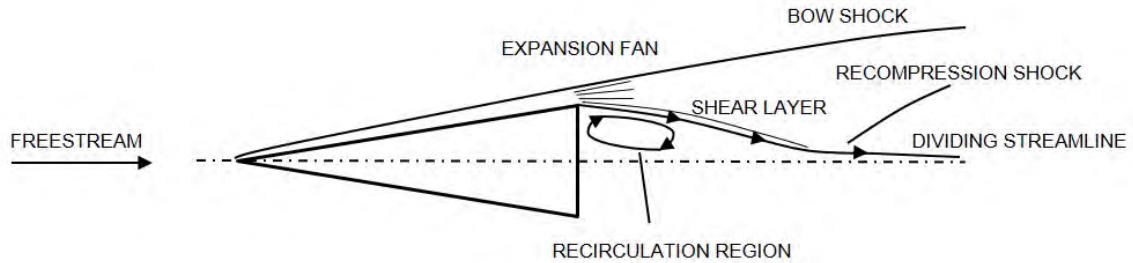


Figure 1. Near-wake flowfield for slender hypersonic body. Based on Park [58].

of these considerations presented, it is imperative that we continue to improve our understanding of these materials and develop the tools used to model them.

The goal of this research is to enhance our knowledge of high-temperature materials in relevant flight environments and assess current state-of-the-art flowfield, ablation, and radiation models. The data collected during experimentation will be the most comprehensive data set of its kind and will be provided to code developers and TPS designers to help improve existing models and designs. Suggested improvements to existing models will also be provided. To assess material performance and evaluate ablation models, a series of experiments were conducted at the X2 superorbital expansion tunnel at UQ, Australia. The X2 facility allows for testing of subscale models at realistic flight temperatures and enthalpies. The materials considered in these experiments were uncoated and SiC-coated reinforced C-C. The materials were tested at 8.6 km/s Earth entry flow monitored by Ultraviolet (UV), Visible/Near Infrared (vis/nIR), and MWIR spectrometry. The experiments utilized a relatively new concept of preheating the model to temperatures in excess of 2500 K to stimulate surface reactions and increase ablation during microseconds of available test time [40]. Such preheating is accomplished by sending an electrical current through the model and allowing the surface temperature to rise due to the natural electrical resistance of the material. These experiments provide benchmark data to validate existing hypersonic flowfield, ablation, and radiation models.

The work outlined in this dissertation aligns itself with the following research objectives:

Research Objective 1: Perform a proof-of-concept to assess the ability to pre-heat and test SiC-coated C-C in a hypersonic expansion tunnel.

Research Objective 2: Perform a comprehensive experimental assessment of expanding hypersonic flowfields targeting atomic Si, CN violet, C₂ Swan, atomic N,

atomic O, CO, and CO₂.

Research Objective 3: Develop a new technique using current state-of-the-art flowfield, ablation, and radiation models to simulate shock tube experiments.

Research Objective 4: Conduct a computational study to assess current state-of-the-art flowfield, ablation, and radiation models and suggest potential improvements.

Research Objective 5: Create a database of experimental data to share with code developers and TPS designers.

Chapter II presents computational theory and methodology. Chapter III provides an overview of the experimental setup used in the X2 facility and the types of instrumentation available. Results from the first and second experimental campaign are discussed in Chapters IV and V, respectively, while computational results will be discussed in Chapter VI, which also compares experimental and computational results. Finally, Chapter VII provides conclusions and suggestions for future work.

II. Computational Theory and Methodology

The hypersonic flows that are of interest cannot be modeled by the perfect gas form of the Navier-Stokes equations due to the physical phenomena present. These phenomena include chemical and thermal nonequilibrium, vibrational and electronic excitation, and weak ionization. In order to account for these phenomena, the use of a real gas model is necessary.

There are a number of different hypersonic flowfield, ablation, and radiation models. Some of the existing hypersonic flowfield models include Data Parallel Line Relaxation (DPLR) [65], Fully Unstructured Navier Stokes 3D (FUN3D) [66], hyFoam [67], Kentucky Aerothermodynamics and Thermal-response Solver (KATS) [68, 69], LeMANS [70, 71], Parallel Hypersonic Aerothermodynamics and Radiation Optimized Solver (PHAROS) [72], Stochastic PARallel Rarefied-gas Time-accurate Analyzer (SPARTA) [73], and US3D [74] while some of the ablation and thermal response models include CHarring Ablator Response (CHAR) [75], Charring Material Thermal Response and Ablation (CMA) [76], Fully Implicit Ablation and Thermal Response Program (FIAT) [77, 78], Icarus [79], Modeling of Pyrolysis and Ablation Response (MOPAR) [71, 80], and Two-dimensional Implicit Thermal Ablation (TITAN) [81, 82]. But perhaps the most robust of the available computational tools is the Langley Aerothermodynamic Upwind Relaxation Algorithm (LAURA) aerothermodynamic simulation code [83].

LAURA is a structured, finite-volume, thin shear layer, shock-capturing aerothermodynamic simulation code that has been applied to a wide range of hypersonic vehicles and flight conditions over the past several decades [83–86]. Originally developed for simulation of hypersonic nonequilibrium flows over blunt bodies including the Aeroassisted Orbital Transfer Vehicle (AOTV) [86–88], the code includes models for perfect gas, equilibrium air, and thermal and chemical nonequilibrium air [84].

Features of the code include the ability to perform one-dimensional grid adaptation (normal to the body) in parallel with the solution to resolve high gradients in the boundary layer and across a bow shock, coupled ablation, and flowfield radiation [83, 84]. Radiation computations are made using the Hypersonic Air Radiation Algorithm (HARA) radiation code, which is coupled to LAURA and is included in standard LAURA releases [83]. The following sections will describe the LAURA Computational Fluid Dynamics (CFD) simulation code in more detail.

2.1 Assumptions

The assumption of fluid as a continuum is foundational to the use of the Navier-Stokes equations. The Knudsen number, which is the ratio of the mean free path to a characteristic length, is commonly used to distinguish between continuum and non-continuum flow conditions. Although there is no definitive threshold for where the continuum model begins to break down, a commonly-used value is a Knudsen number of less than 0.1 [89], though a value of less than 0.2 is also used [90]. For flows with larger Knudsen numbers, there are an insufficient number of molecules within the computational volume for the fluid to be considered a continuum, and thus fluid properties are determined from statistical averages. Further, for flows with a Knudsen number of greater than 0.03, slip effects must be included [90]. Therefore, it is assumed that there are a sufficient number of collisions of gas molecules with the wall so that there is no velocity or temperature slip and the Navier-Stokes equations may be solved to determine the flow conditions.

The thermal state of the gas is assumed to be in nonequilibrium and follows Park's two-temperature model [91]. This two-temperature model uses one temperature, T , to describe the translational energy of the atoms and molecules and the rotational energy of molecules, and another temperature, T_V , to describe the vibrational energy

of molecules, translational energy of electrons, and the electronic excitation energy of atoms and molecules [91]. Conversely, a one-temperature model assumes that all internal energy modes of the gaseous species are in equilibrium with the translational mode [91] while a three-temperature model assumes that the partitioning of energy among the translational, rotational, vibrational, and electronic modes of all gaseous species can be adequately described by three temperatures [92]. The assumption of a single translational-rotational temperature is reasonable given that translational and rotational equilibration require approximately the same number of collisions [58]. The justification for the two-temperature model is based on the rapid energy transfer between the translational mode of free electrons and the vibrational mode of polyatomic species and the rapid equilibration of the low-lying electronic states of heavy particles with the ground electronic states at the electronic temperature [58]. The assumption of the two-temperature model simplifies the conservation equations by combining the conservation of vibrational energy and conservation of electronic energy equations into a single vibrational-electronic energy conservation equation. While the two-temperature model may not be valid for all high-speed flow problems, it has been shown to provide accurate predictions of the aerodynamic coefficients and convective heating rates for hypersonic vehicles [92].

2.2 CFD Solver

Conservation Equations.

The conservation equations for simulating hypersonic flows in thermal and chemical nonequilibrium used in LAURA are derived in this section. Conservation of mass, momentum, and energy for a species s can be expressed as follows [46, 92, 93]:

Species Conservation:

$$\frac{\partial \rho_s}{\partial t} + \frac{\partial}{\partial x_j} \rho_s u_j = \frac{\partial}{\partial x_j} \left(\rho D_s \frac{\partial y_s}{\partial x_j} \right) + \dot{w}_s, \quad (1)$$

where ρ_s is the density of species s , u_j is the velocity in the j -direction, D_s is the effective diffusion coefficient for species s , and $\dot{w}_s$ is the mass rate of production of species s per unit volume. The mixture density, ρ , is defined by

$$\rho = \sum_{s=1}^{ns} \rho_s, \quad (2)$$

where ns is the number of species. The mole fraction of species s , y_s , is defined by

$$y_s = \frac{(\rho_s/M_s)}{\sum_{k=1}^{ns} (\rho_k/M_k)}, \quad (3)$$

where M_s is the molecular weight of species s . The mass diffusion fluxes of species s , J_s , are modeled using Fick's law

$$J_s = \rho_s \nu_{sj} = -\rho D_s \frac{\partial y_s}{\partial x_j}. \quad (4)$$

Mixture Momentum Equation:

$$\frac{\partial}{\partial t} \rho u_i + \frac{\partial}{\partial x_j} \rho u_i u_j = -\frac{\partial P}{\partial x_i} \delta_{ij} + \frac{\partial \tau_{ij}}{\partial x_j}, \quad (5)$$

where u_i is the velocity in the i -direction and δ_{ij} is the Kronecker delta. The pressure, P , is defined by

$$P = \sum_{k=1}^{ns} P_s, \quad (6)$$

and the partial pressure of species s , P_s is defined by

$$P_s = \frac{\rho_s \bar{R} T}{M_s}, \quad (7a)$$

where s represents an atomic, molecular, or ionic species, and

$$P_s = \frac{\rho_s \bar{R} T_e}{M_s}, \quad (7b)$$

where s represents the free electron species and T_e is the electron-electronic excitation temperature. In both Equations (7a) and (7b), $\bar{R}$ is the universal gas constant. The viscous shear stresses, τ_{ij} , are modeled assuming a Newtonian fluid and are given by

$$\tau_{ij} = \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \lambda \frac{\partial u_k}{\partial x_k} \delta_{ij}, \quad (8)$$

where μ is the mixture coefficient of viscosity and u_k is the velocity in the k -direction. From Stoke's hypothesis, the second coefficient of viscosity, λ , is given as $\lambda = -2/3\mu$.

Total Energy Conservation:

$$\begin{aligned} \frac{\partial}{\partial t} \rho E + \frac{\partial}{\partial x_j} \rho H u_j = & \frac{\partial}{\partial x_j} \left[\eta \frac{\partial T}{\partial x_j} + (\eta_v + \eta_e) \frac{\partial T_V}{\partial x_j} \right] + \frac{\partial}{\partial x_j} \left(\rho \sum_{s=1}^{ns} h_s D_s \frac{\partial y_s}{\partial x_j} \right) \\ & + \frac{\partial}{\partial x_j} \left[u_i \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} u_i \mu \frac{\partial u_k}{\partial x_k} \delta_{ij} \right] - Q_{rad}, \end{aligned} \quad (9)$$

where η is the frozen thermal conductivity for translational-rotational energy of heavy particles, η_v is the frozen thermal conductivity for vibrational energy due to collisions between molecules and all particles, η_e is the frozen thermal conductivity for electronic energy due to collisions between electrons and all particles, h_s is the enthalpy per unit mass of species s , and Q_{rad} is the radiative energy transfer rate. The total energy per unit mass of the mixture, E , is defined by

$$E = \frac{u_i u_i}{2} + \sum_{s=1}^{ns} \frac{\rho_s e_s}{\rho}, \quad (10)$$

where e_s is the energy per unit mass of species s . The total enthalpy per unit mass of the mixture, H , is defined by

$$H = E + \frac{P}{\rho}. \quad (11)$$

Vibrational-Electronic Energy Conservation:

$$\begin{aligned} \frac{\partial}{\partial t} \rho e_V + \frac{\partial}{\partial x_j} \rho e_V u_j = & -P_e \frac{\partial u_j}{\partial x_j} + \frac{\partial}{\partial x_j} \left[(\eta_v + \eta_e) \frac{\partial T_V}{\partial x_j} \right] + \frac{\partial}{\partial x_j} \left(\rho \sum_{s=1}^{ns} h_{V,s} D_s \frac{\partial y_s}{\partial x_j} \right) \\ & + \sum_{s=mol.} \rho_s \frac{(e_{v,s}^* - e_{v,s})}{\langle \tau_s \rangle} + 2\rho_e \frac{3}{2} \bar{R}(T - T_V) \sum_{s=1}^{ns-1} \frac{\nu_{es}}{M_s} - \sum_{s=6}^{ns-1} \dot{n}_{e,s} \hat{I}_s + \sum_{s=mol.} \dot{w}_s \hat{D}_s - Q_{rad}, \end{aligned} \quad (12)$$

where P_e is the electron pressure, $h_{V,s}$ is the vibrational-electronic enthalpy per unit mass of species s , $e_{v,s}^*$ is the vibrational energy per unit mass of species s evaluated at temperature T , $e_{v,s}$ is the vibrational energy per unit mass of species s , $\langle \tau_s \rangle$ is the translational-vibrational energy relaxation time for molecular species s , ρ_e is the electron density, ν_{es} is the effective collision frequency for electrons and heavy particles in electronic-translational energy relaxation, $\dot{n}_{e,s}$ is the molar rate of production of species s per unit volume by electron impact ionization, $\hat{I}_s$ is the first ionization energy of species s per kmol, $\dot{w}_s$ is the mass rate of production of species s per unit volume, and $\hat{D}_s$ is the average vibrational energy per unit mass of molecule s , which is created or destroyed at rate $\dot{w}_s$. The mixture vibrational-electronic energy per unit mass, e_V , and the vibrational-electronic enthalpy per unit mass for species s , $h_{V,s}$, are defined by

$$e_V = e_v + e_e, \quad (13)$$

$$h_{V,s} = h_{v,s} + h_{e,s}, \quad (14)$$

where the mixture vibrational energy per unit mass, e_v , and the mixture electronic energy per unit mass, e_e , are defined by

$$e_v = \sum_{s=1}^{ns} \frac{\rho_s e_{v,s}}{\rho}, \quad (15)$$

$$e_e = \sum_{s=1}^{ns} \frac{\rho_s e_{e,s}}{\rho}, \quad (16)$$

where $e_{e,s}$ is the electronic energy per unit mass of species s , which is identical to the electronic enthalpy per unit mass of species s for all species except free electrons. In this case, this quantity is defined as

$$h_{e,e} = e_{e,e} + \frac{\bar{R}T_e}{M_e}. \quad (17)$$

The following sections provide more details on how these terms are modeled.

Thermodynamic Relations.

In thermal nonequilibrium, e_s and h_s are functions of several temperatures, depending on the number of parameters required to describe the partitioning of energy in the gas [92]. For the temperature range of $200 \text{ K} \leq T \leq 50,000 \text{ K}$, both the translational and rotational modes are assumed to be fully excited and therefore the heat capacities of these modes are assumed to be independent of temperature. This assumption results in

$$C_{v,tr}^s = \frac{3}{2} \frac{\bar{R}}{M_s}, \quad (18)$$

for the translational mode and

$$C_{v,rot}^s = \frac{\bar{R}}{M_s}, \quad (19)$$

for the rotational mode where $C_{v,tr}^s$ is the specific heat at constant volume for species s for translational energy and $C_{v,rot}^s$ is the specific heat at constant volume for species s for rotational energy. The energy per unit mass of species s can then be expressed as

$$e_s = C_v^s T + e_{v,s} + e_{s,o}, \quad (20)$$

where C_v^s is the specific heat at constant volume for species s and $e_{s,o}$ is the energy of formation of species s . The enthalpy per unit mass of species s can be expressed as

$$h_s = C_v^s T + \bar{R}T + e_{v,s} + h_{s,o}, \quad (21)$$

where $h_{s,o}$ is the enthalpy of formation of species s .

The species thermodynamic data is taken from work of Gordon and McBride [94]. The data are expressed as least-squares coefficients for the calculation of specific heat at constant pressure for species s , C_p^s , enthalpy per unit mass of species s , h_s , and entropy per unit mass of species s , s_s .

$$\frac{C_p^s(T)}{\bar{R}} = \frac{a_1}{T^2} + \frac{a_2}{T} + a_3 + a_4 T + a_5 T^2 + a_6 T^3 + a_7 T^4, \quad (22)$$

$$\frac{h_s(T)}{\bar{R}T} = -\frac{a_1}{T^2} + \frac{a_2}{T} \ln T + a_3 + a_4 \frac{T}{2} + a_5 \frac{T^2}{3} + a_6 \frac{T^3}{4} + a_7 \frac{T^4}{5} + \frac{a_9}{T}, \quad (23)$$

$$\frac{s_s(T)}{\bar{R}} = -\frac{a_1}{2T^2} - \frac{a_2}{T} + a_3 \ln T + a_4 T + a_5 \frac{T^2}{2} + a_6 \frac{T^3}{3} + a_7 \frac{T^4}{4} + a_{10}, \quad (24)$$

where the a_i are the curve fit coefficients. The species specific heat at constant volume can be evaluated as

$$C_v^s = C_p^s - \frac{\bar{R}}{M_s}. \quad (25)$$

From these thermodynamic quantities, the species energy per unit mass and species enthalpy per unit mass can be found using Equations (20) and (21). Once the total thermodynamic quantities are known, the vibrational-electronic contributions can be found by subtracting the translational and rotational contributions.

If the gas temperature is out of the given range for a particular species, the following correction will be applied

$$C_p(T) = C_p(T^*), \quad (26)$$

$$h(T) = h(T^*) + (T - T^*)C_p(T^*), \quad (27)$$

$$s(T) = s(T^*) + \ln \frac{T}{T^*} C_p(T^*), \quad (28)$$

where

$$T^* = \begin{cases} T_{lower} & \text{for } T < T_{lower}, \\ T_{upper} & \text{for } T > T_{upper}. \end{cases} \quad (29)$$

Equations (20), (21), (22), (23), (24), and (25) are utilized for a single species.

Mixture thermodynamic quantities can be expressed as

$$C_{p,q} = \frac{1}{\rho} \sum \rho_s C_{p,q}^s, \quad (30)$$

$$C_{v,q} = \frac{1}{\rho} \sum \rho_s C_{v,q}^s, \quad (31)$$

$$h = \frac{1}{\rho} \sum \rho_s h_s, \quad (32)$$

where q is a dummy index for a particular energy storage mode (translational, rotational, vibrational, or electronic).

Transport Properties.

The viscosity and thermal conductivity for each energy mode are calculated following the convention of Gupta et al. [92, 95]. The collision integrals for heavy particles are evaluated using the heavy particle translational-rotational temperature, T , while those for electrons with any other partner are obtained using the vibrational-electron-electronic temperature, T_V . For a gas in thermal nonequilibrium, the viscosity of the mixture can be expressed as

$$\mu = \sum_{s=1}^{ns-1} \left[\frac{m_s \gamma_s}{\sum_{r=1}^{ns-1} \gamma_r \Delta_{sr}^{(2)}(T) + \gamma_e \Delta_{se}^{(2)}(T_e)} \right] + \frac{m_e \gamma_e}{\sum_{r=1}^{ns} \gamma_r \Delta_{er}^{(2)}(T_e)}, \quad (33)$$

where m_s is the mass of species s per particle and Δ_{sr} are the collision integrals for species s and r . The molar concentration of species s , γ_s , is defined by

$$\gamma_s = \frac{\rho_s}{\rho M_s}. \quad (34)$$

The translational energy thermal conductivity of heavy particles, η_t , is expressed

as

$$\eta_t = \frac{15}{4}k \sum_{s=1}^{ns-1} \frac{\gamma_s}{\sum_{r=1}^{ns-1} \alpha_{sr} \gamma_r \Delta_{sr}^{(2)}(T) + 3.54 \gamma_e \Delta_{se}^{(2)}(T_e)}, \quad (35)$$

where k is the Boltzmann constant and the non-dimensional parameter for collision of species s and r used in defining thermal conductivity, a_{sr} , is defined as

$$a_{sr} = 1 + \frac{[1 + (m_s/m_r)][0.045 - 2.54(m_s/m_r)]}{[1 + (m_s/m_r)]^2}. \quad (36)$$

The rotational energy thermal conductivity, η_r , is expressed as

$$\eta_r = k \sum_{s=mol.} \frac{\gamma_s}{\sum_{r=1}^{ns-1} \gamma_r \Delta_{sr}^{(1)}(T) + \gamma_e \Delta_{se}^{(1)}(T_e)}. \quad (37)$$

The mixture translational-rotational thermal conductivity, η , is given by

$$\eta = \eta_t + \eta_r. \quad (38)$$

The vibrational energy thermal conductivity, η_v , is expressed as

$$\eta_v = k \frac{C_{v,vib}}{R} \sum_{s=mol.} \frac{\gamma_s}{\sum_{r=1}^{ns-1} \gamma_r \Delta_{sr}^{(1)}(T) + \gamma_e \Delta_{se}^{(1)}(T_e)}, \quad (39)$$

where $C_{v,vib}$ is the specific heat at constant volume for vibrational energy. The vibrational thermal conductivity is equal to the rotational thermal conductivity when that energy mode is fully excited.

The electronic energy thermal conductivity, η_e , is expressed as

$$\eta_e = k \frac{C_{v,vib}}{R} \sum_{s=mol.} \frac{\gamma_s}{\sum_{r=1}^{ns-1} \gamma_r \Delta_{sr}^{(1)}(T) + \gamma_e \Delta_{se}^{(1)}(T_e)}. \quad (40)$$

The binary diffusion coefficient for a pair of heavy particles s and r , D_{sr} , is defined as

$$D_{sr} = \frac{kT}{P\Delta_{sr}^{(1)}(T)}. \quad (41)$$

The binary diffusion coefficient between electrons and heavy particles, D_{er} , is expressed as

$$D_{er} = \frac{kT_e}{P\Delta_{er}^{(1)}(T_e)}. \quad (42)$$

The effective diffusion coefficient of species s in the mixture, D_s , is expressed as

$$D_s = \frac{\gamma_t^2 M_s (1 - M_s \gamma_s)}{\sum_{r=1, r \neq s}^{ns} (\gamma_r / D_{sr})}, \quad (43)$$

where γ_t is defined by

$$\gamma_t = \sum_{s=1}^{ns} \gamma_s. \quad (44)$$

The diffusion coefficient of electrons, D_e , is expressed as

$$D_e = m_e \frac{\sum_{s=6}^{ns-1} D_s^a \gamma_s}{\sum_{s=6}^{ns-1} m_s \gamma_s}, \quad (45)$$

where D_s^a is the effective diffusion coefficient for ions.

The collision integrals, Δ_{sr} , are defined as

$$\Delta_{sr}^{(1)} = \frac{8}{3} \left[\frac{2M_i M_j}{\pi \bar{R} T (M_i + M_j)} \right]^{\frac{1}{2}} \pi \Omega_{ij}^{(1,1)}, \quad (46)$$

and

$$\Delta_{sr}^{(2)} = \frac{16}{5} \left[\frac{2M_i M_j}{\pi \bar{R} T (M_i + M_j)} \right]^{\frac{1}{2}} \pi \Omega_{ij}^{(2,2)}. \quad (47)$$

The collision cross-section terms are computed utilizing curve-fits of the form

$$\pi \Omega_{ij}^{(1,1)} = D_1 T^{(A_1 \ln^2 T + B_1 \ln T + C_1)}, \quad (48)$$

$$\pi \Omega_{ij}^{(2,2)} = D_2 T^{(A_2 \ln^2 T + B_2 \ln T + C_2)}, \quad (49)$$

where A_1 , B_1 , C_1 , D_1 , A_2 , B_2 , C_2 , and D_2 are curve-fit coefficients taken from Wright et al. [96, 97].

Source Terms.

There are a number of source terms appearing in the conservation equations. These terms will be discussed in the subsequent sections.

Chemical Reactions.

The species mass production rate source terms, $\dot{w}_s$, are derived from the chemical reactions that take place in the gas. For C-C, a 20-species, 55-reaction chemistry model for reacting air that includes carbon species is used in this work. The species considered are: N, N⁺, NO, NO⁺, N₂, N₂⁺, O, O⁺, O₂, O₂⁺, e⁻, C, C⁺, CO, CO⁺, CO₂, C₂, C₃, C₅, and CN. For SiC, 26 species and 64 reactions are considered. The additional species considered are Si, Si⁺, SiO, SiO₂, SiC, and SiN.

The mass rate of production of species s is expressed as [92]

$$\dot{w}_s = M_s \sum_{r=1}^{N_r} (\beta_{s,r} - \alpha_{s,r}) (R_{f,r} - R_{b,r}), \quad (50)$$

where N_r is the number of reactions, $\beta_{s,r}$ are the stoichiometric coefficients for

products in reaction r , and $\alpha_{s,r}$ are the stoichiometric coefficients for reactants in reaction r . The forward and backward reaction rates for the r reaction, $R_{f,r}$ and $R_{b,r}$, respectively, are defined by

$$R_{f,r} = k_{f,r} \prod_{s=1}^{ns} (\rho_s/M_s)^{\alpha_{s,r}}, \quad (51)$$

and

$$R_{b,r} = k_{b,r} \prod_{s=1}^{ns} (\rho_s/M_s)^{\beta_{s,r}}. \quad (52)$$

The forward reaction rate coefficient, $k_{f,r}$, is expressed as

$$k_{f,r} = A_{f,r} T_{f,r}^{n_{f,r}} \exp\left(\frac{-E_{f,r}}{kT_{f,r}}\right), \quad (53)$$

where $A_{f,r}$ is the pre-exponential term used in evaluating the forward reaction rate coefficient, $n_{f,r}$ is the power of temperature dependence on pre-exponential factor for forward reaction r , and $E_{f,r}$ is the activation energy for forward reaction r . These values are determined experimentally and are listed in Tables 1, 2, and 3 along with their source data references. The temperature governing a reaction is either the translational-rotational temperature, the vibrational-electron-electronic temperature, or in the case of dissociation reactions, a temperature that is a combination of these two temperatures. This temperature, T_d , is defined by [91]

$$T_d = T^q T_V^{1-q}. \quad (54)$$

T_d is often taken as the geometric average of two temperatures (i.e $q = 0.5$), though some sources use a value of 0.7 for q .

The backward reaction rate coefficient, $k_{b,r}$, can then be expressed as

$$k_{b,r} = \frac{k_{f,r}}{K_{eq,r}}, \quad (55)$$

where $K_{eq,r}$ is the equilibrium constant for reaction r . The equilibrium constant is found from curve fits of the form

$$K_{eq,r} = \exp\left(\frac{A_1}{Z} + A_2 + A_3 \ln Z + A_4 Z + A_5 Z^2\right), \quad (56)$$

where $Z = 10,000/T$ and A_1, A_2, A_3, A_4 , and A_5 are constants for each reaction r .

Table 1. Chemical Kinetics for air species.

r	Reaction	$A_{f,r}$	$n_{f,r}$	$E_{f,r}/k$	$T_{f,r}$	Third Body, M	Ref.
1	$N_2 + M \rightleftharpoons N + N + M$	3.0e+22	-1.60	1.132e+5	T_d	N, C, O	[58]
		6e+3	2.6	1.132e+5	T_V	e^-	[98]
		7.0e+21	-1.60	1.132e+5	T_d	others	[58]
2	$NO + M \rightleftharpoons N + O + M$	4.40e+16	0.00	7.55e+4	T_d	N, C, O, NO, CO_2	[58]
		2.0e+15	0.00	7.55e+4	T_d	others	[58]
3	$O_2 + M \rightleftharpoons O + O + M$	1.0e+22	-1.50	5.936e+4	T_d	N, C, O	[58]
		2.0e+21	-1.50	7.55e+4	T_d	others	[58]
4	$N_2 + O \rightleftharpoons NO + N$	1.0e+22	-1.50	5.936e+4	T_d		[99]
5	$O_2 + N \rightleftharpoons NO + O$	2.49e+9	1.18	4.01e+3	T		[100]
6	$N + O \rightleftharpoons NO^+ + e^-$	5.30e+12	0.0	3.19e+4	T		[101]
7	$NO^+ + N \rightleftharpoons O^+ + N_2$	3.40e+13	-1.08	1.28e+4	T		[58]
8	$NO^+ + O \rightleftharpoons O_2^+ + N$	7.20e+12	0.29	4.86e+4	T		[58]
9	$NO^+ + O^2 \rightleftharpoons NO + O_2^+$	2.40e+13	0.41	3.26e+4	T		[58]
10	$O + O \rightleftharpoons O_2^+ + e^-$	7.10e+02	2.7	8.06e+4	T		[101]
11	$O + e^- \rightleftharpoons O^+ + e^- + e^-$	3.90e+33	-3.78	1.585e+5	T_V		[58]
12	$O_2^+ + O \rightleftharpoons O^+ + O_2$	4.00e+12	-0.09	1.80e+4	T		[101]
13	$O_2 + e^- \rightleftharpoons O_2^+ + e^- + e^-$	2.19e+10	1.16	1.30e+5	T_V		[102]
14	$N + N \rightleftharpoons N_2^+ + e^-$	4.40e+07	1.50	6.750e+4	T		[103]
15	$N + e^- \rightleftharpoons N^+ + e^- + e^-$	2.50e+34	-3.82	1.682e+5	T_V		[103]
16	$N^+ + N_2 \rightleftharpoons N_2^+ + N$	1.00e+12	0.50	1.220e+4	T		[98]
17	$N^2 + O^+ \rightleftharpoons N_2^+ + O$	9.10e+11	0.36	2.280e+4	T		[101]
18	$N^2 + e^- \rightleftharpoons 2N + e^-$	6.00e+3	2.6	1.132e+5	T_V		[98]
19	$NO + O^+ \rightleftharpoons N^+ + O_2$	1.40e+05	1.90	2.660e+4	T		[101]
20	$NO^+ + C \rightleftharpoons C^+ + NO$	1.00e+13	0.0	2.32e+4	T		[99]
21	$NO^+ + N \rightleftharpoons N_2^+ + O$	7.20e+13	0.00	3.550e+4	T		[101]
22	$NO^+ + N \rightleftharpoons O^+ + N_2$	3.40e+13	-1.08	1.280e+4	T		[101]
23	$NO^+ + O \rightleftharpoons N^+ + O_2$	1.00e+12	0.50	7.720e+4	T		[101]
24	$NO^+ + O \rightleftharpoons O_2^+ + N$	7.20e+12	0.29	4.860e+4	T		[99]
25	$NO^+ + O_2 \rightleftharpoons NO + O_2^+$	2.40e+13	0.41	3.260e+4	T		[101]
26	$O_2^+ + N \rightleftharpoons O_2 + N^+$	8.70e+13	0.14	2.860e+4	T		[101]
27	$O_2^+ + N_2 \rightleftharpoons N_2^+ + O_2$	9.90e+12	0.00	4.070e+4	T		[101]

Table 2. Chemical Kinetics for carbon ablation products.

r	Reaction	$A_{f,r}$	$n_{f,r}$	$E_{f,r}/k$	$T_{f,r}$	Third Body, M	Ref.
1	$CO_2 + M \rightleftharpoons CO + O + M$	1.38e+22	-1.50	6.328e+4	T_d	N, C, O	[104]
		6.9e+20	-1.50	6.328e+4	T_d	Ar	[104]
		6.9e+21	-1.50	6.328e+4	T_d	others	[104]
2	$CO + M \rightleftharpoons C + O + M$	1.80e+21	-1.00	1.29e+5	T_d	N, C, O	[104]
		1.20e+20	-1.00	1.29e+5	T_d	Ar	[104]
		1.20e+21	-1.00	1.29e+5	T_d	others	[104]
3	$C_2 + M \rightleftharpoons C + C + M$	4.5e+18	-1.00	7.15e+4	T_d	All	[104]
4	$CN + M \rightleftharpoons C + N + M$	6.0e+15	-0.4	7.10e+4	T_d	All	[99]
5	$CO_2 + O \rightleftharpoons O_2 + CO$	2.71e+14	0.0	3.38e+4	T		[105]
6	$CO + C \rightleftharpoons C_2 + O$	2.4e+17	-1.00	5.80e+4	T		[106]
7	$CO + N \rightleftharpoons CN + O$	1.0e+15	0.00	3.86e+4	T		[104]
8	$CO + NO \rightleftharpoons CO_2 + N$	3.0e+6	0.88	1.33e+4	T		[99]
9	$CO + O \rightleftharpoons O_2 + C$	3.9e+13	-0.18	6.92e+4	T		[106]
10	$C_2 + N_2 \rightleftharpoons CN + CN$	1.5e+13	0.0	2.1e+4	T		[107]
11	$CN + C \rightleftharpoons C_2 + N$	3.0e+14	0.00	1.81e+4	T		[99]
12	$CN + O \rightleftharpoons NO + C$	1.6e+12	0.10	1.46e+4	T		[104]
13	$N + CO \rightleftharpoons NO + C$	1.1e+14	0.07	5.35e+4	T		[99]
14	$N_2 + C \rightleftharpoons CN + N$	1.1e+14	-0.11	2.32e+4	T		[106]
15	$N_2 + CO \rightleftharpoons CN + NO$	1.2e+16	-1.23	7.70e+4	T		[99]
16	$C_3 + C \rightleftharpoons C_2 + C_2$	6.00e+11	1.07	1.650e+4	T		[99]
17	$C_3 + M \rightleftharpoons C_2 + C + M$	1.60e+21	-1.5	8.774e+4	T_d	N, C, O	[99]
		8.40e+20	-1.5	8.774e+4	T_d	others	[99]
18	$C_3 + N \rightleftharpoons CN + C_2$	1.00e+12	0.00	3.420e+4	T_V		[103]
19	$C_5 + M \rightleftharpoons C_3 + C_2 + M$	4.00e+14	0.0	81549.0	T_d		[104]
20	$CO + C_2 \rightleftharpoons C_3 + O$	1.00e+12	0.00	4.120e+4	T_V		[103]
21	$C + O \rightleftharpoons CO^+ + e^-$	8.8e+8	1.0	3.31e+4	T		[106]
22	$C + e^- \rightleftharpoons C^+ + e^- + e^-$	3.9e+33	-3.78	1.307e+5	T_V		[106]
23	$C^+ + CO \rightleftharpoons CO^+ + C$	1.0e+13	0.0	3.14e+4	T		[106]
24	$CO + e^- \rightleftharpoons CO^+ + e^- + e^-$	4.5e+14	0.275	1.63e+5	T_V		[107]
25	$NO^+ + C \rightleftharpoons C^+ + NO$	1.0e+13	0.0	2.32e+4	T		[106]
26	$O_2 + C^+ \rightleftharpoons O_2^+ + C$	1.00e+13	0.0	9.40e+3	T		[106]
27	$C + N \rightleftharpoons CN^+ + e^-$	1.00e+15	1.50	1.6444e+5	T		[107]
28	$C^+ + N_2 \rightleftharpoons N_2^+ + C$	1.11e+14	-0.11	5.0000e+4	T		[107]

Table 3. Chemical Kinetics for silicon ablation products.

*Based on code developers' estimates.

r	Reaction	$A_{f,r}$	$n_{f,r}$	$E_{f,r}/k$	$T_{f,r}$	Third Body, M	Ref.
1	$Si + e^- \rightleftharpoons Si^+ + e^- + e^-$	2.500e+21	-3.82	9.462e+04	T_V		*
2	$Si + CO \rightleftharpoons SiO + C$	7.8e+14	0.0	34510.0	T		[108]
3	$Si + CO_2 \rightleftharpoons SiO + CO$	6.0e+14	0.0	9420.0	T		[108]
4	$Si + NO \rightleftharpoons SiO + N$	3.2e+13	0.0	1775.0	T		[109]
5	$Si + O_2 \rightleftharpoons SiO + O$	3.2e+13	0.0	1775.0	T		[110]
6	$SiO + M \rightleftharpoons Si + O + M$	4.0e+14	0.0	95617.0	T		*
7	$SiO_2 + M \rightleftharpoons SiO + O + M$	4.0e+14	0.0	89591.0	T		*
8	$SiC + M \rightleftharpoons Si + C + M$	4.0e+14	0.0	53773.0	T		*
9	$SiN + M \rightleftharpoons Si + N + M$	4.0e+14	0.0	65673.0	T		*

Vibrational Energy.

The variable $\hat{D}_s$, which appears in Equation (12), represents the average vibrational energy per unit mass of diatomic molecule s , which is created or destroyed at rate $\dot{w}_s$. This term can be defined with a preferential or non-preferential model for dissociation. The preferential model for dissociation assumes that a molecule is more likely to dissociate if it is at a higher vibrational state and that atoms that recombine are more likely to create molecules in a higher vibrational state. Consequently, the value for $\hat{D}_s$ should be larger than the average vibrational energy. The non-preferential model assumes that molecules are created or destroyed at the average vibrational energy [92]. Currently, the LAURA code does not employ a preferential dissociation model. The vibrational energy lost or gained due to dissociation or recombination is defined as

$$\sum_{s=mol.} \dot{w}_s \hat{D}_s, \quad (57)$$

where $\hat{D}_s$ is taken as $e_{V,s}$.

Electronic Energy.

The term $\sum_{s=6}^{ns-1} \dot{n}_{e,s} \hat{I}_s$, which appears in Equation (12), accounts for the rate of electron energy loss when a free electron strikes a neutral particle and frees another electron (i.e. ionizes the particle), resulting in a loss in electron translational energy. For these reactions, the molar rate of ionization, $\dot{s}_{e,s}$, is given as the forward reaction rate, $R_{f,r}$, for reaction r . This model assumes that all of the energy required to ionize the species comes from the electron translational energy and that the ionization energy is taken from the ground state, which likely overestimates the electronic energy loss rate due to electron impact ionization [92].

Relaxation Processes.

The term $\sum_{s=mol.} \rho_s \frac{(e_{v,s}^* - e_{v,s})}{\langle \tau_s \rangle}$ in Equation (12) is the energy exchange rate between the vibrational-electron-electronic and translational-rotational energy modes. This term follows the Landau-Teller formulation, where it is assumed that molecules behave as harmonic oscillators and the vibrational level can only change one quantum level at a time [111]. The relaxation time, $\langle \tau_s \rangle$, is defined as

$$\langle \tau_s \rangle = \tau_s^{MW} + \tau_s^P. \quad (58)$$

The first term, τ_s^{MW} , is the vibrational relaxation time for species s due to inelastic collisions. Millikan and White [112] proposed

$$\tau_s^{MW} = \frac{1}{P} \frac{\sum_{j=1}^{ns-1} n_j \exp \left[A_s (T^{1/3} - 0.015 \mu_{sj}^{1/4} - 18.42) \right]}{\sum_{j=1}^{ns-1} n_j}, \quad (59)$$

where P is in atmospheres and n_j is the number density of species j . The reduced molecular weight of the colliding species s and j , μ_{sj} , is expressed as

$$\mu_{sj} = \frac{M_s M_j}{M_s + M_j}, \quad (60)$$

while the parameter A_{sj} can often be approximated by

$$A_{sj} = 1.16 \times 10^{-3} \mu_{sj}^{1/2} \theta_{sj}^{4/3}, \quad (61)$$

where θ_{sj} is the characteristic vibrational temperature. At temperatures above 8000 K, the kinetic energy of a gas molecule is much higher than the characteristic vibrational temperature which results in an overprediction of the collision cross-section resulting in an unrealistically large relaxation time. To correct this overprediction,

Park proposed adding the second term of Equation (58) [113]. This term, known as a collision-limited cross-section, is written as

$$\tau_s^P = \frac{1}{\sigma_s \bar{c}_s n_s}, \quad (62)$$

where $\bar{c}_s$, the average molecular velocity of molecule s is expressed as

$$\bar{c}_s = \left(\frac{8kT}{\pi m_s} \right)^{1/2}, \quad (63)$$

where n_s is the number density of molecule s and σ_s is the effective cross-section for vibrational relaxation. Park noted that this cross-section must be smaller than the elastic cross-section, which is of the order of 10^{-16} cm^2 at temperatures above 8000 K. Therefore, it is assumed that the effective cross-section for vibrational relaxation is an order of magnitude smaller than the elastic cross-section.

The energy relaxation term in Equation (12), $\sum_{s=mol.} \rho_s \frac{(e_{v,s}^* - e_{v,s})}{\langle \tau_s \rangle}$, is further simplified by making the following approximations:

$$e_{v,s}^* - e_{v,s} \approx C_{v,vib}^s (T - T_V), \quad (64)$$

$$\sum_{s=mol.} \frac{\rho_s C_{v,vib}^s}{\langle \tau_s \rangle} \approx \frac{\rho C_{v,vib} \sum_{s=mol.} \rho_s / M_s \langle \tau_s \rangle}{\sum_{s=mol.} \rho_s / M_s}. \quad (65)$$

Thus, the energy relaxation term becomes

$$\sum_{s=mol.} \frac{\rho_s (e_{v,s}^* - e_{v,s})}{\langle \tau_s \rangle} \approx \frac{\rho C_{v,vib} (T - T_V) \sum_{s=mol.} \rho_s / M_s \langle \tau_s \rangle}{\sum_{s=mol.} \rho_s / M_s}. \quad (66)$$

Numerical Methods.

In the LAURA code, which is derived using a finite-volume formulation of the conservation equations, the inviscid and viscous contributions are considered separately for convenience [114]. The inviscid components of the flux across a cell are calculated using a modified Roe’s averaging and Harten’s entropy fix with second-order corrections based on Yee’s Symmetric Total Variation Diminishing (TVD) scheme [92]. Upwind-biased numerical dissipation is applied, retaining strong stability over a range of numerical tests. Roe’s scheme is employed because it appeared well suited for capturing the strong bow shock associated with the hypersonic flows over blunt bodies during the development of the LAURA code. Harten’s entropy correction [115] is employed to correct nonphysical weak solutions of the governing equations obtained for waves associated with eigenvalues equal to zero. This correction restricts the minimum value of the eigenvalue magnitude. A TVD scheme, which is satisfied by use of a limiting procedure, can be second-order accurate and prevents introduction of any new maxima or minima, which can contribute to a negative artificial dissipation. The limiters used in the LAURA code are based on the work of Yee [116, 117]. Algorithms based on such limiters are referred to as symmetric TVD schemes as they involve symmetric functions of gradients near the cell face. The viscous terms are approximated using second-order accurate central differences. The governing equations are simplified by the thin shear layer approximation, eliminating gradients parallel to the surface [114] and thus reducing computational time. While this simplification may not be suitable for areas of separated or reversed flow, it is often used when simulating flows around bodies for high Reynolds numbers, such as these experiments [93, 118].

The relaxation scheme employed by LAURA requires only a single level of storage for the unknowns for steady-state solutions. Time-accurate solutions can be

constructed by employing additional storage levels to save the results of previous iterations. The use of relaxation factors with the inviscid contribution of the flux Jacobian enhances stability for the second-order accurate implementation of the scheme. Convergence is accelerated by applying separate relaxation factors to the inviscid and viscous contributions to the Jacobian. LAURA remains stable at high Courant numbers due to the point-implicit relaxation strategy [92, 114].

LAURA includes many different boundary conditions including symmetry, reflection, venting, subsonic inflow and outflow, and solid surface. Users may specify up to ten solid surface boundaries. Surface properties including blowing model, catalysis model, and surface temperature type must be specified for each solid surface boundary. The next section will discuss the available options for an ablating wall boundary condition [83].

2.3 Ablation Modeling

Coupled ablation is governed by two primary equations: surface energy balance and surface mass balance. The surface energy balance at the surface of a charring ablator is expressed as [85, 119–121]

$$q_{conv} + \alpha q_{rad} - \epsilon \sigma T_w^4 - \dot{m}_c(h_w - h_c) - \dot{m}_g(h_w - h_g) - q_{cond} = 0. \quad (67)$$

The first two terms, the convective heat flux, q_{conv} , and the radiative heat flux, αq_{rad} , where α is the surface absorptivity, are functions of the flight conditions, vehicle geometry, wall temperature, and injection of ablation products. The third term, $\epsilon \sigma T_w^4$, is the re-radiation from the ablator surface, which is a function of only wall temperature, T_w , and surface emissivity, ϵ , where σ is the Stefan-Boltzmann constant. The next two terms represent the enthalpy of the solid char and pyrolysis gas, respectively. The enthalpy of the gas at the wall, h_w , is computed from the species

composition obtained from the species mass balance and surface temperature while the solid char and pyrolysis gas enthalpies, h_c and h_g , respectively, are determined experimentally and provided in tabular or curve-fit form. $\dot{m}_c$ is the mass flux of surface char and $\dot{m}_g$ is the mass flux of pyrolysis gas at the surface. The last term is the heat conducted into the surface which represents the inability of the previous terms to relieve incoming convective and radiative fluxes.

The species mass balance is

$$\dot{m}_c(c_{c,k} - c_{w,k}) + \dot{m}_g(c_{g,k} - c_{w,k}) - J_k = 0, \quad (68)$$

where $c_{c,k}$ is the mass fraction of species k in the char gas, $c_{w,k}$ is the mass fraction of species k at the wall, and $c_{g,k}$ is the mass fraction of species k in the pyrolysis gas. The diffusion mass flux of species k , J_k , can be written as [14, 46, 122]

$$J_k = \rho_w D_k \nabla c_k|_w, \quad (69)$$

where ρ_w is the density at the wall, D_k is the diffusion coefficient for species k , and c_k is the mass fraction of species k .

For a non-charring ablator, such as those considered in this work, there is no pyrolysis contribution to ablation. As a result, Equations (67) and (68) reduce to

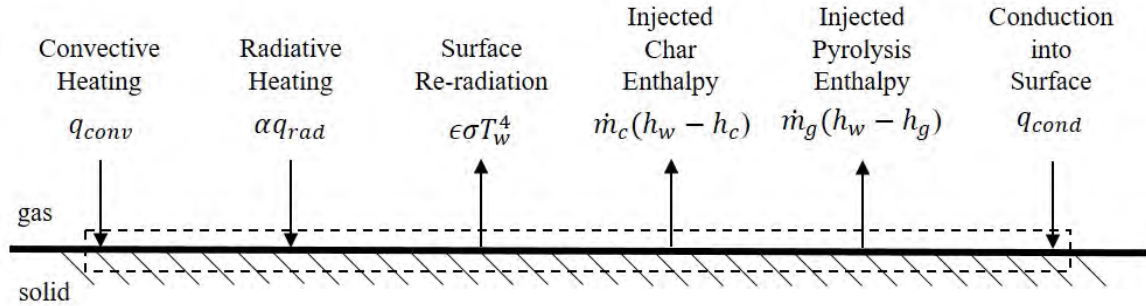


Figure 2. Surface energy balance

[14, 85]

$$q_{conv} + \alpha q_{rad} - \epsilon \sigma T_w^4 - \dot{m}(h_w - h_s) - q_{cond} = 0, \quad (70)$$

and

$$\dot{m}(c_{s,k} - c_{w,k}) - J_k = 0, \quad (71)$$

where $\dot{m}$ is the mass flux at the surface and $c_{s,k}$ is the mass fraction of species k at the gas-solid interface.

The LAURA code presently contains two ablation models: the equilibrium-char (which is sometimes referred to as steady-state or equilibrium ablation approximation) model and finite-rate surface chemistry model, which will be discussed in the following sub-sections.

Equilibrium-Char Model.

The equilibrium-char model assumes that the solid carbon at the surface is in chemical equilibrium at the wall temperature, pressure, and elemental composition with the gas at the surface [85, 120, 123]. Under this assumption, the species mass balance at the surface reduces to solving for the elemental mass balance. This simplification results in the following relation, assuming a solid carbon surface

$$\rho_w \frac{c_{w,C}}{M_C} - K_{s,C} = 0, \quad (72)$$

where $c_{w,C}$ is the mass fraction of atomic carbon at the wall, M_C is the molecular weight of atomic carbon, and $K_{s,C}$ is the equilibrium constant for heterogeneous reaction $C(solid) \rightarrow C(gas)$. The wall pressure, P_w , is computed from the normal momentum equation

$$\frac{dP_w}{dz} + \rho_w v_w \frac{dv_w}{dz} = 0. \quad (73)$$

The normal velocity, v_w , is found from the mass continuity equation

$$\rho_w v_w = \dot{m}. \quad (74)$$

Under the steady-state approximation, the heat flux conducted into the surface, q_{cond} , is approximately equal to the steady-state value [14]

$$q_{cond} \approx \dot{m} h_s. \quad (75)$$

This approximation results in the surface energy balance reducing to [123]

$$q_{conv} + \alpha q_{rad} - \epsilon \sigma T_w^4 - \dot{m} h_w = 0. \quad (76)$$

Finite-Rate Surface Chemistry Model.

Application of finite-rate surface chemistry models allows for higher simulation fidelity in hypersonic aerothermodynamic environments by allowing the processes of oxidation, sublimation, and surface catalysis to be modeled in detail rather than relying on assumptions of chemical equilibrium at the surface elemental composition and temperature [85]. The rate model included in the LAURA code is based on values proposed by Park [103], Driver and Maclean [124], and Keenan and Candler [125]. This model, presented by Johnston [85], is applicable over a wide range of conditions, ranging from low-temperature rate-limited regime to the high-temperature sublimation regime and is discussed in the following sub-sections.

Oxidation.

The forward reaction rate for the primary carbon oxidation reaction $O + C(s) \rightarrow CO$, $k_{f,O}$, is expressed as

$$k_{f,O} = \gamma_O \left(\frac{\bar{R}T}{2\pi M_O} \right)^{1/2}, \quad (77)$$

where Park [103] suggests a value for γ_O of

$$\gamma_O = 0.63 \exp \left(\frac{-1160}{T} \right). \quad (78)$$

The forward reaction rate for the secondary carbon oxidation reaction $O_2 + 2C(s) \rightarrow 2CO$, k_{f,O_2} is written as

$$k_{f,O_2} = \gamma_{O_2} 2 \left(\frac{\bar{R}T}{2\pi M_{O_2}} \right)^{1/2}. \quad (79)$$

For this reaction, Park proposes [103]

$$\gamma_{O_2} = \frac{1.43 \times 10^{-3} + 0.01 \exp \left[\frac{-1450}{T} \right]}{1 + 2.0 \times 10^{-4} \exp \left[\frac{13000}{T} \right]}. \quad (80)$$

The resulting species mass fluxes are

$$\dot{m}_{CO} = \frac{M_{CO}}{M_O} k_{f,O,\rho_O} + 2 \frac{M_{CO}}{M_{O_2} k_{f,O_2,\rho_{O_2}}}, \quad (81)$$

$$\dot{m}_O = -k_{f,O,\rho_O}, \quad (82)$$

$$\dot{m}_{O_2} = -k_{f,O_2,\rho_{O_2}}, \quad (83)$$

where ρ_s are the species densities and M_s are the species molecular weights.

Sublimation.

The rate of sublimation of carbon molecules, expressed as $x\text{C}(s) \rightarrow C_x$, is written as

$$\dot{m}_{C_x} = \alpha_{C_x} (\rho_{E,C_x} - \rho_{C_x}) \left(\frac{\bar{R}T}{2\pi M_{C_x}} \right)^{1/2}, \quad (84)$$

where the equilibrium vapor pressure, ρ_{E,C_x} , is given as

$$\rho_{E,C_x} = A_x T^{n_x} \exp \left[\frac{-E_x}{T} \right]. \quad (85)$$

The coefficients for ρ_{E,C_x} are computed by McBride, Zehe, and Gordon [126] while the values for α_{C_x} are taken from Keenan and Candler [125]. These coefficients are listed in Table 4.

Table 4. Coefficients for sublimation rate equations.

C_x	α_x	A_x	n_x	E_x
C	0.14	$1.486e + 12$	-1.487	87,110
C_2	0.26	$1.8399e + 17$	-2.318	101,715
C_3	0.03	$4.3197e + 22$	-3.459	103,339
C_5	0.015	$2.6559e + 15$	-1.266	117,049

Nitridation.

The rate of nitridation $N + C(s) \rightarrow CN$, $k_{f,N}$, is written as

$$k_{f,N} = \gamma_N \left(\frac{\bar{R}T}{2\pi M_N} \right)^{1/2}, \quad (86)$$

where γ_N is set to the value proposed by Driver and Maclean of 0.001 [124]. The resulting species mass fluxes are

$$\dot{m}_{CN} = \frac{M_{CN}}{M_N} k_{f,N} \rho_N, \quad (87)$$

$$\dot{m}_N = -k_{f,N,\rho_N}, \quad (88)$$

where ρ_s are the species densities and M_s are the species molecular weights.

It should be noted that the finite-rate surface chemistry model that exists in LAURA is only for pure carbon. There are no known finite-rate chemistry models for SiC or any other high-temperature material discussed in this dissertation. Therefore, application of the finite-rate chemistry model will be limited to simulating experimental results for C-C only.

2.4 Radiative Solver

The electromagnetic spectrum is shown in Figure 3, which represents the spectral regions and approximate spectral ranges for emission and absorption due to atomic and molecular processes [47]. Radiative transitions occur when a photon of energy is released, resulting from the internal energy state of an atom or molecule going from an upper to a lower level [58]. The transitions of atoms and molecules are different due to the differing degrees of freedom of their motion.

Radiative transitions of atoms can occur between two bound electronic states by a number of processes. An atom with its outermost electron in an excited state (i.e. in a high energy orbit) can spontaneously move to a lower energy state, emitting a photon of energy in a process known as spontaneous emission. Another nearby atom can absorb the emitted photon of energy and be excited to a higher energy state. This absorption process can also induce a stimulated emission. The total emission rate is the sum of these three processes [58].

Radiative transitions of molecules are far more complicated with vibrational and rotational mechanisms, as well as coupling effects, and need to be considered. Transitions are modeled by treating molecules as vibrating rotators and applying correction

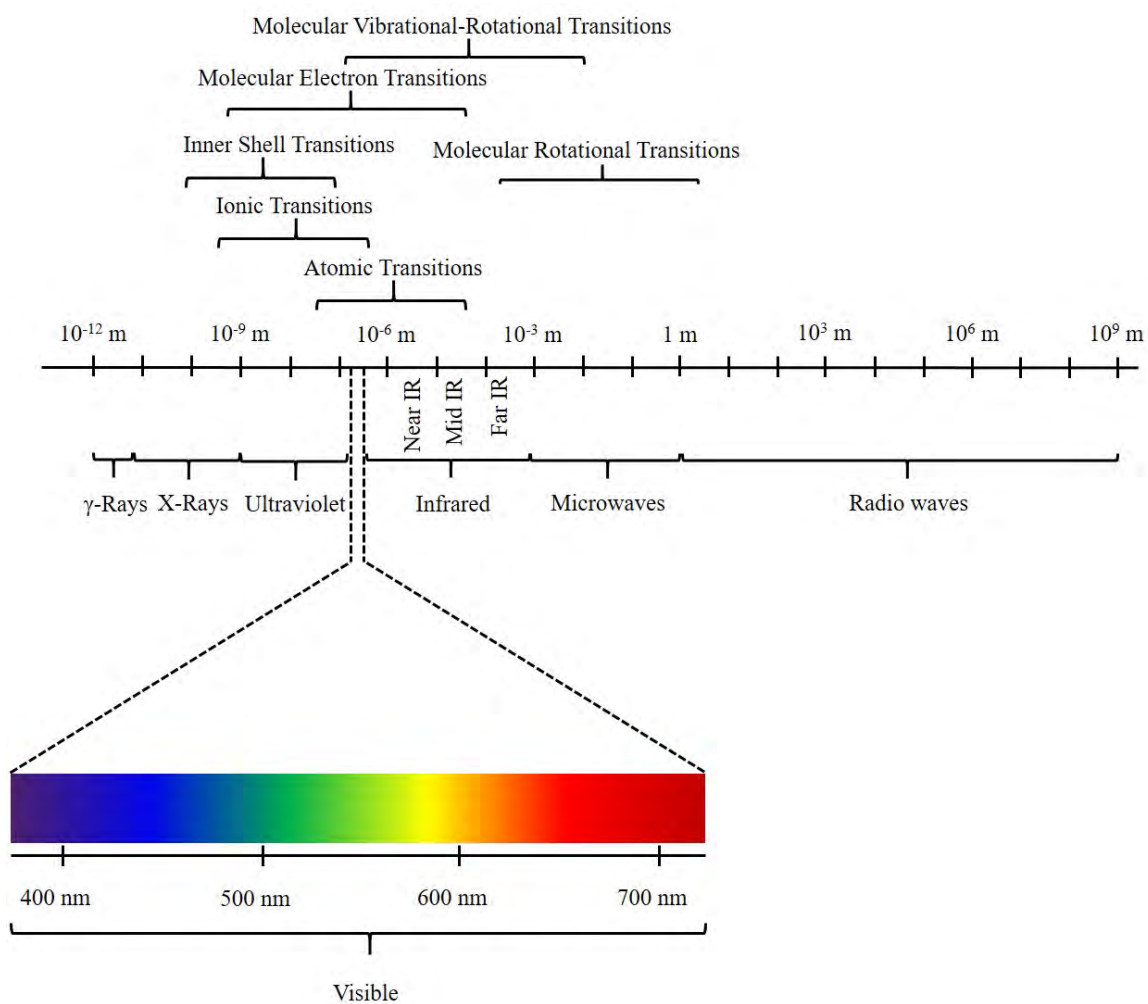


Figure 3. The electromagnetic spectrum. Based on Eichmann [47].

terms to account for non-rigid motion. Rotational transitions occur preferentially when the colliding particle has a similar mass, because energy transfer is more efficient when the masses of colliding partners are nearly equal. Therefore, electrons are inefficient at causing rotational transitions because they possess little momentum, but they can cause vibrational transitions since only the transfer of energy is required [58].

The collisions between electrons and molecules can also cause electronic transitions in molecules. Electronic transitions occur with a preference for certain rotational-vibrational combinations within a given electronic state, known as the Franck-Condon principle. For an electronic transition to occur, the vibrational ranges of the initial and final electronic states must spatially overlap [58]. Such simultaneous changes in electronic and vibrational energy levels of a molecule are known as “vibronic” transitions.

The radiation solver used in this work is Hypersonic Air Radiation Algorithm (HARA) nonequilibrium radiation code. HARA was created to be applied to coupled radiation and ablation simulations [120] and is included in standard LAURA releases [83]. The high accuracy of HARA is achieved through its comprehensive set of radiation properties, including spectral data and non-Boltzmann models for atoms and diatomic molecules [85].

HARA has the ability to treat molecular bands using either the Smeared Rotational Band (SRB) approach, which applies a simplified and efficient treatment of each molecular band system or a significantly more computationally-expensive line-by-line approach. The SRB approach applies an approximation for the rotational energy, which simplifies the calculation of the absorption coefficient. Further details on the SRB approach can be found in Johnston [127].

The SRB approach has been shown to be accurate for optically thin conditions.

Therefore, the line-by-line approach is not recommended for most coupled radiation-flowfield computations of interest [83]. Johnston et al. [127] found that for lunar-return conditions, the SRB approach for both strongly emitting and strongly absorbing band systems was in excellent agreement with the line-by-line approach. Johnston et al. [123] also noted that only the CO 4th Positive band requires the line-by-line approach, which may be optically thick for Mars entry conditions [83].

If not specified by the user, HARA will choose which radiation mechanisms to include based on species present in the flow with number densities of at least 1000 particles/cm³. Emission and absorption of atomic carbon (C), hydrogen (H), oxygen (O), and nitrogen (N) is treated, which includes bound-free (photoionization), free-free, and bound-bound (atomic lines) radiative processes [83, 104]. HARA also allows for treatment of radiation resulting from a number of molecular band systems including the C₂ Swan, CN red (A-X), CN violet (B-X), CO₂ infrared, and N₂⁺ first negative band systems, where the CN red (A-X) and CN violet (B-X) are the transitions of the first two excited electronic states of CN. The electronic states are represented by the letters X, A, B, etc. with X designating the ground state. Although not mentioned in the LAURA users manual, HARA does in fact contain radiation models for atomic silicon (Si) and the SiO molecule, which will be investigated in this research.

The following subsections will discuss in greater detail how HARA models atomic and molecular radiation.

Radiative Transfer.

The HARA radiation code calculates the frequency-dependent radiative intensity, I_ν , by solving the radiative transfer equation

$$\frac{dI_\nu}{ds} = j_\nu - k_\nu I_\nu, \quad (89)$$

where j_ν is the frequency-dependent emission coefficient and k_ν is the frequency-dependent absorption coefficient [90]. The following subsections will describe how the emission and absorption coefficients are calculated for atomic and molecular species.

Bound-Bound Atomic Transitions.

Bound-bound transitions are the result of the spontaneous emission of a photon, which is accompanied by a transition from an upper energy state to a lower energy state. The frequency-dependent absorption coefficient for a bound-bound atomic transition from an ungrouped lower level i' to an upgrouped upper level j' is written as [128]

$$k_{\nu,i'j'}^{bb} = N_{i'} \frac{\pi e^2}{mc} f_{i'j'} b_\nu, \quad (90)$$

where e is the electron charge, m is the electron mass, c is the velocity of light, $f_{i'j'}$ is the absorption oscillator strength for a line with an upper level j' and a lower level i' , and b_ν is the line-shape function.

The HARA code groups closely spaced levels for improved computational efficiency, while lower levels are left ungrouped for higher precision in the calculation of these levels, which are most important to the radiation calculation [127]. The levels contained in a group are assumed to be in a local Boltzmann distribution, which allows the individual number density, $N_{i'}$, to be related to the group number density, N_i , as

$$N_{i'} = N_i \frac{g_{i'}}{g_i} \exp \left[-\frac{hc}{kT_e} (E_{i'} - E_i) \right]. \quad (91)$$

Similarly, the relationship between the energy for a grouped level i and a set of ungrouped levels i' is

$$E_i = \frac{\sum g_{i'} E_{i'}}{\sum g_{i'}}, \quad (92)$$

while for the degeneracy, it is

$$g_i = \sum g_{i'}. \quad (93)$$

In the equations above, g_i is the degeneracy for an atomic level i , h is Planck's constant, and E_i is the electronic energy for an atomic level i . Similarly, the frequency-dependent bound-bound emission coefficient is written as

$$j_{\nu, i' j'}^{bb} = N_{j'} \frac{2\pi h e^2}{m c^3} \left(\frac{c}{\lambda_{CL}} \right)^3 \frac{g_{i'}}{g_{j'}} f_{i' j'} b_{\nu}, \quad (94)$$

where λ_{CL} is the wavelength of the centerline in the spectrum of an atomic or molecular line.

Bound-Free Atomic Transitions.

Bound-free radiation is the result of a bound electron being excited to an energy level above the ionization energy, which results in the bound electron becoming a free electron [128]. The absorption coefficient resulting from this process is

$$k_{\nu, i' j'}^{bf} = \sigma_{\nu, i}^{bf} N_i, \quad (95)$$

where $\sigma_{\nu, i}^{bf}$ is the bound-free absorption cross-section of level i . Similarly, the bound-free emission coefficient from a single level i is calculated as

$$j_{\nu, i' j'}^{bf} = N_+ N_e \frac{2h\nu^3}{c^2} \frac{g_i}{2Q_+} \left(\frac{h^2}{2\pi m k T_e} \right)^{3/2} \sigma_{\nu, i}^{bf} \exp \left[\frac{hc(E_{ionize} - E_i) - h\nu}{k T_e} \right], \quad (96)$$

where N_+ is the ion number density, N_e is the electron number density, Q_+ is the ion partition function, and E_{ionize} is the ionization energy of an atomic level i .

A significant challenge in calculating bound-free atomic radiation is determining the bound-free absorption cross-section. HARA models the lowest three levels of atomic N and O using a step-model consisting of enough steps to sufficiently model any “spikes” in the spectrum [127, 128]. The cross-sections for all other levels are approximated by

$$\sigma_{\nu,i}^{bf} = \sigma_{thresh,i}^{bf} \left(\frac{h\nu_{thresh,i}}{h\nu} \right)^{\theta_i}. \quad (97)$$

The parameters $\sigma_{thresh,i}^{bf}$, $h\nu_{thresh,i}$, and θ_i are chosen to give the best fit through the TOPbase data and are contained in Appendix B of Johnston [128].

Free-Free Atomic Radiation.

Free-free radiation, also called Bremsstrahlung emission, results from electrons being slowed down in the external electric field of positive ions. The loss of kinetic energy of each electron is accompanied by the emission of a photon of equal energy. The absorption coefficient for this process is [128]

$$k_{\nu}^{ff} = \frac{4}{3} \left(\frac{2\pi}{3mkT_e} \right)^{1/2} \frac{Z^2 e^6}{hcm\nu^3} N_+ N_e, \quad (98)$$

where Z is the charge number of the species ($Z = 1$ for neutral atoms). Similarly, the emission coefficient is written as

$$j_{\nu}^{ff} = \frac{8}{3} \left(\frac{2\pi}{3mkT_e} \right)^{1/2} \frac{Z^2 e^6}{mc^3} N_+ N_e \exp \left(-\frac{h\nu}{kT_e} \right). \quad (99)$$

Molecular Band Radiation.

Radiative transitions of molecules result from a change in the electronic energy level, as well as possible vibrational and rotational level changes. In such transitions, the upper state, referred to as u , is defined by e' , V' , and J' , while the lower state, referred to as l , is defined by e'' , V'' , and J'' , where e , V , and J are the electronic, vibrational, and rotational quantum numbers, respectively. The absorption coefficient of a single rotational line resulting from a transition from u to l is written as [128]

$$k_{\nu,ul} = N_{e''} \frac{1}{Q_{V''}Q_{J''}} \exp \left(-\frac{hc}{kT_V} E_{V''} - \frac{hc}{kT} E_{J''} \right) \frac{1}{g_{e''}} \frac{\pi e^2}{mc} f_{V'V''} S_{J'J''} b_\nu, \quad (100)$$

where $N_{e''}$ is the number density of the lower electronic state, $Q_{V''}$ and $Q_{J''}$ are the partition functions of the lower vibrational and rotational states, respectively, $g_{e''}$ is the degeneracy of the lower electronic state, $f_{V'V''}$ is the band absorption oscillator strength, and $S_{J'J''}$ is the line-intensity factor. Similarly, the emission coefficient is written as

$$j_{\nu,ul} = N_{e'} \frac{1}{Q_{V'}Q_{J'}} \exp \left(-\frac{hc}{kT_V} E_{V'} - \frac{hc}{kT} E_{J'} \right) \frac{1}{g_{e'}} \frac{2\pi e^2 h}{c^3 m} \nu_{CL}^3 f_{V'V''} S_{J'J''} b_\nu, \quad (101)$$

where $N_{e'}$ is the number density of the upper electronic state, $Q_{V'}$ and $Q_{J'}$ are the partition functions of the upper vibrational and rotational states, respectively, and $g_{e'}$ is the degeneracy of the upper electronic state.

As was mentioned previously, the HARA code has the ability to model many atomic and molecular radiative mechanisms. These different models will be presented in the following subsections.

Modeling of Atomic Radiation.

The HARA radiation code has the ability to model radiation of atomic C, H, O, N, and Si. Each of these species can be modeled assuming a Boltzmann distribution of the electronic states. For these cases, the excited state number densities can be calculated using the Boltzmann equation [129]

$$N_i^B = N_a \frac{g_i \exp(-hcE_i/kT_e)}{Q_a}. \quad (102)$$

The HARA code also allows a number of species to be modeled assuming a non-Boltzmann distribution. The two available non-Boltzmann models for atomic species are the “Gally First-Order Local Thermodynamic Nonequilibrium (LTNE)” model and the “Collisional Radiative (CR)” model. The Gally LTNE model can be applied to N, O, and Si while the CR model can be applied only to N and O.

The Gally LTNE model was developed in an attempt to improve upon the original non-Boltzmann model developed by Gally [130] based on the work of Carlson [131, 132]. The original non-Boltzmann model applied correction factors to evaluate cross-sections and absorption coefficients [131] but lacked detail in the radiation model, particularly with respect to atomic lines and molecular ion bands [132]. The new model assumes that atomic ionization proceeds by excitation from the three low ground states to the excited states, followed by a rapid ionization [132]. It also assumes that excitation from ground states to higher states is a rate limiting step for the ionization process. Finally, it assumes that the excited states are in equilibrium with the free electrons and ions, due to their energy proximity to the ionized state. These assumptions allow the excited state number densities to be populated using the Saha-Boltzmann equation

$$N_i^{SB} = N_+ N_e \left(\frac{h^2}{2\pi m k T_e} \right)^{3/2} \frac{g_i \exp[-hc(E_i - E_{ionize})/kT_e]}{2Q_+}. \quad (103)$$

The CR model for atomic N and O was developed by Johnston et al. [129] based on a new set of electronic-impact excitation rates. This model, populates the electronic states by solving the master equation, given as

$$\begin{aligned} \frac{\partial N_i}{\partial t} = & \left(\frac{\partial N_i}{\partial t} \right)_{elec-imp-ex} + \left(\frac{\partial N_i}{\partial t} \right)_{hp-imp-ex} + \left(\frac{\partial N_i}{\partial t} \right)_{elec-imp-ion} + \left(\frac{\partial N_i}{\partial t} \right)_{elec-imp-dis} \\ & + \left(\frac{\partial N_i}{\partial t} \right)_{bb-rad} + \left(\frac{\partial N_i}{\partial t} \right)_{bf-rad} \end{aligned} \quad (104)$$

for the processes of electron-impact excitation, heavy particle-impact excitation, electron-impact ionization, electron-impact dissociation, bound-bound radiation, and bound-free radiation. The Quasi-Steady State (QSS) assumption, where $\frac{\partial N_i}{\partial t}$ is assumed to be equal to zero, is made for all levels except the ground state. The population of the ground state is found by equating the sum of the level number densities of the species to the total number density of that species [129].

Figure 4 shows the typical population distribution of the electronic states for atomic N for each of the three models. This figure was produced using the flowfield properties at the cell along the $z = 8$ mm line-of-sight at the midpoint between the shock and the wall. The population distribution of the electronic states of other species is similar. There are several orders of magnitude variation in the population of the excited states between each of the models, which is likely to produce orders of magnitude variation in the radiation computed by each of these models.

The primary source of the atomic line data contained in HARA is the NIST database [127, 129], with the exception of those that group all levels of a single quantum number n , which were taken from Park [58]. The absorption oscillator

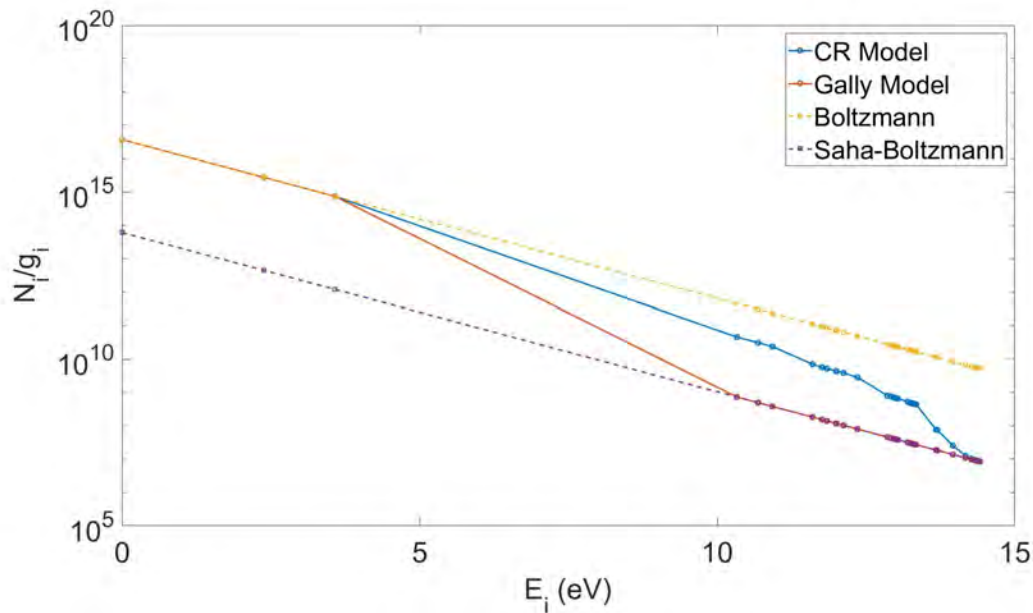


Figure 4. Population of the electronic states of atomic nitrogen. Values shown are from the 1930 K case for SiC-coated C-C in the near-stagnation region.

strengths are from a combination of experimental and theoretical sources [127]. The atomic line data contained in the HARA code can be found in Appendix A of Johnston [128].

Modeling of Molecular Radiation.

As was the case for atomic species, HARA contains the ability to model radiation of polyatomic species assuming a Boltzmann distribution of the electronic states. Additionally, HARA also contains non-Boltzmann models for a number of polyatomic species.

The non-Boltzmann model developed by Johnston et al. for modeling nonequilibrium radiation of C_2 and CN [123] applies oscillator strengths [133] and spectroscopic constants [134] presented by Babou. The current non-Boltzmann model for CN, known as the “CR Park” model, improves upon the previous non-Boltzmann model for CN developed by Johnston et al. [135], which sought to correct an order-of-

magnitude overprediction of the previous Boltzmann model.

A non-Boltzmann model for N_2^+ was developed by Johnston et al. in conjunction with the previously-discussed non-Boltzmann model for atomic N and O [129]. This model considered electron-impact excitation rates from a number of experimental and theoretical sources. There is a large discrepancy between the various sources, with electron-impact excitation rates ranging several orders of magnitude. This discrepancy is particularly true for the electron-impact excitation rates for populating the $N_2^+(B)$ state, which is the upper state of the $N_2^+(1-)$ band system. As such, the model chosen for implementation in HARA was selected as it is approximately in the middle of the available choices [129]. The wide range of electron-impact excitation rates again poses the possibility of overpredicting or underpredicting simulated radiation results.

As was discussed previously in this chapter, many of the features of the LAURA code, including reaction coefficients and ablation rates, are based on experimental data. Similarly, the HARA radiation code also utilizes inputs from the National Institute for Standards and Technology (NIST) Atomic Spectra Database [136], further highlighting the tightly-coupled nature between experimentation and modeling of hypersonic systems. The next chapter will discuss experimental testing and will provide an overview of the X2 facility at the University of Queensland (UQ) and the types of instrumentation available.

III. Experimental Testing

In order to fully investigate all the phenomena encountered during hypersonic flight, flight testing is required. However, given the enormous cost associated with conducting a flight test, great emphasis is placed on ground testing and simulation. While more cost effective, ground test facilities face many challenges in accurately replicating flight conditions; they simply cannot replicate the many different types of phenomena present in the flowfield, which include viscous-inviscid interactions, surface ablation, nonequilibrium thermodynamics, finite-rate chemical reactions, and radiative heat transfer in a fully coupled manner [137]. Integrated testing utilizing both impulse and arc-jet facilities, combined with computational simulations, is necessary to adequately characterize a TPS material.

Given their short time scales, impulse facilities cannot adequately simulate ablating flowfields without preheating the model. Such a preheating technique was developed at the University of Queensland (UQ), Australia, enabling surface temperatures of 2500 K for carbon-based materials [40]. This technique was modified to extend the temperature range to a maximum of 3300 K [43]. This approach results in the correct surface thermal boundary condition, enabling the gas-surface interaction to be simulated, which can then be compared to numerically simulated results. The following sections describe the experimental setup used in the impulse facility tests.

3.1 X2 Facility

The experiments were conducted at the X2 superorbital expansion tunnel at UQ. The tunnel, shown schematically in Figure 5, is a free piston driven facility capable of producing representative reentry flow environments. The tunnel is operated by releasing a piston that is rapidly accelerated by high-pressure reservoir gas. The

piston compresses the driver gas, consisting of a mixture of helium and argon, raising pressure and temperature. At a specified pressure, the steel primary diaphragm bursts, allowing a strong shock wave to propagate through the shock tube. The test gas is accelerated until it reaches a thin secondary aluminum diaphragm which immediately ruptures. The test gas then flows downstream into the lower pressure acceleration tube, where it accelerates and experiences an unsteady (i.e. changing with time) expansion before reaching the test model [43].

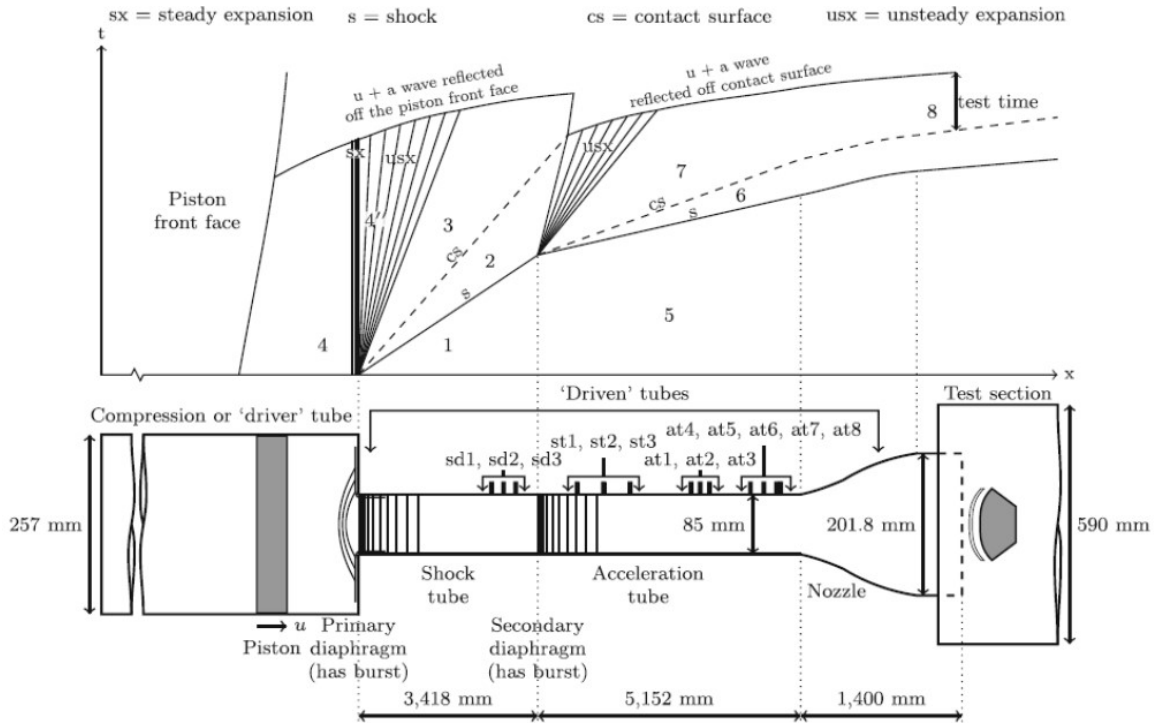


Figure 5. Schematic of X2 the expansion tunnel. Taken from James [138].

The tunnel condition used for these experiments was 8.6 km/s flight speed. Other researchers [40, 43, 46] have used this same condition, which provides approximately 100 μs of steady test time. The freestream conditions of the test flow are shown in Table 6. These values are computed for each experiment, using the procedure described by James et al. [138], to account for any facility performance variation over time. The X2 fill pressures for each section of the expansion tube are shown in Table

5. Optical windows at the side and above the test section allowed for non-invasive optical data collection.

Table 5. X2 fill conditions.

Parameter	Value	Gas
Reservoir	6.85 ± 0.05 MPa	Air
Driver	92.8 ± 0.1 kPa	80% He, 20% Ar
Shock Tube	3.0 ± 0.1 kPa	Instrument Air
Acceleration Tube/Test Section	10.0 ± 0.1 Pa	Air

Table 6. X2 freestream test conditions.

Parameter	Value
Total Enthalpy	37.97 ± 0.11 MJ/kg
Pressure	645 ± 58 Pa
Temperature	2493 ± 18 K
Velocity	8598 ± 9 m/s
Density	$0.867 \pm 0.071 \times 10^{-3}$ kg/m ³
y_{N_2}	0.7807 ± 0.0002
y_{O_2}	0.1618 ± 0.0018
y_{NO}	$1.989 \pm 0.0525 \times 10^{-2}$
y_O	$3.761 \pm 0.1513 \times 10^{-2}$

Throughout this document, shot numbers will be referenced by the tracking number used at the X2 facility. As an example, x2s3570 was one of the shots conducted during the course of these experiments. The first three characters, “x2s”, indicate that this shot was executed at the X2 facility (rather than another facility at UQ). The last four digits are a running tally of the shot number since the facility’s inception. In this example, x2s3570 was the 3570th shot since the X2 facility began operating.

3.2 Test Model

The model used throughout these experiments was a two-dimensional steel compression wedge. The wedge was designed by a PhD student at UQ, Ranjith Ravichan-

dran [139]. Figure 6 shows the model, which measures 100 mm wide, 25 mm tall, and 168 mm in length. The 54 degree turning angle was chosen to keep the post-shock flow supersonic and attached, while providing significant compression [140]. The ramp corner is designed to simulate rapidly expanding hypervelocity flows. A unique feature about this model, which was used for the first time during the first experimental campaign, is that it allows an ablative strip to be attached, releasing ablation products into the flowfield.

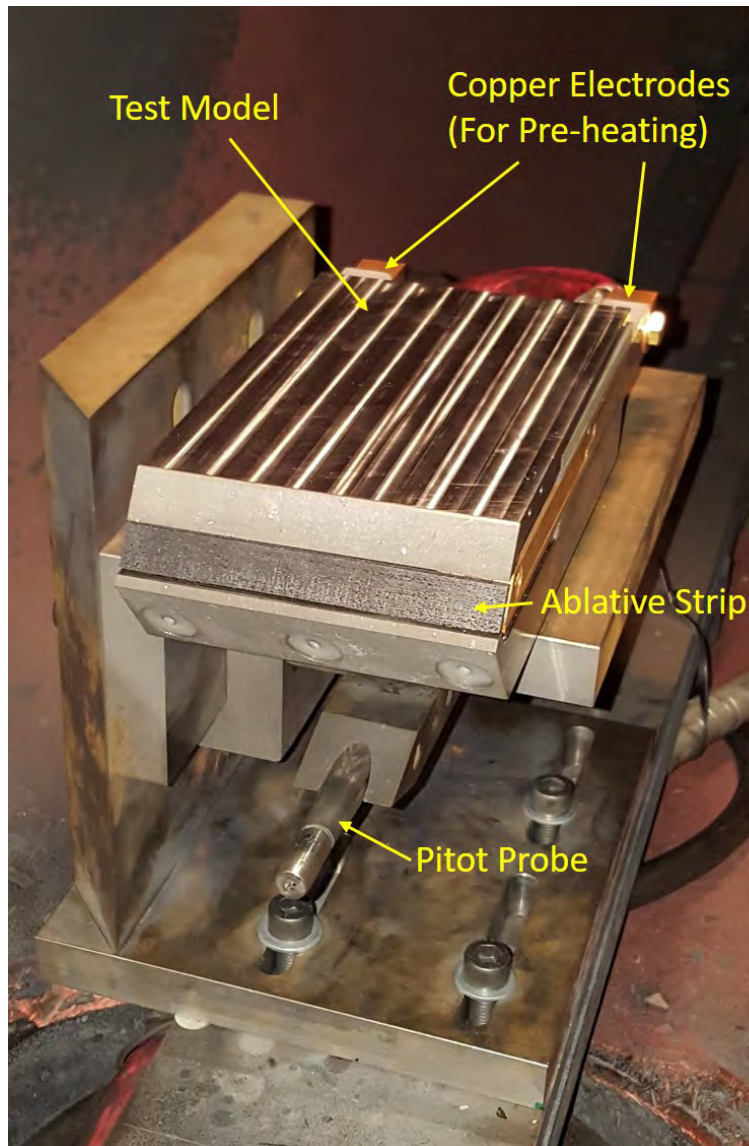


Figure 6. Model in X2 test section

The material used for these strips was reinforced C-C manufactured by Carbon-Carbon Advanced Technologies (C-CAT). The material was procured by the Air Force Research Laboratory's Aerospace Systems Directorate (AFRL/RQ). The C-C was pyrolyzed and densified to an Advanced Carbon-Carbon (ACC)-6 configuration, which was considered as a candidate material for the DARPA HTV-2 program [141]. The C-C parts were cut from solid blocks of C-C using wire Electrical Discharge Machining (EDM), which is perhaps a bit nontraditional given that C-C is not very conductive. In order to increase conductivity, a hole was drilled through the C-C block into which a copper rod was inserted. This machining method was chosen as it is extremely precise, can be automated, and significantly reduces the amount of waste material compared to other machining methods. One drawback is that this method is a bit slow, yielding about one part per working day.

A SiC coating was applied to some of the test articles by the Air Force Research Laboratory's Materials and Manufacturing Directorate (AFRL/RX) using commercially-available SiC powder manufactured by Materion and SMP-10 SiC matrix precursor manufactured by Starfire Systems. The coating on all test articles, with the exception of two samples from the first experimental campaign, was 1 mm thick. Two samples from the first experimental campaign had a 300 μm thick coating, which was simply the result of running out of time for additional coating cycles before the campaign. Energy-dispersive X-ray Spectroscopy (EDS) analysis of several samples conducted prior to the first experimental campaign showed that the samples were a bit more carbon-rich than expected. A total of seven samples were scanned in approximately 15 locations each at a magnification of 200x. These scans showed an average weight percent (i.e. mass fraction) composition of 40.01% C - 59.99% Si, compared to the approximately 30% C - 70% Si that should have been expected. Table 7 shows the results of the EDS scans for the seven samples. An example EDS

result is shown in Figure 7.

Table 7. Summary of EDS results for SiC-coated C-C samples.

Sample Number	Carbon Weight %	Silicon Weight %
1	46.08	53.92
2	40.44	59.56
3	45.86	54.14
4	41.14	58.86
5	34.50	65.50
6	39.30	60.70
7	32.77	67.23
Average	40.01	59.99

Test articles were cut into strips 100 mm wide and 10 mm tall angled at 54 degrees relative to the incoming flow. Thicknesses were varied from 3 mm to 7 mm allowing for a range of surface temperatures, since increasing the thickness increases the cross-sectional area, which in turn reduces the resistance.

3.3 Preheating of Test Articles

The impulse facility time scales are insufficient to allow thermal equilibrium to be reached when the model is initially at room temperature. Under such conditions, approximately 1 to 10 seconds would be necessary to correctly simulate the effects of ablation and surface chemistry on the flowfield [142]. As a result, it is not possible to study fully coupled ablating flowfields in impulse facilities. Preheating a model can eliminate this time requirement, allowing the study of ablation and gas-surface interactions [40]. Such preheating is accomplished by sending an electrical current through the model and allowing the surface temperature to rise due to the natural electrical resistance of the material. For these experiments, preheating occurred immediately before the flow arrives, allowing surface temperatures up to 2700 K to be achieved.

In order to stimulate ablation and gas-surface reactions under relevant flowfield

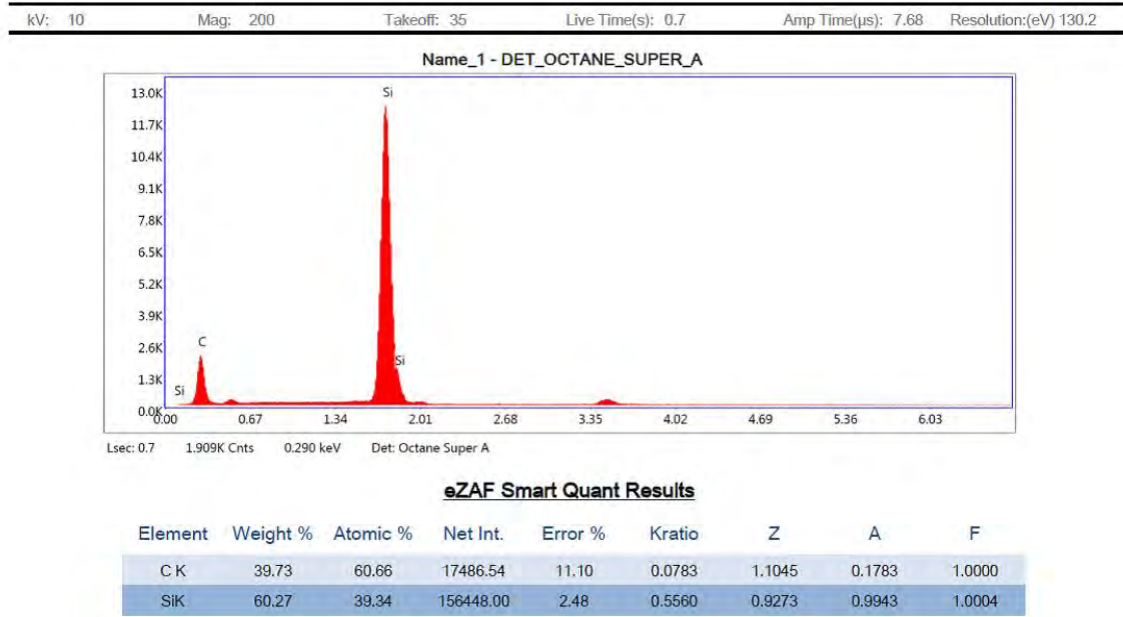


Figure 7. Example EDS result.

conditions, the strips were preheated using the technique detailed by Zander [40]. Heating of the samples was accomplished using a direct current power supply capable of supplying up to 22.5 V and 1500 A [44]. Surface temperature estimates were obtained with a digital single-lens reflex (DSLR) camera using a technique that was developed by Zander [143]. This technique, known as Two Color Ratio Pyrometry (TCRP), captures intensities for red, blue, and green wavelengths then uses two-color ratios to calculate temperature in each pixel.

3.4 Instrumentation

In addition to using a DSLR camera to measure surface temperature, imagery was also taken with UV, vis/nIR, and MWIR spectrometers, while a data acquisition system recorded the tunnel pressures for flow condition determination. Additionally, a camera recorded voltage and current into the test articles, as shown in Figure 8, allowing power to be computed post-shot. The following subsections will describe the instrumentation used in more detail.



Figure 8. Example of voltage and current measurement into the test articles before a shot.

TCRP.

In order to accurately replicate experiments with numerical simulations, it is necessary to know the temperature of the model surface before the flow arrives. A common technique of using thermocouples is impractical due to temperature limitations and the requirement to imbed them into the model. Other techniques such as using optical pyrometers or thermal imaging cameras were not available. For these experiments, a technique developed by Zander [143] for measuring spatially resolved surface temperature using TCRP was implemented using a commercially available DSLR camera.

This technique relies on the ratio of intensities at two different known wavelengths. Digital cameras satisfy this requirement by capturing intensities for red, blue, and green wavelengths. Two-color ratios are then used to calculate the temperature for

each pixel. Test articles are assumed to be radiating as gray bodies (i.e. constant emissivity) which is consistent with previous research of carbon-based materials in near-vacuum conditions [40, 144]. The camera used for these experiments was a Canon 400D DSLR. Settings were varied as necessary to accommodate anticipated surface temperatures. An example DSLR image is shown in Figure 9.

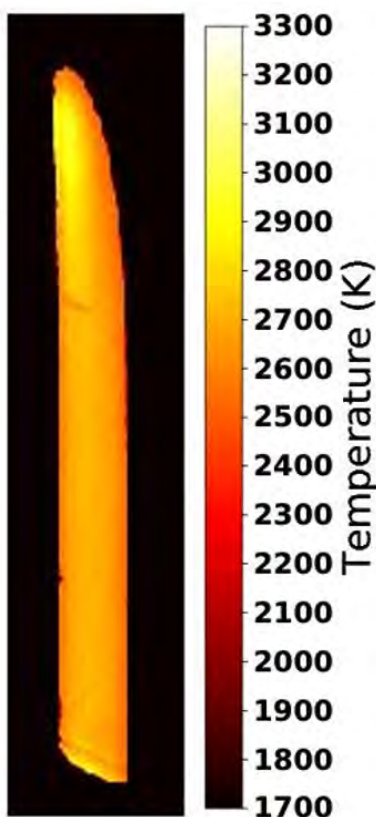


Figure 9. Example of how surface temperature is estimated using a DSLR image using two color ratio pyrometry. Image was taken immediately before test time.

UV Spectrometer.

The UV spectrometer used in the experiments was an Acton Research SpectraPro 2300i coupled to a Princeton Instruments PI-MAX Intensified Charge-Coupled Device (ICCD) UV-sensitive camera. The spectrometer was configured using a grating with a groove density of 600 g/mm centered at 380 nm when targeting CN violet bands

and 255 nm when targeting atomic Si. Additionally, for two shots at the end of the second experimental campaign, the spectrometer was centered at 480 nm to target C₂ Swan bands. The images used an exposure time of 35 μ s during the steady test time. The spectrometer was used to capture spatially-resolved, time-integrated images.

The high-temperature gas emitted light through a window mounted on the side of the test section. When targeting atomic Si lines, this window was a UV-grade fused silica window. For CN violet and C₂ Swan bands, it was a k9 borosilicate window. The light is redirected from the test section to the entrance slit of the spectrometer using a concave focusing mirror, a flat turning mirror, and a periscope. The periscope serves the dual purpose of changing the height of the light path from the test section window to that of the spectrometer entrance slit and also reorients the image by 90 degrees to capture the model surface, shock layer, expansion fan, and freestream flow.

vis/nIR Spectrometer.

The vis/nIR spectrometer used during the second experimental campaign was an Acton Research SpectraPro 2300i coupled to an Andor VUV Enhanced ICCD camera. The spectrometer was configured using a grating with a groove density of 600 g/500 nm centered at 480 nm when targeting C₂ Swan bands and 790 nm when targeting atomic N and O lines. The images used an exposure time of 35 μ s during the steady test time. The window used when targeting C₂ Swan bands and atomic N and O lines was a k9 borosilicate window.

MWIR Spectrometer.

The MWIR spectrometer used during the first experimental campaign was a Prince Instruments Acton SpectraPro SP2500i coupled to an IRCameras IRC800 Liquid Nitrogen Cooled Infrared Camera System. The IR spectrometer was config-

ured using a grating with a groove density of 17 g/mm centered at 4.7 μm . The images used an exposure time of 35 μs during the steady test time. The window used was an IR CaF_2 window.

The optical layout for the first experimental campaign is shown in Figure 10. The optical layout for the second experimental campaign is nearly identical to the first experimental campaign except for the location of the spectrometers: the UV spectrometer was moved to the other side of the tunnel and the vis/nIR spectrometer was placed where the UV spectrometer was.

High Speed Imaging.

The experiments were recorded using a Shimadzu HPV-1 high-speed camera. This camera is capable of frame rates up to 1 MHz and records the luminosity of the flow over the model [46]. The videos for most shots were recorded at 0.5 MHz with a 4 μs exposure time. A recording time of 400 μs was used to ensure observation of flow arrival, steady flow establishment, and arrival of the driver gas.

The camera captured images using a turning mirror through a side window except for a brief period during the first experimental campaign. During this campaign when targeting atomic Si, high-speed video collection was not possible until the camera was relocated to obtain a top down view of the model, as the smaller diameter fused silica window prevented access. This issue was remedied during the second experimental campaign by locating the UV spectrometer on the opposite side of the test section.

3.5 Acquisition of Spectra

Figure 11 show the capture areas for the UV, vis/nIR, and MWIR spectrometers throughout the course of the experiments. For most of the shots, the capture area focused on the expansion region at locations of 0.75, 4.0, and 6.5 mm above the

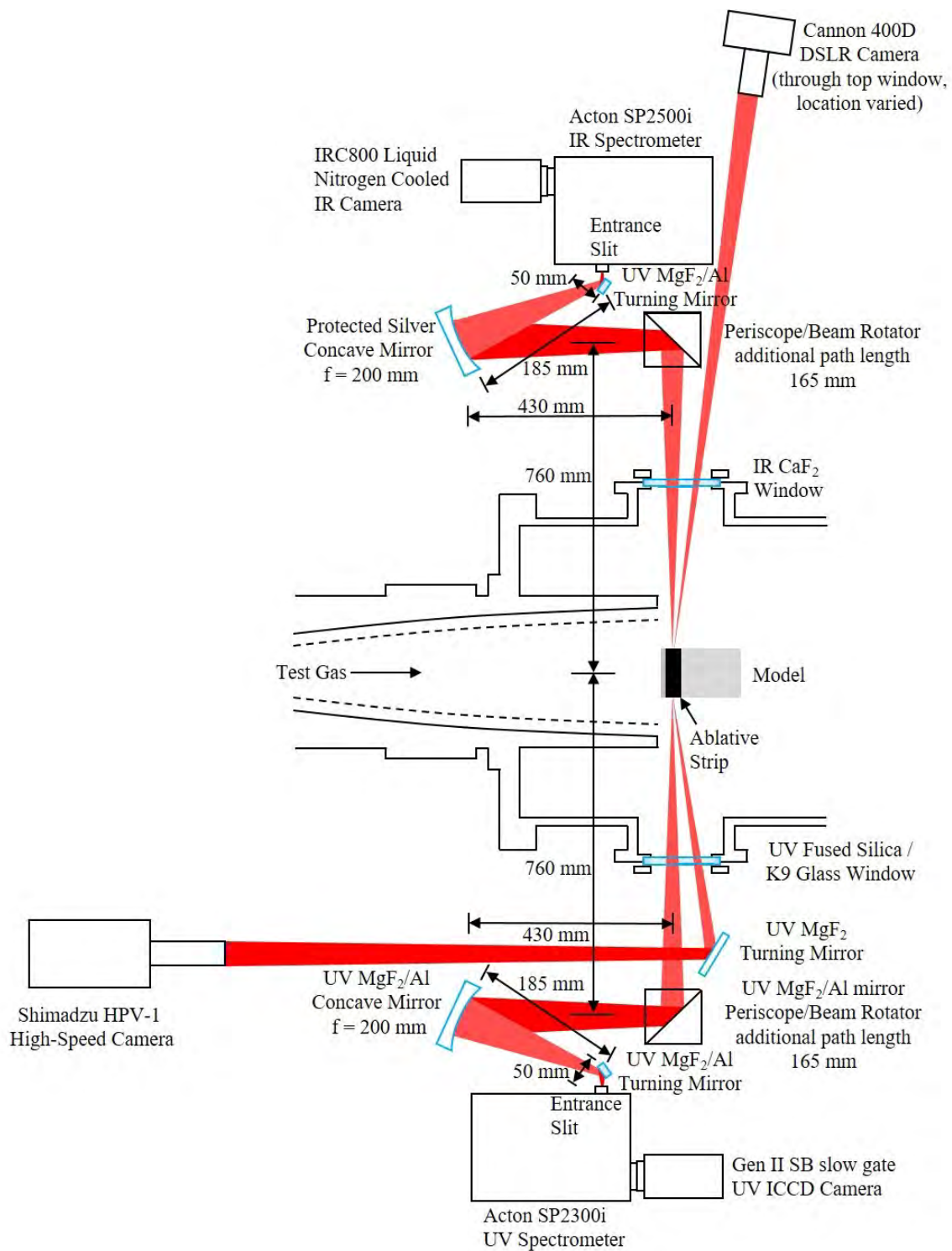


Figure 10. Schematic of optics layout used during X2 experiments.

model. Data was also collected in the near-stagnation region at the center of the ablative strip.

The resultant images from the UV, vis/nIR, and IR spectrometers are spectral intensity contour plots with wavelength and spatial distance as the horizontal and vertical axis, respectively. Intensity is represented by the number of signal counts, which is an arbitrary unit for uncalibrated results. The spatial distance is represented by the number of pixels, while the wavelength is in units of nanometers. After calibration, the intensity is measured by spectral radiance in units of $\text{W}/(\text{cm}^2 * \mu\text{m} * \text{sr})$ and the spatial distance is measured in millimeters. Figure 12 shows uncalibrated UV spectral results for shot x2s3570. The top contour plot in each image is uncalibrated output from the spectrometer, while the bottom line plot is an integration of spectral intensity over the pixel range corresponding to the expansion region. Previous experiments at UQ have shown a 10 – 20% shot-to-shot variation in measured spectral radiance values [47], which results from the error associated with the integrating sphere calibration uncertainty and cumulative error in each integration step [43].

There are three calibrations that must be undertaken when processing experimental results: intensity calibration, wavelength calibration, and spatial calibration. The intensity calibration can be accomplished by using one of two methods. The first method is an in-situ calibration conducted by placing a light source of known spectral radiance, a Labsphere CSTM-LR-2Z-4, in-place of the model and recording an image with the optical system. While this method inherently accounts for the optical efficiency of all optical components, the second method does not. This method uses an Optronic Laboratories OL 200M tungsten calibration lamp with serial number S-1197, of known spectral irradiance. The solid capture angle, magnification, and optical efficiencies of all components of the optical system must be known, making this method more prone to error. The Labsphere intensity calibration method was used

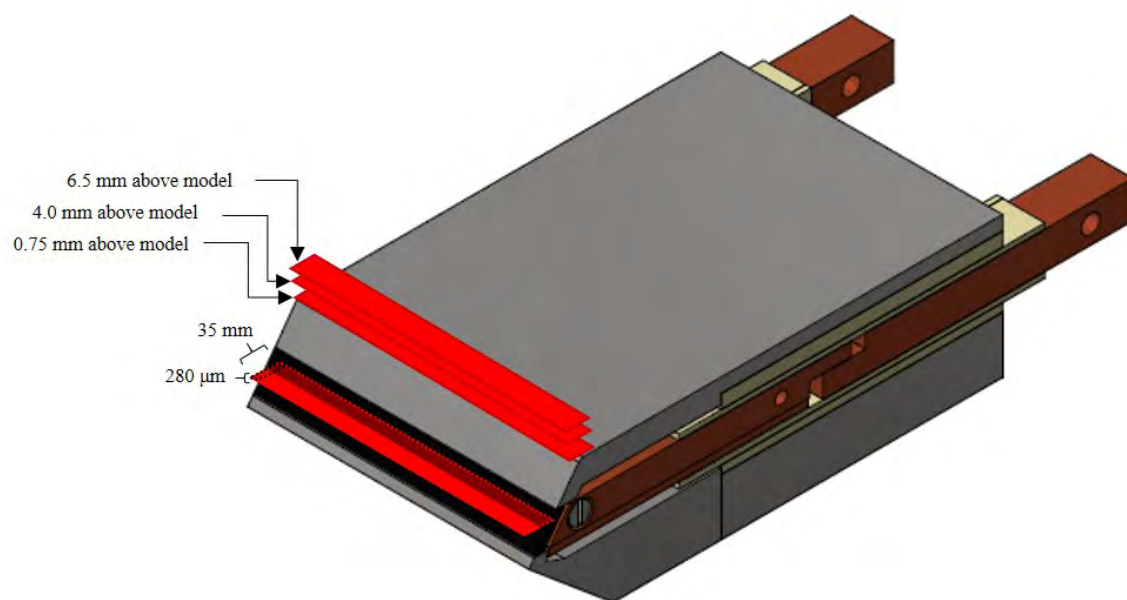


Figure 11. Schematic of spectrometer capture area at various target locations. Adapted from Ravichandran [139].

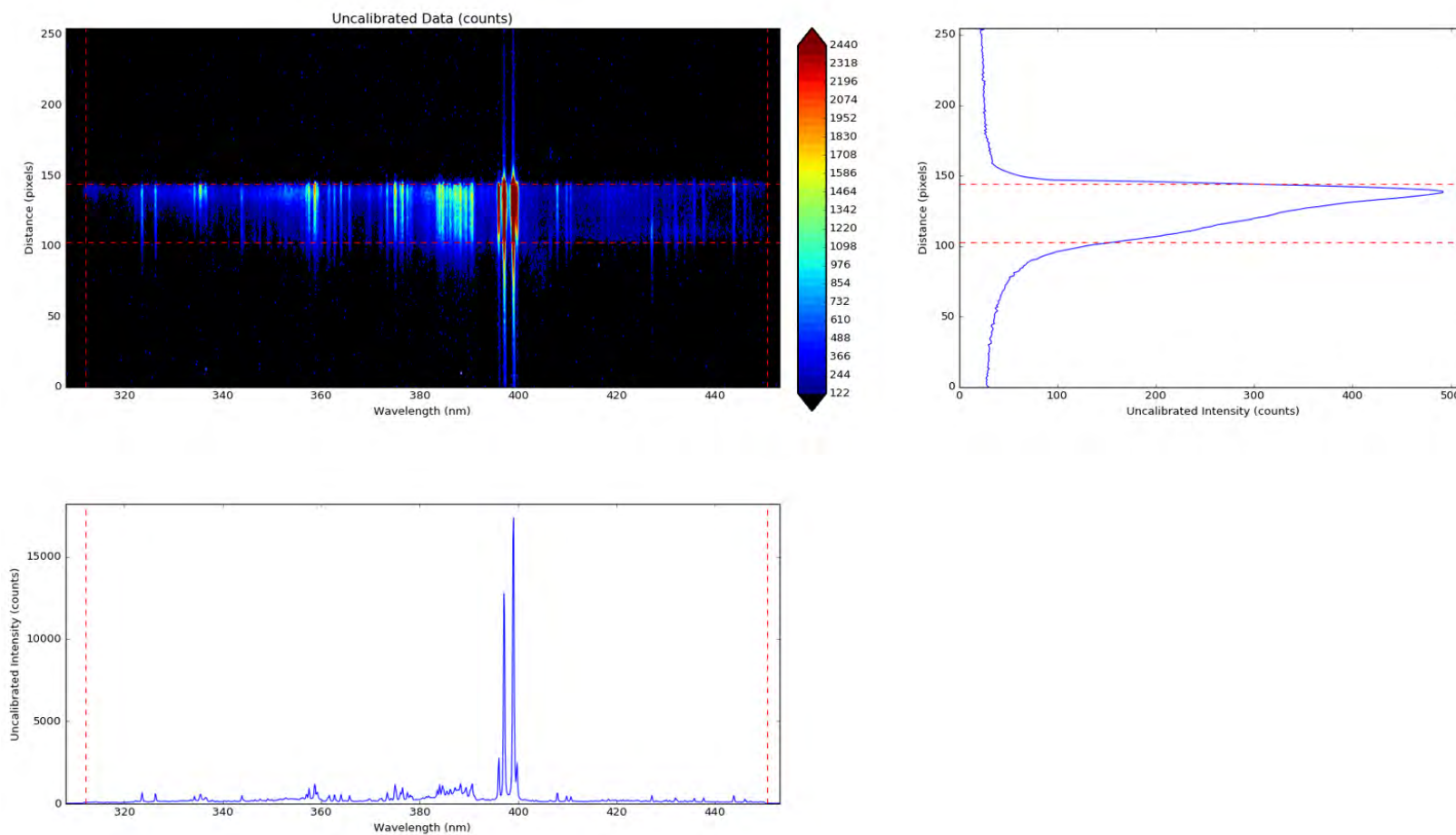


Figure 12. Uncalibrated UV spectral results for shot x2s3570. The top contour image is uncalibrated output from the UV spectrometer. The flow is bottom to top. The bottom line plot represents an integration of spectral intensity from pixel 103 to 144 for all wavelengths.

for all data presented in this dissertation except when targeting atomic Si. The tungsten lamp intensity calibration must be used for atomic Si as the Labsphere method is only valid above approximately 300 nm.

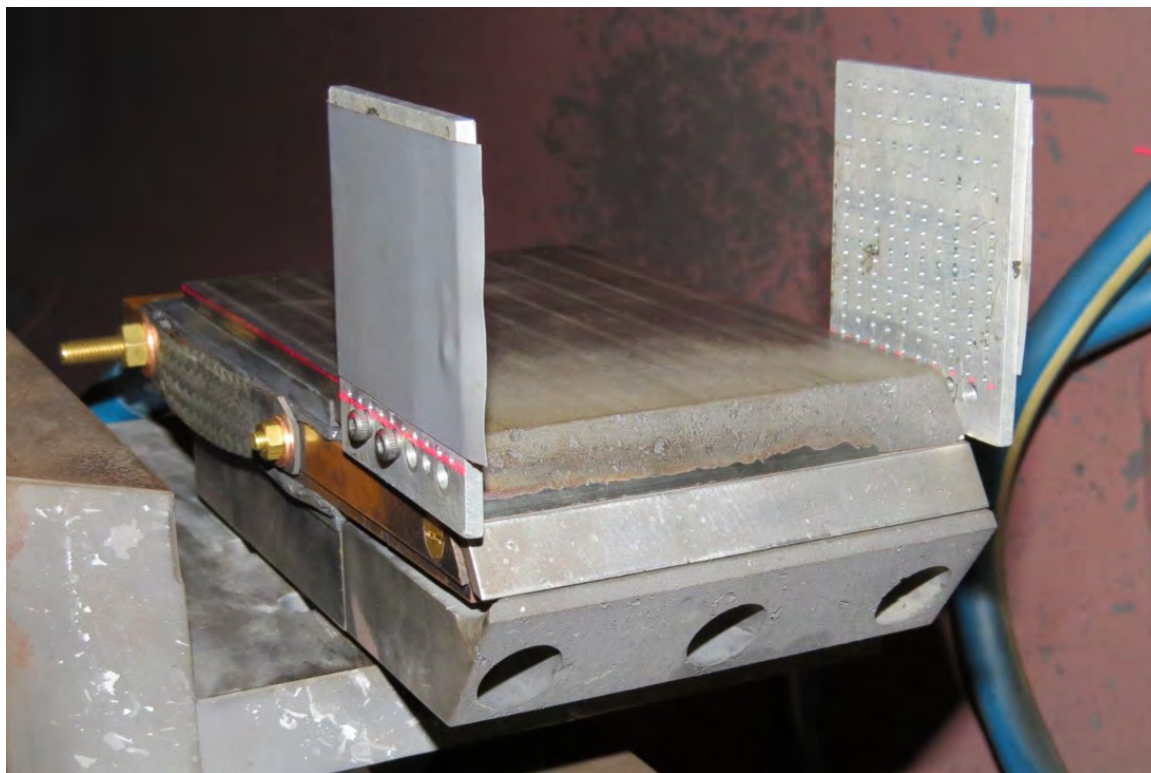


Figure 13. Model in X2 facility during spatial calibration and alignment.

The wavelength and spatial calibration are far simpler. The wavelength calibration is done using a Newport 6035 mercury/argon (Hg/Ar) pencil lamp. An image is captured and a polynomial fit is created by comparing the observed lines to the actual lines in the users manual. The spatial calibration is done by capturing an image while shining a light source through the alignment plate and counting the number of pixels between holes that are a known distance apart. The model in the X2 facility during spatial calibration and alignment is shown in Figure 13.

The unique capabilities of the X2 facility and its full suite of optical equipment make it ideally suited for characterizing high-temperature materials. The next two chapters will discuss the results of the two experimental campaigns.

IV. First Experimental Campaign

The following results are from the first experimental campaign conducted at UQ from 15 May - 2 June 2017. During this campaign, a total of 25 shots were completed, including four shots that were completed later by UQ personnel. A summary of the shots discussed in this chapter is shown in Table 8. Some of the shots were unsuccessful for various reasons (optics misaligned, sample failed to heat, etc.) and are not included in this table. All shots with the exception of x2s3585 were with C-C cut with the fibers parallel to the incoming flow. Shot x2s3585 was with C-C cut with the fibers perpendicular to the incoming flow to assess the effects of machining parts in this orientation. Additional parts were manufactured in this orientation but were not used during the experiments.

Table 8. Summary of shots completed during first X2 experimental campaign.

Material	Heating Condition	Feature Investigated	UV Target	MWIR Target	Temperature (K)	X2 Shot ID
Cold Steel	Unheated	Near-Stagnation	CN Violet	CO/CO ₂	N/A	x2s3559
C-C	100 A	Near-Stagnation	CN Violet	CO/CO ₂		x2s3560
C-C	200 A	Near-Stagnation	CN Violet	CO/CO ₂		x2s3562
C-C	300 A	Near-Stagnation	CN Violet	CO/CO ₂		x2s3564
C-C	100 A	Expansion, 6.5 mm above model	CN Violet	CO/CO ₂		x2s3566
C-C	200 A	Expansion, 6.5 mm above model	CN Violet	CO/CO ₂	2521	x2s3567
C-C	300 A	Expansion, 6.5 mm above model	CN Violet	CO/CO ₂	2713	x2s3568
C-C	300 A	Expansion, 4.0 mm above model	CN Violet	CO/CO ₂		x2s3570
C-C	300 A	Expansion, 0.75 mm above model	CN Violet	CO/CO ₂		x2s3565
C-C ($\perp$)	300 A	Expansion, 0.75 mm above model	CN Violet	CO/CO ₂		x2s3585
SiC	125 A	Expansion, 0.75 mm above model	CN Violet	CO/CO ₂	2232	x2s3571
SiC	250 A	Expansion, 0.75 mm above model	CN Violet	CO/CO ₂	2451	x2s3572
SiC	Unheated	Expansion, 0.75 mm above model	Atomic Si	CO/CO ₂	N/A	x2s3576
SiC	125 A	Expansion, 0.75 mm above model	Atomic Si	CO/CO ₂	2287	x2s3578
SiC	250 A	Expansion, 0.75 mm above model	Atomic Si	CO/CO ₂		x2s3577

The main objectives of this first experimental campaign were to assess the effectiveness of the SiC coating at introducing ablative species into the flowfield and evaluate the effects of using C-C cut to varying thicknesses and fiber orientations (i.e. perpendicular or parallel) to the flowfield. Going into the experimental campaign, there were concerns that the SiC coating would be too brittle and fragile to survive the extreme conditions of the X2 tunnel. As will be discussed in this chapter, the

SiC coating far exceeded expectations. Additionally, it was suspected that it may be difficult to heat C-C cut with the fibers perpendicular to the flow given the inherent porosity of the material, however, this concern also proved to be invalid.

4.1 Bench Testing

Prior to commencing with actual shots, a number of “bench tests” were performed to gain an understanding of what surface temperatures might be expected. The power supply available for the bench test was capable of supplying up to 12.5 V and 300 A. Figure 14 shows this power supply and a C-C sample being heated. The 12.5 V limit was reached at current values of about 150 to 175 A, limiting the temperatures that could be achieved. Table 9 shows the temperatures that were measured during bench testing.

Table 9. Temperatures measured during bench testing during the first experimental campaign.

Material	Condition	Temperature (K)
C-C ($\parallel$)	100 A	1700
C-C ($\parallel$)	150 A	2000
C-C ($\perp$)	130 A	2250
C-C ($\perp$)	150 A	2200
SiC	145 A	1650
SiC	175 A	1900

The C-C sample cut with the fibers perpendicular to the flow direction reached a higher temperature than the C-C sample with the fibers cut perpendicular to the flow direction. This difference is likely explained by the fact that the perpendicular-cut samples were actually about 2.5 mm thick rather than 3 mm thick as the parallel cut samples were, increasing their resistance. Thus, it can be concluded that fiber direction has little effect on the ability to resistively heat the samples. It should be noted, however, that samples cut perpendicular to the flow were more difficult to



Figure 14. Power supply used for bench testing. Sample being heated was C-C.

work with, as the first attempt to tighten the screws attaching the sample to the copper electrodes resulted in the tabs cracking along the fiber direction.

Photos of the SiC-coated sample used for bench testing before and after heating are shown in Figure 15. The post-test photo clearly shows that the sample has oxidized. It should be noted that the bench testing took place under atmospheric conditions while heating of actual shots took place under near-vacuum. Therefore, samples evaluated during bench testing will likely experience higher levels of oxidation than actual shots.

4.2 Results

During the first experimental campaign, two shots with stainless steel, 15 shots with C-C, and eight shots with SiC-coated C-C were conducted. The two steel shots were used to establish a baseline for the collection of CN violet bands in the near-stagnation region and to ensure that all of the optical equipment was properly con-

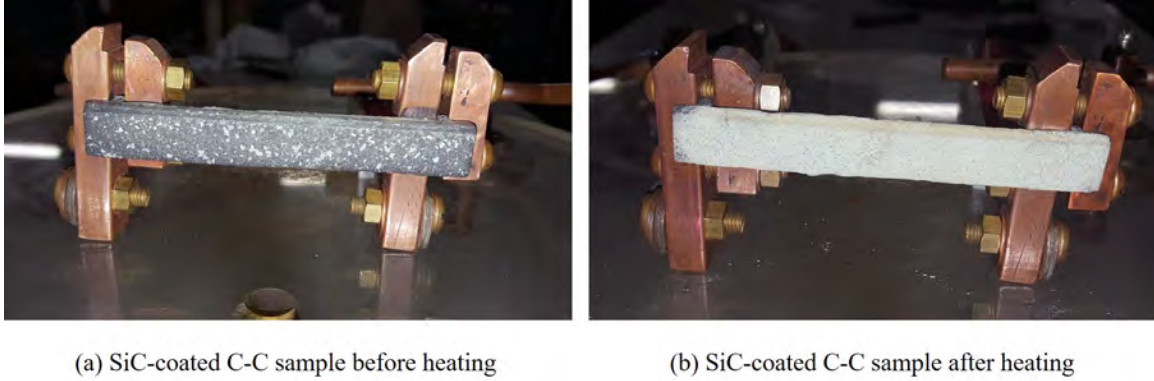


Figure 15. SiC-coated C-C sample before and after heating.

figured for shots with ablative specimens. Only eight SiC-coated samples were used during testing since only 10 were made given the concerns over the ability to heat coated samples. One sample was used during bench testing while another sample, which was 3 mm thick, was deemed too deformed as a result of the coating process to be used, leaving eight samples to test. Of the eight samples tested, the substrates of five were 3 mm thick while three were 6 mm thick. One of the 3 mm thick coated samples had a 300 μm thick coating while the other four had a 1 mm thick coating. One of the 6 mm thick coated samples had a 300 μm thick coating while the other two had a 1 mm thick coating. All of the C-C samples tested were 3 mm thick and were cut with the fibers parallel to the flow.

Assessment of Test Samples.

After completing two shots with steel strips, the first C-C shot was attempted. This shot was successful in heating the sample and collecting data, however the model was badly damaged during the shot, as shown in Figure 16. The model had to be removed, the spare set of copper electrodes had to be installed, and the alignment process had to be repeated. It was thought that the C-C sample broke due to the force of the driver gas, allowing it to fill the cavity behind the strip. The force of the driver gas resulted in the copper electrodes being violently expelled from the model

causing significant damage, as shown in Figure 17. To prevent significant damage from happening after every shot, the cavity behind the strip was filled with a V-shaped aluminum piece to channel the driver gas in the event that the strip continued to break, with the hope of preventing the copper electrodes from being deflected away from the model. This change proved successful as future shots did not result in such significant damage to the model, though the copper electrodes did deflect slightly from the model from time to time, requiring minor adjustments.

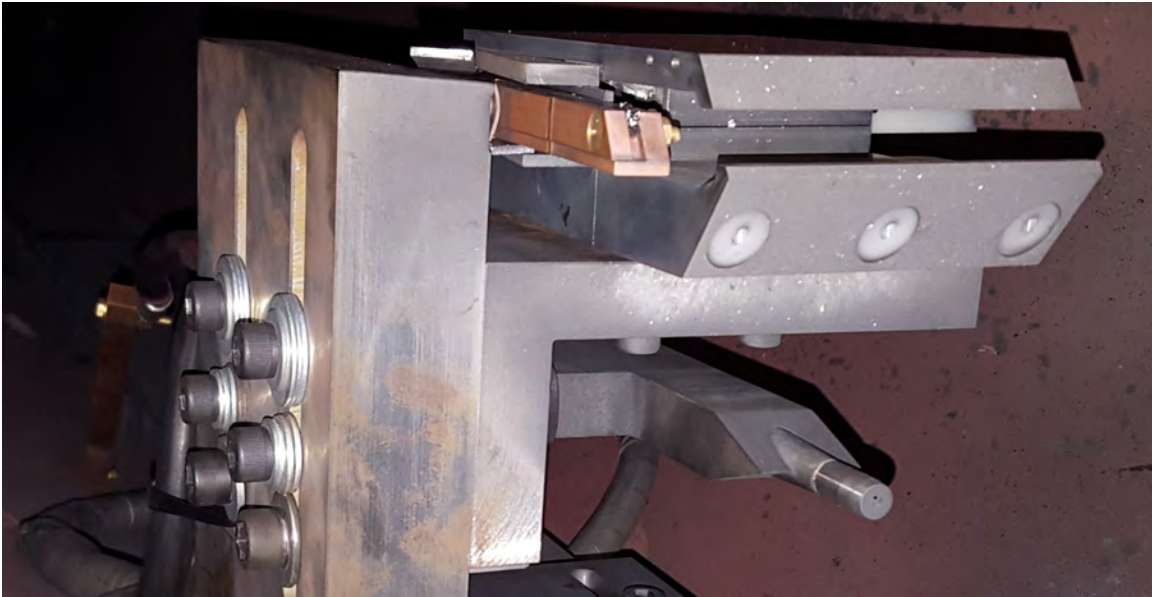


Figure 16. Model after first shot with C-C (x2s3560).

Of the 15 C-C samples tested, most broke during the shot while two survived fully intact. Figure 18 shows a C-C strip mounted in the model before a shot while Figures 19, 20, and 21 show C-C samples after the shot. Figure 19 is representative of how most of the C-C samples that broke looked after the shot, displaying cracking in the fiber direction. Figure 21 shows charring not exhibited by any other samples, possibly the result of a small pocket of resin that was not pyrolyzed during the manufacturing process but does not appear to have affected the data collection.

The 3 mm thick SiC-coated samples displayed a similar trait of breaking during

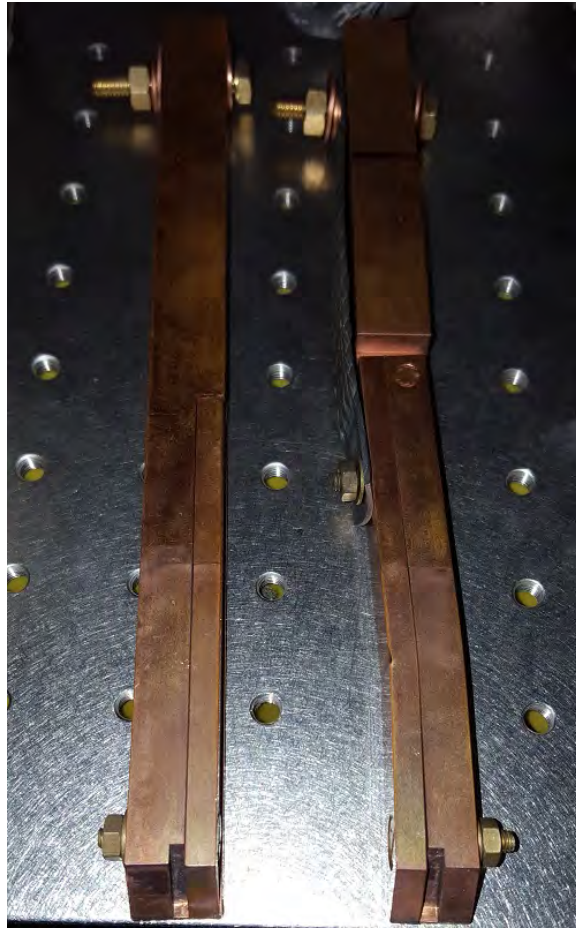


Figure 17. Copper electrodes after first shot with C-C (x2s3560).



Figure 18. Model before first shot with C-C (x2s3560).



Figure 19. Model with C-C sample after shot x2s3564.



Figure 20. Model with C-C sample after shot x2s3567.



Figure 21. Model with C-C sample after shot x2s3570.

testing. In general, it appears as though the 3 mm thick coated samples broke into more and smaller pieces than their uncoated counterparts, which suggests that the coating process made the samples more brittle. Most of the 3 mm thick coated samples displayed some degree of warping as a result of the coating process with one of the samples being deemed too deformed to be used. Figure 22 shows a 3 mm thick coated sample before testing. It can be noted that the bottom left corner of the strip does not line up with the model due to the warping. Since all of the 3 mm thick coated samples broke, it is difficult to assess whether the different coating thickness were adequate. Figures 23, 24, 25, 26, and 27 show each of the 3 mm thick coated samples after the shot.

The 6 mm thick SiC-coated samples fared far better than the 3 mm thick coated and uncoated samples with all three of the samples tested surviving intact. Figures 28, 29, and 30 show these samples after the shot. The first two of these samples had a 1 mm thick coating while the other sample had a 300 μm thick coating. There is a distinct difference in the appearance of these samples. The C-C substrate is clearly visible in the sample that had the thinner coating, while the coating is still completely intact for the samples with the thicker coating.



Figure 22. Model with SiC-coated C-C sample before shot x2s3572.



Figure 23. Model with SiC-coated C-C sample after shot x2s3571.



Figure 24. Model with SiC-coated C-C sample after shot x2s3572.



Figure 25. Model with SiC-coated C-C sample after shot x2s3573.



Figure 26. Model with SiC-coated C-C sample after shot x2s3574.



Figure 27. Model with SiC-coated C-C sample after shot x2s3575.



Figure 28. Model with SiC-coated C-C sample after shot x2s3576.



Figure 29. Model with SiC-coated C-C sample after shot x2s3577.



Figure 30. Model with SiC-coated C-C sample after shot x2s3578.

Temperature Measurements.

Heating of the test samples was accomplished by adjusting the current on the power supply. For C-C, 100 A, 200 A, and 300 A were chosen to provide a range of surface temperatures that were expected to cover approximately 1700 K to 2800 K. Due to the limited number of samples available, only two heating levels were used for the SiC-coated samples. 125 A and 250 A were selected based on the desire to obtain data below and above the expected transition from passive to active oxidation to see if there was a noticeable difference in the spectra.

Actual temperature measurements for C-C samples ranged from approximately 1900 K to 2700 K. For SiC-coated C-C, the range was roughly 2100 K to 2450 K. A summary of each heating condition (i.e. 100 A, 200 A, etc.), taken by averaging all measurements at that condition is contained in Table 10. It should be noted that additional bench testing was conducted during the second experimental campaign to provide additional data points for the values shown in this table. Further details on this testing as well as the rest of the second experimental campaign will be discussed in the next chapter.

The temperature measurements shown in Table 8 are quite sparse. A new technique that uses several wavelength ratios (theoretically making it more accurate) rather than the red/blue/green wavelengths of the DSLR camera was attempted during the start of this campaign. Unfortunately, the camera either overexposed or underexposed on many of these shots. This technique was eventually abandoned and the DSLR camera was used. However, there were still a few shots where the DSLR camera overexposed or underexposed, or there were not enough people available to operate this camera and the X2 tunnel (such as on weekends). The camera settings from the first experimental campaign were noted and applied to the second experimental campaign, which led to much better results for obtaining surface temperature

measurements.

Table 10. Average temperature for each heating condition during first experimental campaign.

Sample	Current (A)	Average Temperature (K)	Standard Deviation (K)	Measurements
C-C	100	1960	6	2
C-C	200	2521	0	1
C-C	300	2624	90	2
SiC	125	2077	99	4
SiC	250	2451	0	1

High-Speed Video.

High-speed video footage was utilized to ensure that data collection occurred during steady test time. The high-speed camera was triggered using a pitot probe to sense the pressure rise of the arriving shock. Figure 31 shows an uncoated C-C sample with a surface temperature of approximately 2600 K while Figure 32 shows a SiC-coated C-C sample with a surface temperature of roughly 2400 K. In the first figure, ablative products, likely CN, can be observed entering the shock layer. Such an observation could not be made utilizing the top-down high-speed video footage. As a result, such video footage did not prove to be very useful. These images appear as expected, however the gaps required between the ablative strip and the model led to multiple shocks forming. To simplify the simulated results, the gaps between the ablative strip and the model will not be modeled.

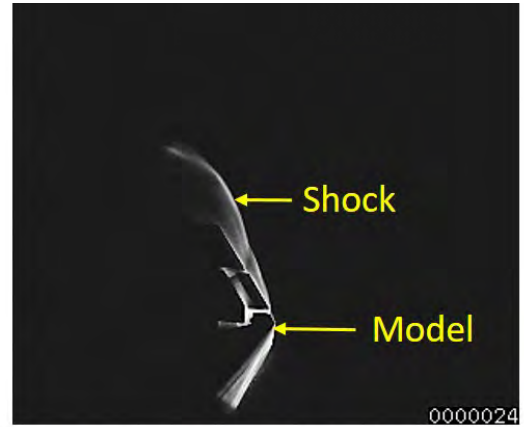
UV Spectra.

CN violet.

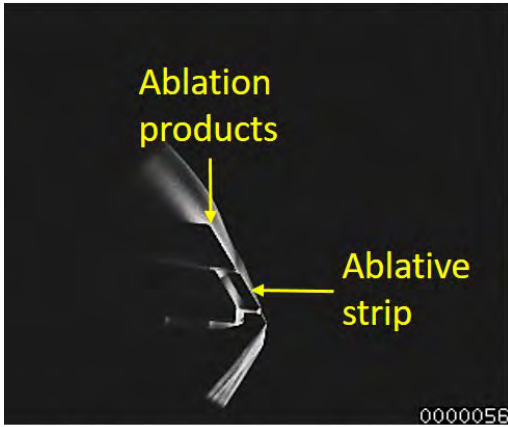
Figures 35, 36, 37, and 38 show UV spectra of C-C samples targeting CN violet bands. Figure 35 shows the UV spectra averaged across the near-stagnation region while Figures 36 and 37 show the UV spectra averaged across the expansion at a fixed



(a) Shock arrival ($t = 6 \mu\text{s}$)



(b) Flow structure established ($t = 24 \mu\text{s}$)



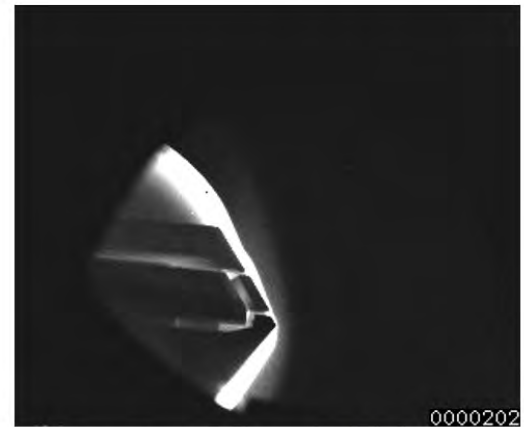
(c) Spectrometer start ($t = 56 \mu\text{s}$)



(d) Spectrometer finish ($t = 90 \mu\text{s}$)

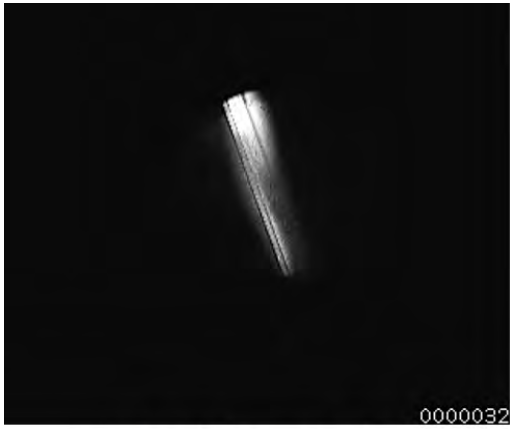


(e) Driver gas arrival ($t = 118 \mu\text{s}$)

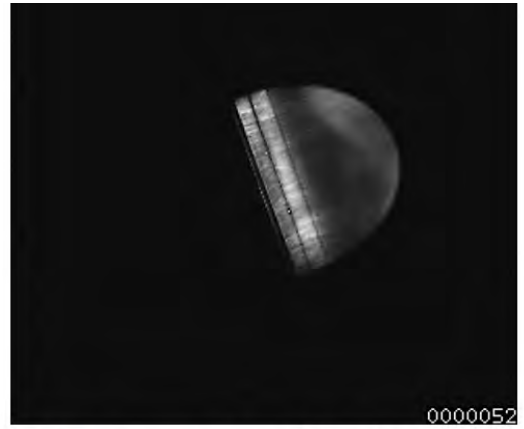


(f) Steady test time ended ($t = 202 \mu\text{s}$)

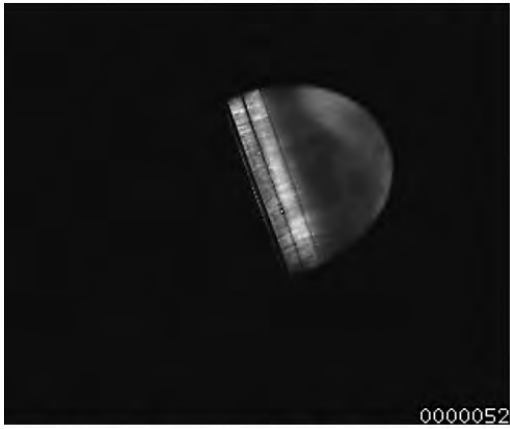
Figure 31. Example analysis of high speed footage from side (times shown are with respect to start of video).



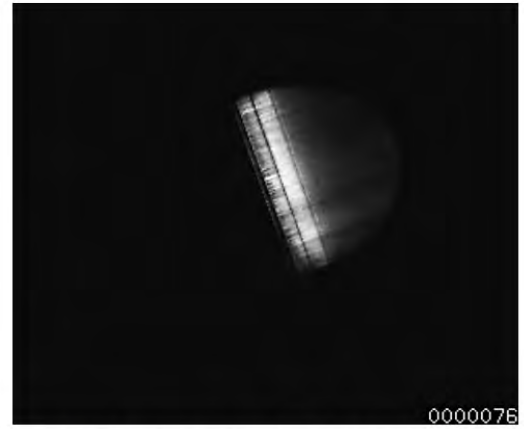
(a) Shock arrival ($t = 32 \mu\text{s}$)



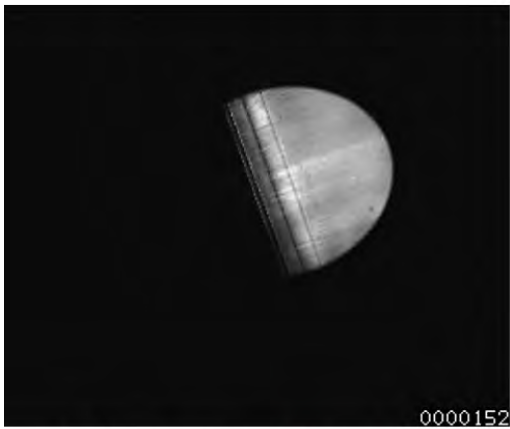
(b) Flow structure established ($t = 52 \mu\text{s}$)



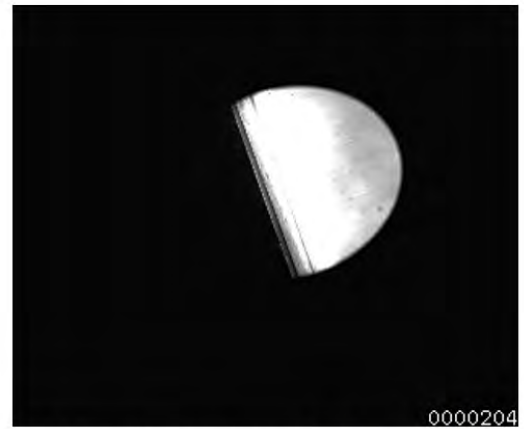
(c) Spectrometer start ($t = 52 \mu\text{s}$)



(d) Spectrometer finish ($t = 76 \mu\text{s}$)



(e) Driver gas arrival ($t = 152 \mu\text{s}$)



(f) Steady test time ended ($t = 204 \mu\text{s}$)

Figure 32. Example analysis of high speed footage from top (times shown are with respect to start of video).

location of 6.5 mm above the model at multiple temperatures and at multiple heights above the model at a constant temperature, respectively, as depicted in Figure 11. Lastly, Figure 38 shows the UV spectra for C-C samples cut with fibers perpendicular and parallel to the flow at the same expansion location and temperature.

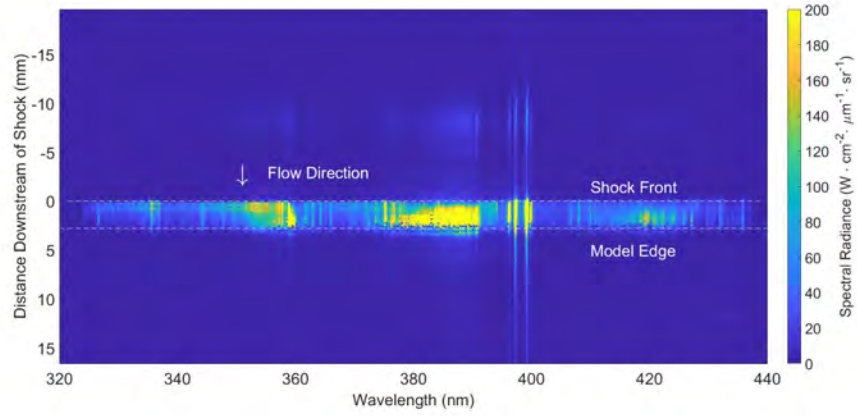


Figure 33. Example of calibrated UV spectra for the near-stagnation region.

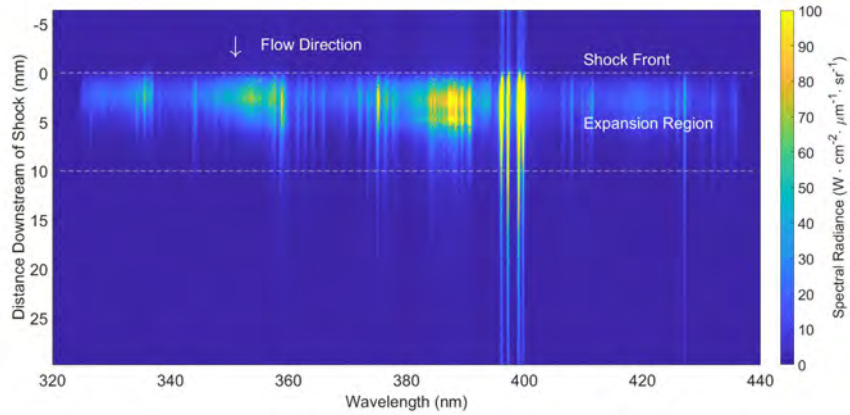


Figure 34. Example of calibrated UV spectra for the expansion region.

In each of these cases, the averaged spectra were extracted by averaging between the rows depicted by horizontal lines in Figures 33 and 34. For the near-stagnation region, this averaging was from the shock front to the model edge. For the expansion

region, this averaging was from the shock front to a distance approximately 10 mm downstream of the shock, where radiating species are no longer observed. Temperatures with an asterisk (*) indicate that a temperature measurement was not obtained for that shot and the value shown is the average of all measurements at this condition. Identification of spectra was accomplished using the NIST Atomic Spectra Database [136] and Pearse and Gaydon [145].

As expected, the spectral emissions are higher in the near-stagnation region compared to the expansion. The spectra averaged in the near-stagnation region show increasing emissions with surface temperature, which was expected based on past work by Lewis et al. [43]. The spectral radiance averaged in the expansion, conversely, does not appear to be influenced by increasing surface temperature. Curiously, the CN (B-X) $\Delta v = 0$ emission is higher for unheated steel than C-C heated to 1960 K. Carbon is a known contaminant [43], which potentially explains this observation.

The height above the model seems to have some influence on the spectral emissions. The measurements taken 6.5 mm above the model are clearly the least intense while the measurements taken 4.0 mm above the model appear to be the most intense. The fact that the spectra 4.0 mm above the model is slightly more intense than the spectra 0.75 mm above the model is likely a result of that shot being heated slightly more or from shot-to-shot variation.

Figure 38 shows that the UV spectra of the C-C sample cut with the fibers perpendicular to the flow is more intense compared to the sample cut with the fibers parallel to the flow. Based on the Scanning Electron Microscope (SEM) images taken at 50x magnification, shown in Figures 39 and 40, this outcome was not expected. It was anticipated that the radiation of the parallel-cut sample would be more intense because it is significantly more porous with large sections of exposed carbon fibers able to interact with the incoming test gas. After testing, this sample looked mostly

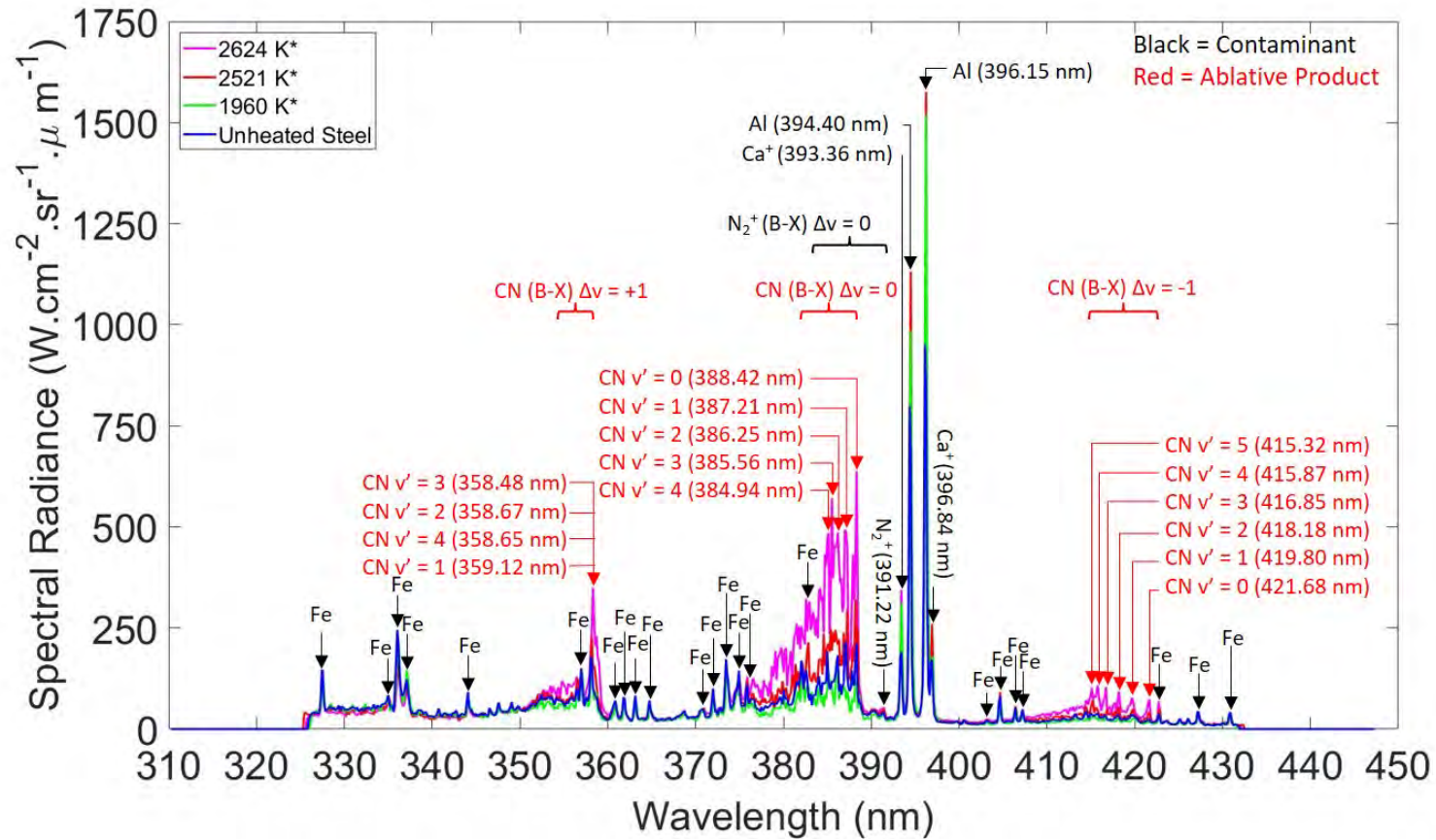


Figure 35. Spectral radiance comparison for C-C at three temperatures with unheated steel targeting CN violet bands. All measurements were taken by averaging in the near-stagnation region.

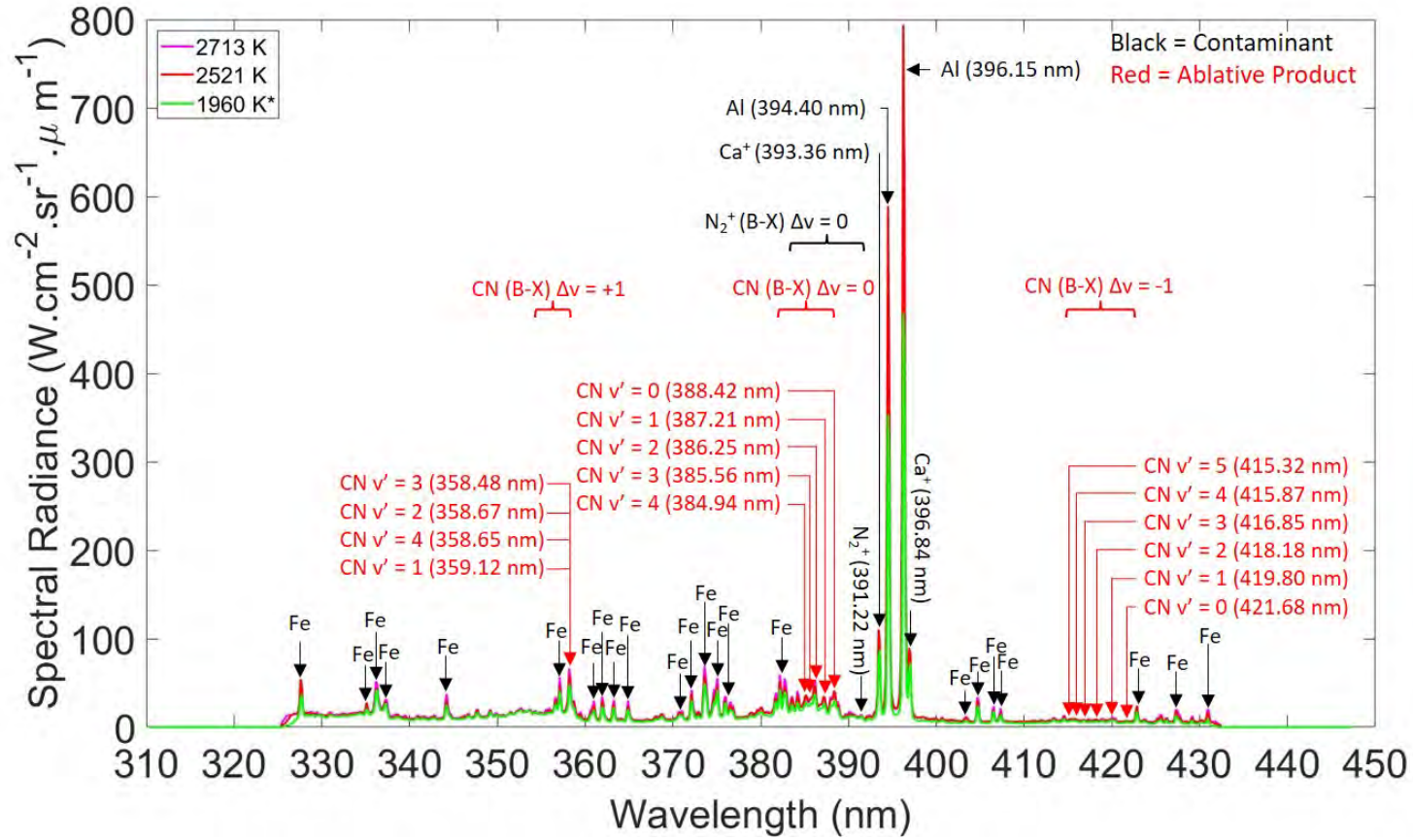


Figure 36. Spectral radiance comparison for C-C in the expansion region at three temperatures targeting CN violet bands. All measurements were taken by averaging in the expansion region 6.5 mm above the model.

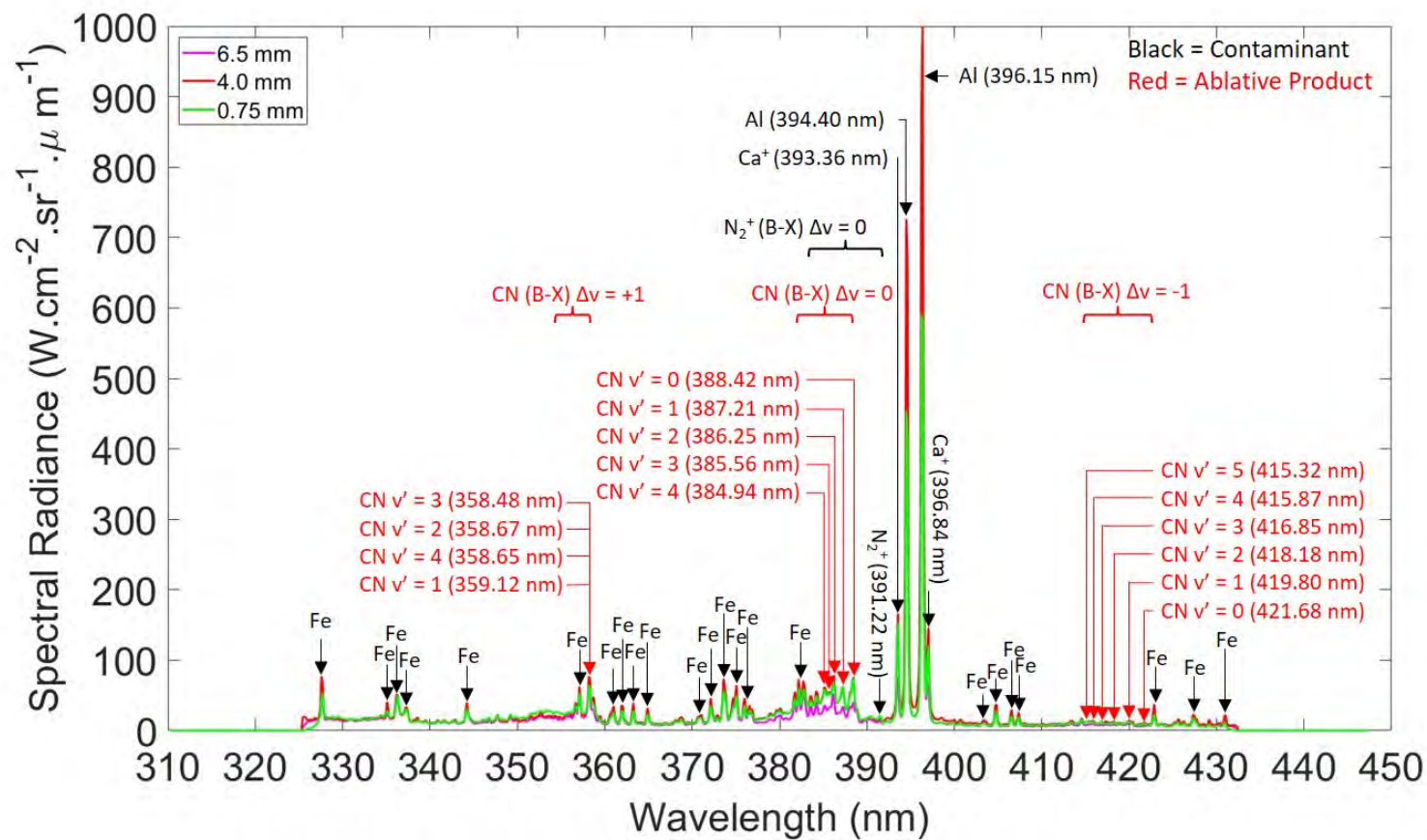


Figure 37. Spectral radiance comparison for C-C at three expansion heights. All measurements were taken by averaging in the expansion region above the model targeting CN violet bands. All samples had a temperature of approximately 2600 K.

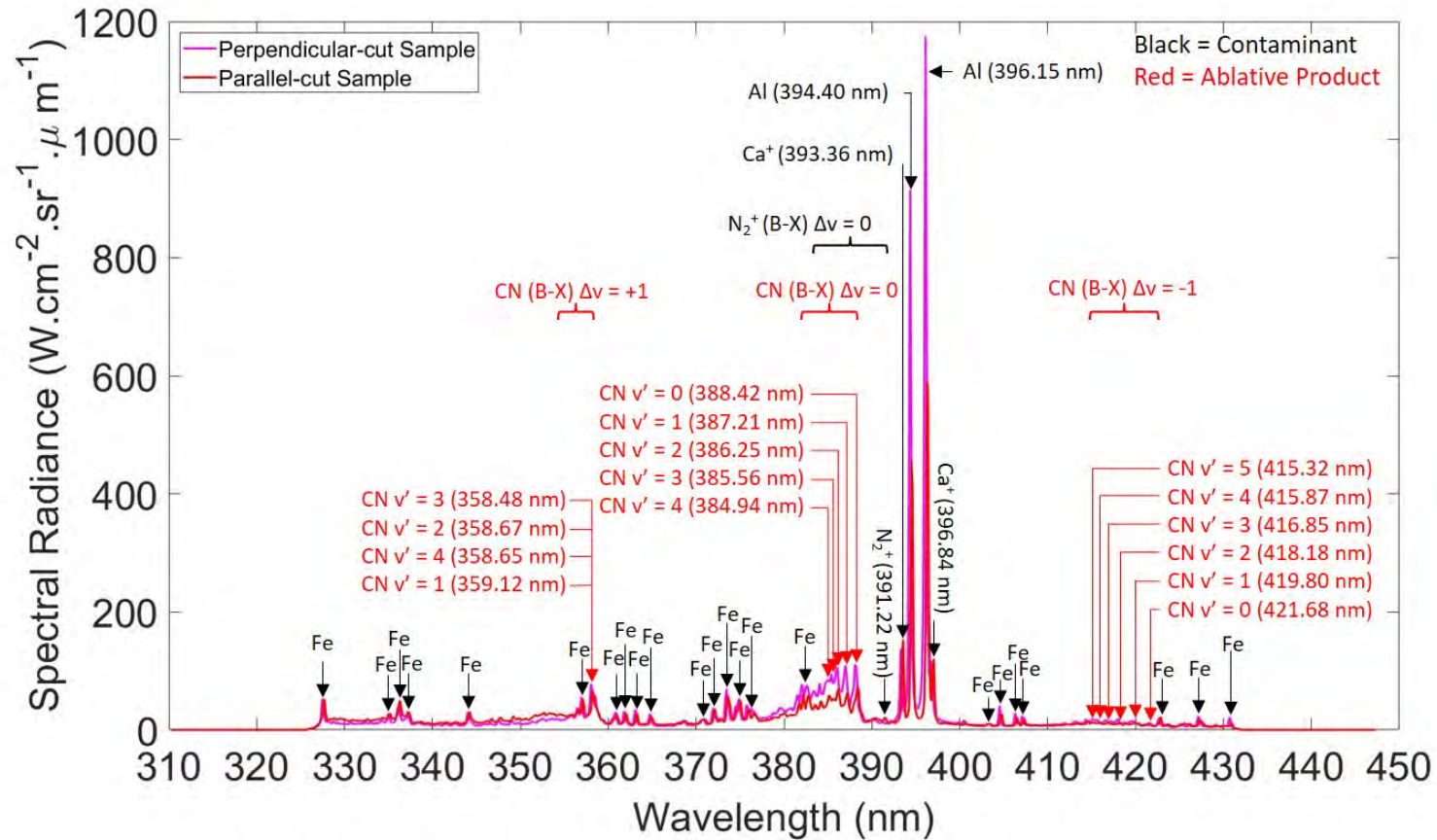


Figure 38. Spectral radiance comparison for 3 mm thick C-C samples cut with fibers perpendicular and parallel to the flow. Both measurements were taken by averaging in the expansion region 0.75 mm above the model targeting CN violet bands. Both samples had a temperature of approximately 2600 K.

the same with some surface degradation. The perpendicular-cut sample is tightly compact with no exposed fibers, though there appears to be some graphite matrix on the surface which could interact with the test gas. After testing, nearly all of the graphite on the surface is gone with many more exposed carbon fibers. Both of these samples are drastically different than the graphite sample, shown in Figure 41, which appears nearly featureless. Note that it is not possible to obtain post-test SEM images of graphite samples as they are always destroyed during the shot.

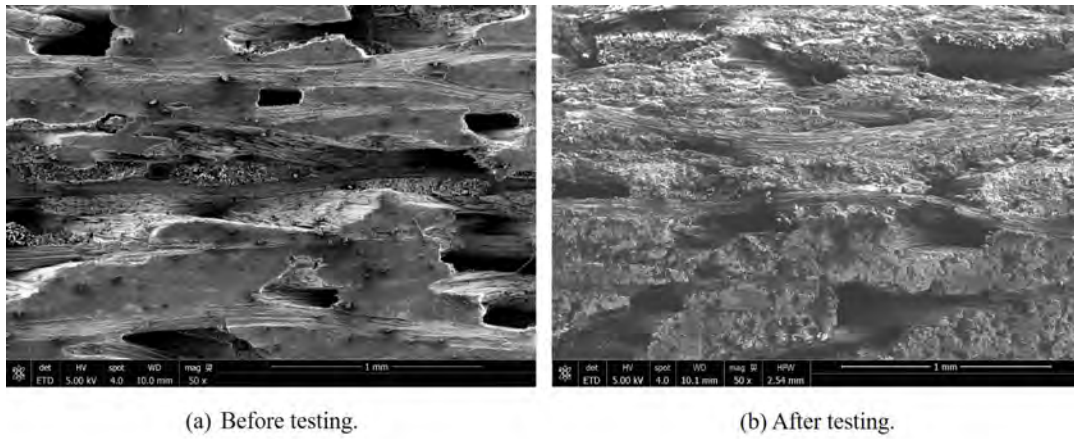


Figure 39. SEM images of C-C sample cut with fibers parallel to the flow before and after testing taken at 50x magnification.

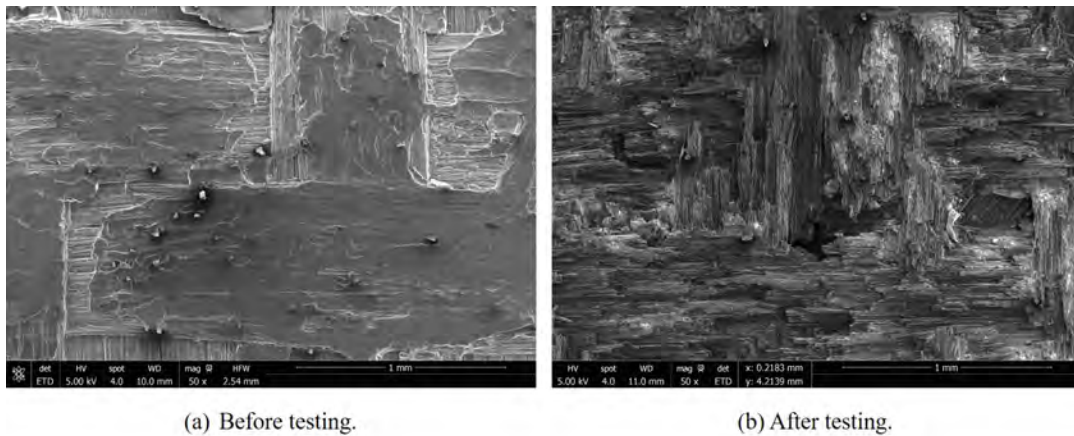


Figure 40. SEM images of C-C sample cut with fibers perpendicular to the flow before and after testing taken at 50x magnification.

Figure 42 shows before and after SEM images of SiC-coated C-C. The post-test

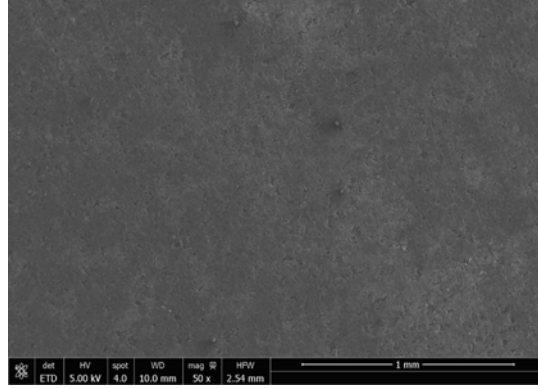
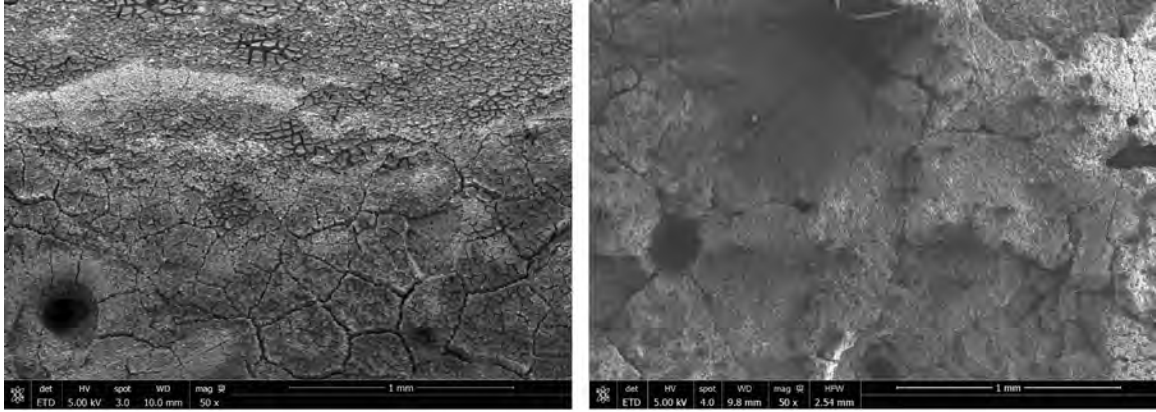


Figure 41. SEM image of graphite before testing taken at 50x magnification.

image shows some signs of surface degradation and oxidation, but the sample is largely undamaged. Although performing an assessment of the SiC-coating as an oxidation solution to C-C was not an objective of these experiments, the coating clearly seems to be providing oxidation protection to the underlying C-C surface.



(a) Before testing.

(b) After testing.

Figure 42. SEM images of SiC-coated C-C sample before and after testing taken at 50x magnification.

Figure 43 shows the UV spectra of SiC-coated C-C samples targeting CN violet bands. This image shows inconsistent results compared to the previously-discussed results with the lower temperature sample having significantly higher spectral radiance. Further analysis has determined that a portion of the UV spectra for the 2451 K case was cut off. It is believed that the portion of the spectra cut off corresponds

to the shock up to a distance of 5 mm downstream, which is why it appears so much less intense.

Atomic Si.

Figure 44 shows UV spectra of SiC-coated C-C samples targeting atomic Si lines. This image shows the expected trend of spectral emissions being higher with increased surface temperature. A number of potential atomic Si lines corresponding to those observed by Panerai [26] have been identified. However, the resolution of the data combined with the number of contaminants present in the flow make it difficult to determine if these lines are indeed atomic Si lines. The second experimental campaign investigated atomic Si lines further. Results will be discussed in the next chapter.

MWIR Spectra.

Though it was thought that perhaps oxidation products, (i.e. CO_2 and CO), might be observed in the MWIR region, only known facility contaminants (i.e. Fe and aluminum (Al)) were observed. CO_2 emissions have been observed in the MWIR region in simulations and experiments conducted by other researchers [48–51], however they were conducted in a Martian atmosphere, which is predominantly CO_2 . Based on this observation, the MWIR spectrometer was not used in the second experimental campaign. Examples of MWIR spectra are shown in Figures 45, 46, and 47.

4.3 Summary

The first experimental campaign marked the first time that SiC-coated C-C had been resistively heated and tested in the X2 shock expansion facility, expanding a relatively new preheating concept and enabling testing of additional materials. A minimal number of SiC-coated samples were tested as it was unknown prior to com-

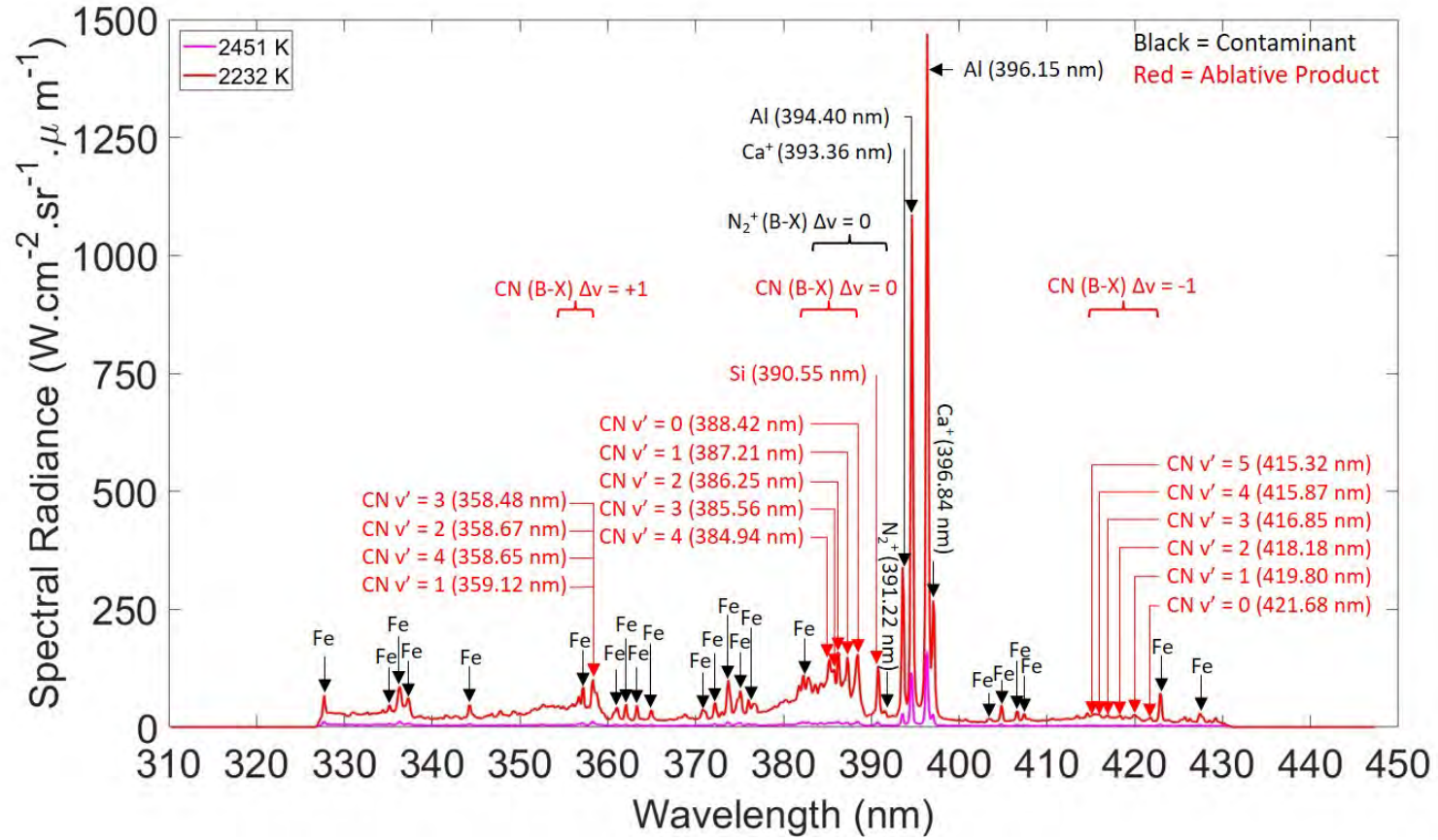


Figure 43. Spectral radiance comparison for SiC-coated C-C at two temperatures. All measurements were taken by averaging in the expansion region 0.75 mm above the model targeting CN violet bands.

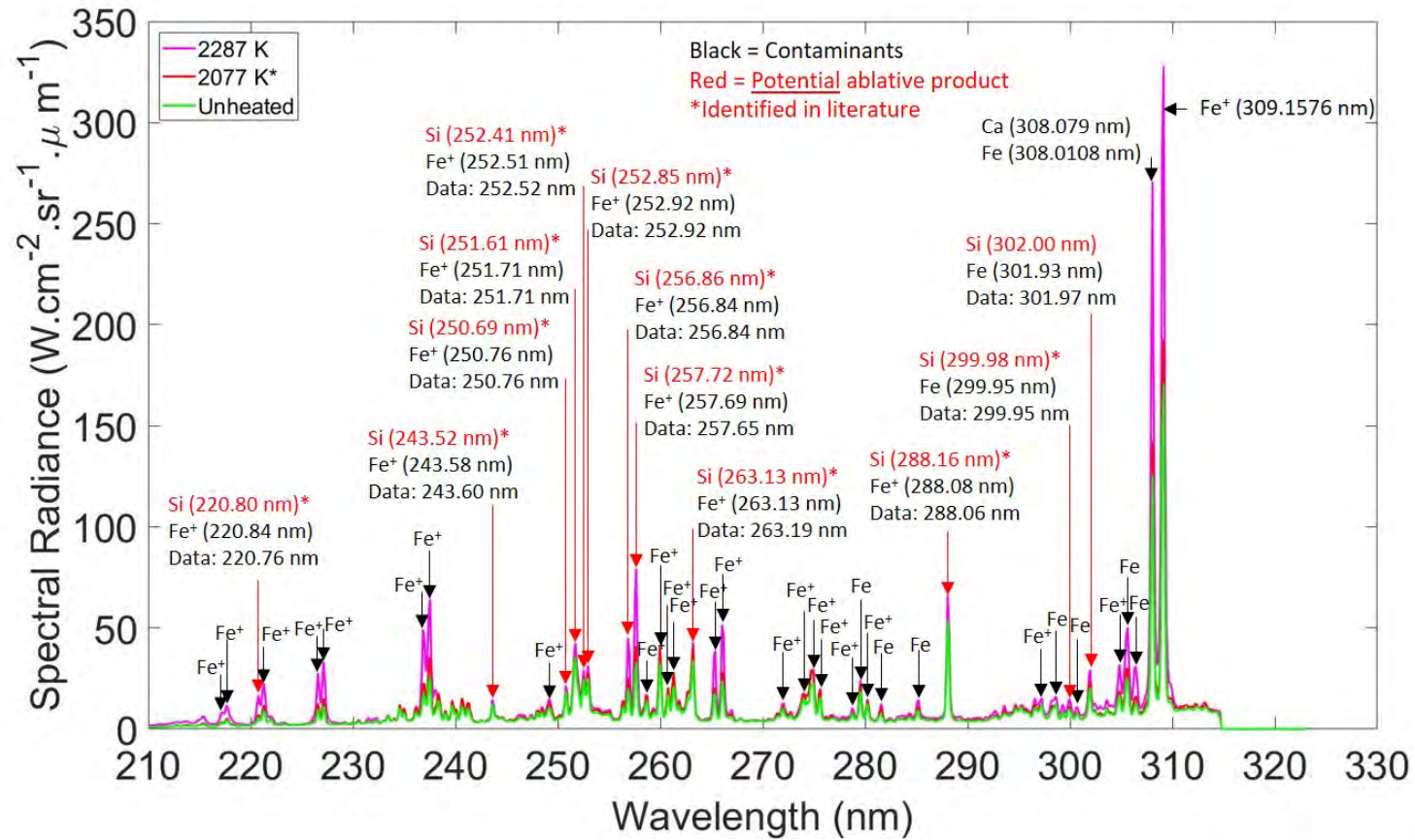


Figure 44. Spectral radiance comparison for SiC-coated C-C at two temperatures. All measurements were taken by averaging in the expansion region 0.75 mm above the model targeting atomic Si lines.

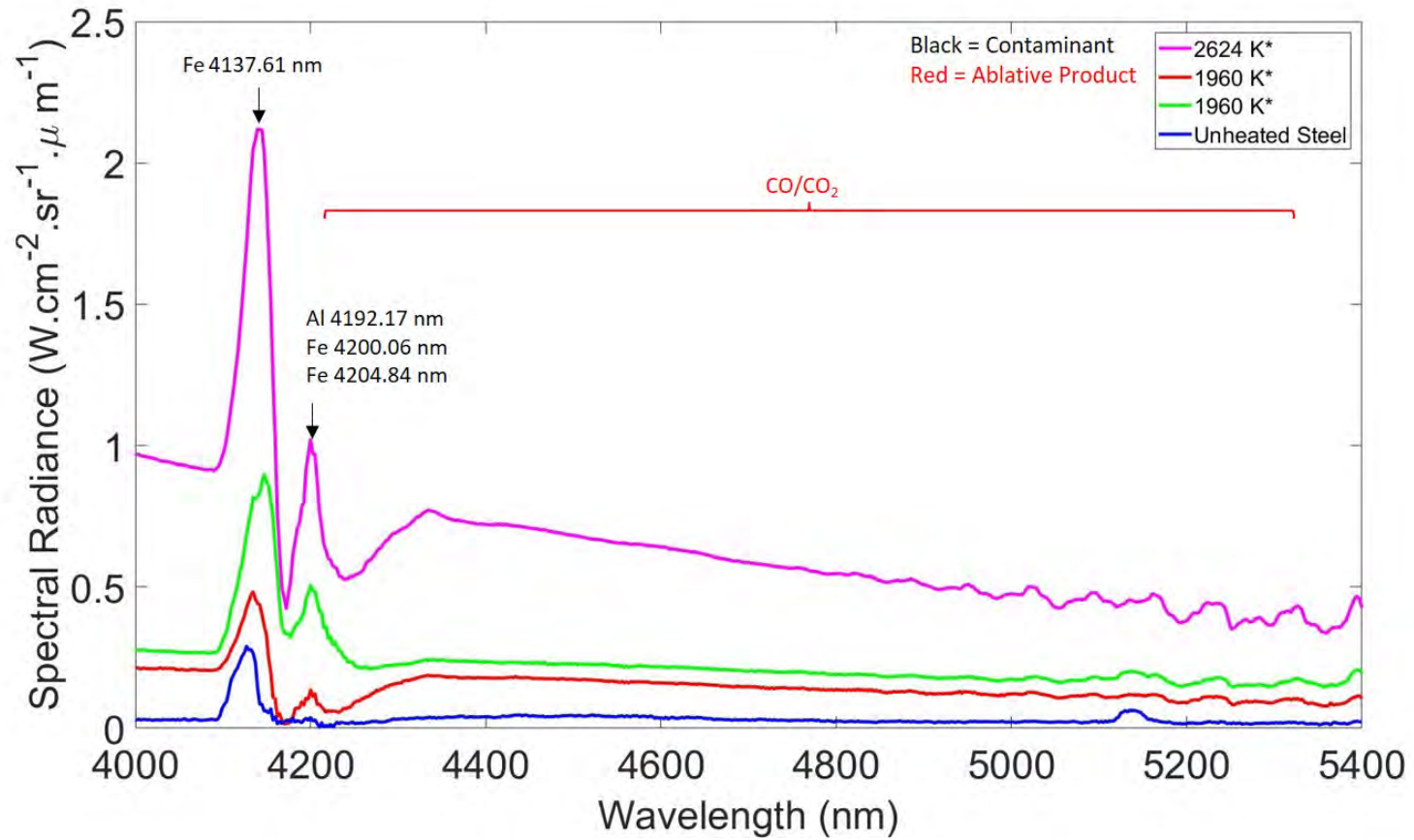


Figure 45. Spectral radiance comparison for C-C at three temperatures with unheated steel. All measurements were taken by averaging in the near-stagnation region targeting CO and CO₂.

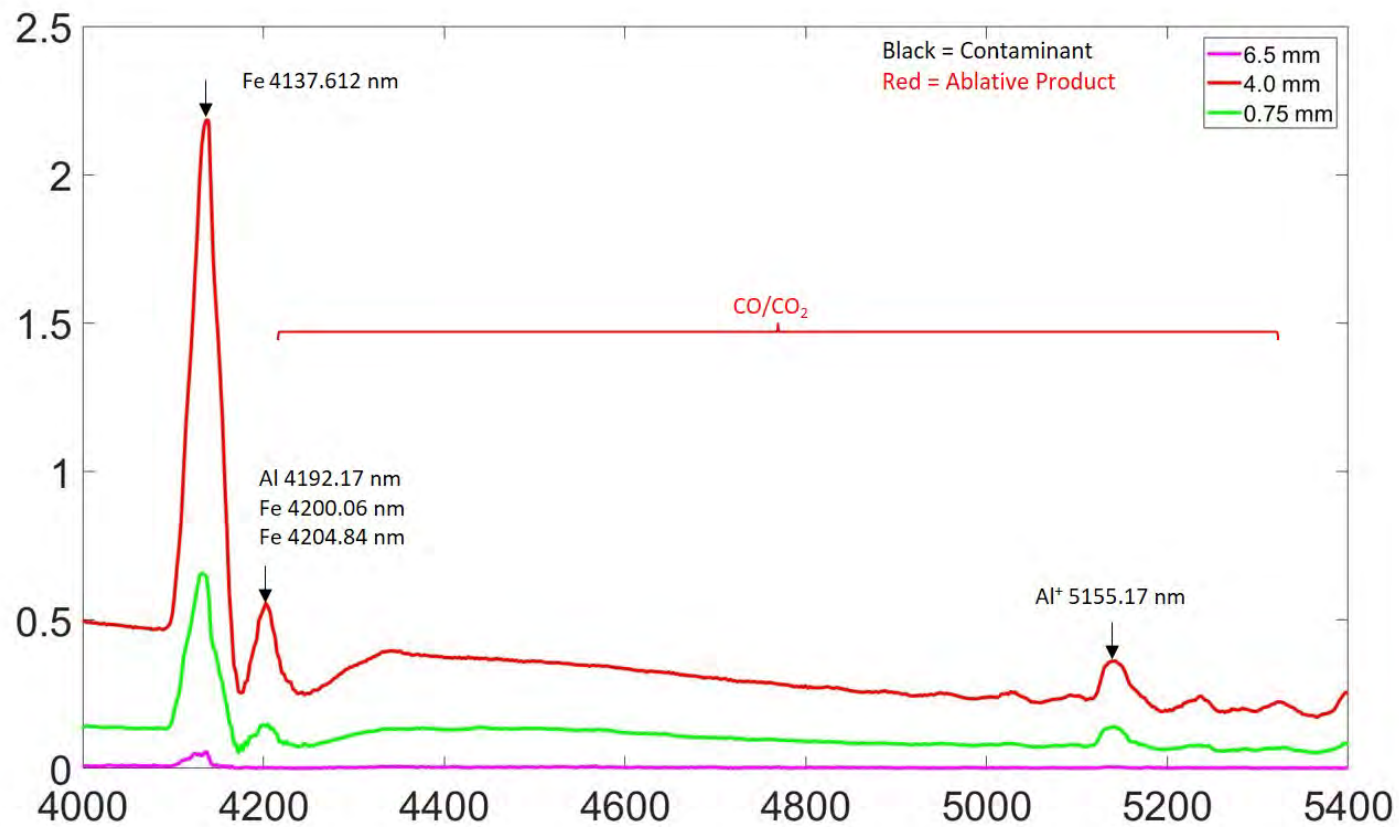


Figure 46. Spectral radiance comparison for C-C at three expansion heights. All measurements were taken by averaging in the expansion region above the model targeting CO and CO₂. All samples had a temperature of approximately 2600 K.

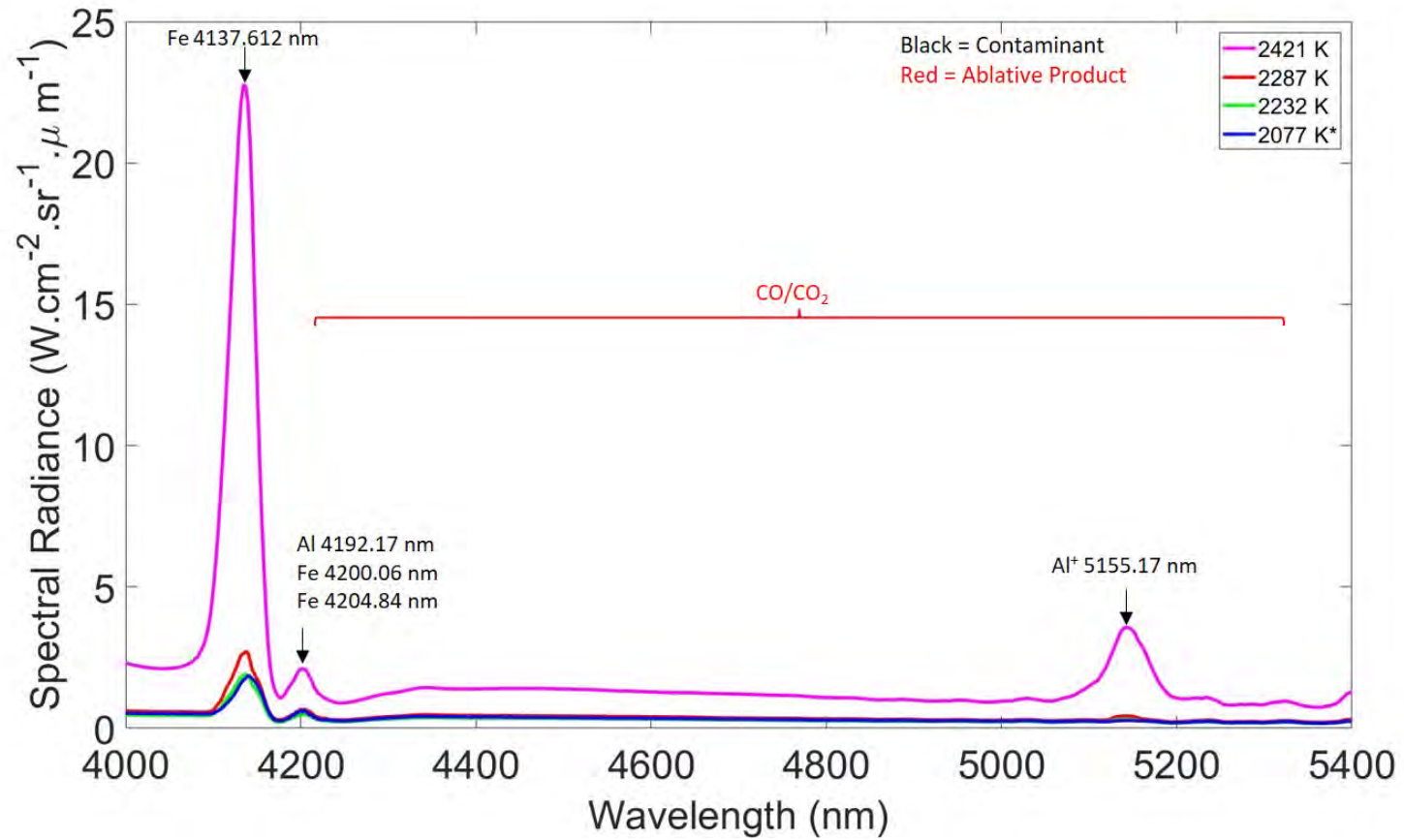


Figure 47. Spectral radiance comparison for SiC-coated C-C at four temperatures. All measurements were taken by averaging in the expansion region 0.75 mm above the model targeting CO and CO₂.

mencement of the experiments if such a material would work in this facility; the coating seemed quite brittle and there was concern that it would not be durable enough to survive the test time. Fortunately, the SiC-coated samples far exceeded expectations. As such, the second experimental campaign built on this success and focused heavily on SiC-coated C-C.

The uncoated C-C samples performed as expected. Most of the samples tested, which were all 3 mm thick, were damaged during the shot, which was likely the result of the heavier helium/argon driver gas rather than the test gas. It should be noted that samples breaking has no impact on data collection as it occurs after steady test time; many researchers at UQ have successfully utilized graphite test articles, which are far less durable than C-C. Surface temperature estimation for both coated and uncoated C-C proved to be a challenge during the campaign, as the camera used at the start of the campaign overexposed or underexposed frequently. As a result, an experimental campaign was planned with AFRL to build comprehensive heating profiles to assist in planning for the second experimental campaign. The results of this experimental campaign are discussed in detail in Appendix A.

Similarly, all of the SiC-coated samples with a 3 mm substrate broke during the shot, though they tended to shatter rather than simply crack along fiber boundaries. This breaking is likely a result of material degradation from the repeated cycles of coating, which also caused 3 mm thick samples to warp slightly, making them more difficult to mount in the model than uncoated samples. It was also observed that for the SiC-coated samples with a thin (300 μm) coating, the underlying C-C substrate was exposed after the shot, which was likely due to the helium/argon driver gas. Future test specimens were made with a 1 mm coating to eliminate any uncertainty. Similarly, all test articles used in the second experimental campaign were 6 mm thick. This design choice was made to avoid the warping that was experienced by the SiC-

coated samples made for the first experimental campaign and to avoid damaging the model with the hope of improving turnaround time between shots and potentially enabling reuse of test articles for the first time at X2.

Post-test analysis of test articles is typically not conducted for experiments in the X2 facility. Weighing to measure mass loss would have been desirable but would not be useful even if the test articles survived intact. Regardless of whether the samples were destroyed, interaction with post-test flow from the helium/argon driver gas combined with possible impacts from shrapnel resulting from ruptured diaphragms prevent any useful data from being obtained. SEM images were taken pre- and post-test for uncoated C-C and SiC-coated C-C samples that survived intact. Example images are shown in Figures 39, 40, and 42. Despite the extremely short test time, the C-C samples are clearly oxidized while the SiC-coated C-C sample also shows signs of oxidation.

CN violet emissions were clearly observed, displaying an increase with surface temperature in the near-stagnation region. This trend was not seen in the expansion region 6.5 mm above the model. Based on this observation, the second experimental campaign focused on the expansion region 0.75 mm above the model, which somewhat simplified the transition from investigating the near-stagnation region to the expansion region since the height of the tables containing all of the optical equipment have to be manually adjusted. An atomic Si line was observed at 390.55 nm, which is consistent with what Panerai [26] observed during his experiments, though other potential atomic Si lines could not be definitively identified. The second experimental campaign continued investigating to determine if atomic Si is a significant radiator. Additionally, since no ablation-related phenomena were observed in the MWIR region, it was decided to make use of the vis/nIR spectrometer in the second experimental campaign to investigate C₂ Swan, atomic N, and atomic O, in addition

to continuing to investigate CN violet and atomic Si. Chapter V will discuss the second experimental campaign in greater detail.

V. Second Experimental Campaign

Building on the lessons learned during the first experimental campaign, a second experimental campaign was conducted at UQ from 12 - 30 March 2018. During this campaign, a total of 26 shots were completed. A summary of the shots discussed in this chapter is shown in Table 11. As was mentioned in the previous chapter, all of the test articles used in the second campaign were 6 mm thick and all SiC-coated samples had a 1 mm thick coating. All parts were machined with the fibers parallel to the flow direction since the first experimental campaign showed that fiber direction was not significant and parts made in this fashion were easier to work with. Additionally, bandpass filters were used with the high-speed camera and with the ICCD cameras, which were decoupled from the spectrometers to attempt to allow emissions to be resolved in two spatial dimensions.

Table 11. Summary of shots completed during second X2 experimental campaign. Shots x2s3843 and x2s3844 had a filter blocking wavelengths below 495 nm when targeting atomic N and O.

Material	Heating Condition	Feature Investigated	UV Target	vis/nIR Target	Temperature (K)	X2 Shot ID
C-C	300 A	Near-Stagnation	CN Violet	C ₂ Swan	2048	x2s3842
C-C	400 A	Near-Stagnation	CN Violet	C ₂ Swan	2286	x2s3841
SiC	250 A	Near-Stagnation	CN Violet	C ₂ Swan	2005	x2s3840
SiC	350 A	Near-Stagnation	CN Violet	C ₂ Swan	2439	x2s3839
Cold Steel	Unheated	Near-Stagnation	Atomic Si	Atomic N/O	N/A	x2s3836
SiC	250 A	Near-Stagnation	Atomic Si	Atomic N/O	1839	x2s3838
SiC	350 A	Near-Stagnation	Atomic Si	Atomic N/O	2352	x2s3837
Cold Steel	Unheated	Near-Stagnation	C ₂ Swan	Atomic N/O*	N/A	x2s3844
SiC	250 A	Near-Stagnation	C ₂ Swan	Atomic N/O*	1930	x2s3843
C-C	200 A	Expansion, 0.75 mm above model	CN Violet	C ₂ Swan		x2s3829
C-C	300 A	Expansion, 0.75 mm above model	CN Violet	C ₂ Swan		x2s3828
C-C	400 A	Expansion, 0.75 mm above model	CN Violet	C ₂ Swan	2499	x2s3830
SiC	250 A	Expansion, 0.75 mm above model	CN Violet	C ₂ Swan	2077	x2s3831
SiC	350 A	Expansion, 0.75 mm above model	CN Violet	C ₂ Swan	2435	x2s3832
SiC	250 A	Expansion, 0.75 mm above model	Atomic Si	Atomic N/O	2014	x2s3834
SiC	350 A	Expansion, 0.75 mm above model	Atomic Si	Atomic N/O	1968	x2s3835
SiC	250 A	Expansion, 0.75 mm above model	Atomic Si	Atomic N/O	2333	x2s3833
C-C	Unheated	2D Decouple	CN Violet	C ₂ Swan	N/A	x2s3849
SiC	Unheated	2D Decouple	Atomic Si	CN Violet	N/A	x2s3845
SiC	350 A	2D Decouple	Atomic Si	CN Violet	2281	x2s3846
SiC	350 A	2D Decouple	Atomic Si	C ₂ Swan	2264	x2s3847
SiC2	350 A	2D Decouple	Atomic Si	CN Violet	2244	x2s3848

The objectives of the second campaign were to continue building a dataset targeting CN violet and atomic Si spectra, to investigate C₂ bands to see if they could be

observed, and to target atomic N and atomic O to see if their emissions are significant relative to CN violet.

5.1 Bench Testing

Additional bench testing was performed during the second experimental campaign. Unlike with the first experimental campaign, bench testing was performed on an as-needed basis to provide additional data points for temperature estimation to aid with simulations. Table 12 shows the results of this bench testing. This table also contains voltage, current, and power for each sample which, with few exceptions, was not captured during the first set of experiments. Additionally, for the 6 mm thick samples, temperature estimates calculated using the temperature profiles produced during the AFRL heating experiment are included. These heating profiles were used throughout the experiments to estimate the surface temperature and as will be shown, were generally in good agreement with measured values. It should be noted that these temperature estimates are calculated after the shot since the video of the heating needs to be viewed to determine voltage and current. Once those values are obtained, power can be calculated. Additional details on the AFRL heating experiment are contained in Appendix A.

Table 12. Temperatures measured during bench testing during the second experimental campaign.

Material	Current (A)	Voltage (V)	Power (W)	Estimated Temperature (K)	Temperature (K)
C-C (3 mm thick)	100	7.5	750	N/A	1954
C-C (3 mm thick)	100	9.25	925	N/A	1966
C-C (6 mm thick)	200	10.5	2100	1974	1970
C-C (6 mm thick)	200	10.5	2100	1974	2049
C-C (6 mm thick)	300	13.5	4050	2366	2349
C-C (6 mm thick)	300	13.5	4050	2366	2476

5.2 Results

During the second experimental campaign, five shots with stainless steel, seven shots with C-C, and 13 shots with SiC-coated C-C were conducted. Additionally, one shot was done with a second SiC coating. This coating was made with Si_3N_4 powder with the intended result of obtaining Si_3N_4 -coated C-C although the coating process seemingly reacted away all of the nitrogen. To distinguish between the different SiC coatings, the coating made with Si_3N_4 powder will be referred to as the “new” SiC coating or SiC2 and the coating made with the SiC powder (i.e. the one used on the other 13 shots and during the first set of experiments) will be referred to as the “original” SiC coating or SiC1.

As with the first set of experiments, the steel shots were used to establish a baseline and ensure that all of the optical equipment was properly configured. This task was not trivial since a new piece of optical equipment, the vis/nIR spectrometer, was being introduced into the experiments and was used with a camera that it is not typically used with since the usual camera was unavailable.

Assessment of Test Samples.

The choice of configuration of the test articles (i.e. 6 mm thick with a 1 mm coating) proved wise as all of the samples survived intact and the 1 mm thick coating proved to be more than adequate, even when samples were used for more than one shot. Several samples, including both coated and uncoated, were used for multiple shots. The reuse of test articles, which had never been accomplished at UQ prior to these experiments, reduces turnaround time between shots and requires less test articles to be made. A SiC-coated C-C sample that was used for two shots is shown in Figure 48. Aside from some minor damage to the bottom right corner after the first shot, likely from shrapnel from the steel diaphragm, the sample is still in excellent

shape even after two shots. Measuring the thickness of the sample after the second shot showed that the coating is still about 0.9 mm thick, suggesting it could potentially have been reused more times.



(a) Unused SiC-coated sample before shot x2s3833



(b) SiC-coated sample after shot x2s3833



(c) Reused SiC-coated sample after shot x2s3834

Figure 48. SiC-coated C-C sample that was used for multiple shots.

Temperature Measurements.

Heating of the test samples was conducted in the same manner as during the first experiments. However, since the test samples were thicker, higher power settings were selected to achieve approximately the same temperature range measured during the first set of experiments. For C-C, 200 A, 300 A, and 400 A were chosen, producing surface temperatures of approximately 2000 K to 2500 K. For SiC-coated C-C, 250 A and 350 A yielded temperatures of roughly 1900 K to 2400 K. Table 13 shows heating conditions for all shots during the second experimental campaign. With the exception of the first two heated shots of the campaign, both of which underexposed the DSLR

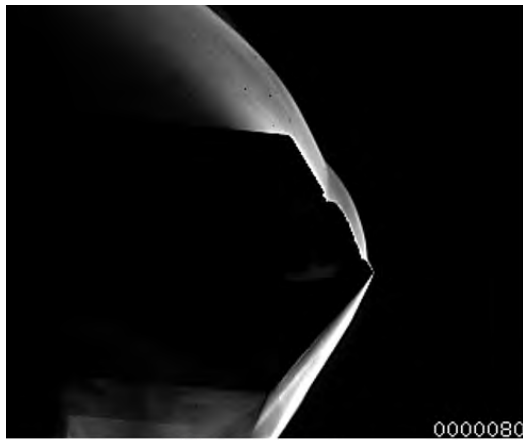
camera, temperature measurements were obtained for all shots. Further, voltage, current, and power were also obtained for all shots as were estimated temperatures from using the heating profiles produced from the AFRL heating experiment. The general trend was for actual temperatures to be lower than estimated values, which is most likely the result of not allowing the material to reach a steady temperature before firing the shot. The AFRL heating experiment showed that it takes far longer than the 5 to 10 seconds previously believed, especially for SiC-coated samples, to reach steady surface temperature.

Table 13. Summary of temperature measurements during second X2 experimental campaign.

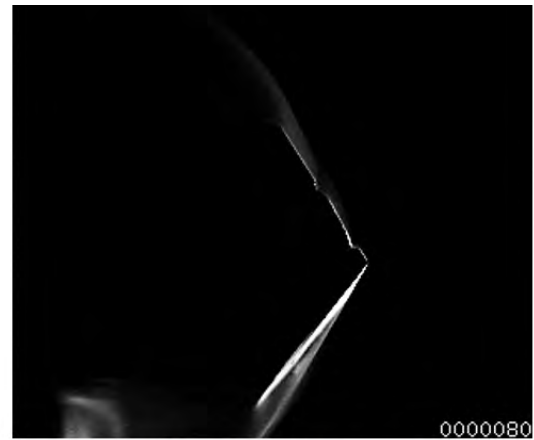
Material	Current (A)	Voltage (V)	Power (W)	Estimated Temperature (K)	Temperature (K)	X2 Shot ID
C-C	300	13	3900	2344	2048	x2s3842
C-C	400	15	6000	2601	2286	x2s3841
SiC	250	11.25	2813	2126	2005	x2s3840
SiC	350	11.5	4025	2505	2439	x2s3839
Cold Steel	Unheated	N/A	N/A	N/A	N/A	x2s3836
SiC	250	9.75	2438	1980	1839	x2s3838
SiC	350	12	4200	2547	2352	x2s3837
Cold Steel	Unheated	N/A	N/A	N/A	N/A	x2s3844
SiC	250	10.5	2625	2055	1930	x2s3843
C-C	200	10	2000	1945		x2s3829
C-C	300	12.5	3750	2320		x2s3828
C-C	400	15	6000	2601	2499	x2s3830
SiC	250	12	3000	2195	2077	x2s3831
SiC	350	12.5	4375	2587	2435	x2s3832
SiC	250	10.75	2688	2079	2014	x2s3834
SiC	350	11.25	2813	2126	1968	x2s3835
SiC	250	13	4550	2623	2333	x2s3833
C-C	Unheated	N/A	N/A	N/A	N/A	x2s3849
SiC	Unheated	N/A	N/A	N/A	N/A	x2s3845
SiC	350	13	4550	2623	2281	x2s3846
SiC	350	13	4550	2623	2264	x2s3847
SiC2	350	12.75	4463	2532	2244	x2s3848

High-Speed Video.

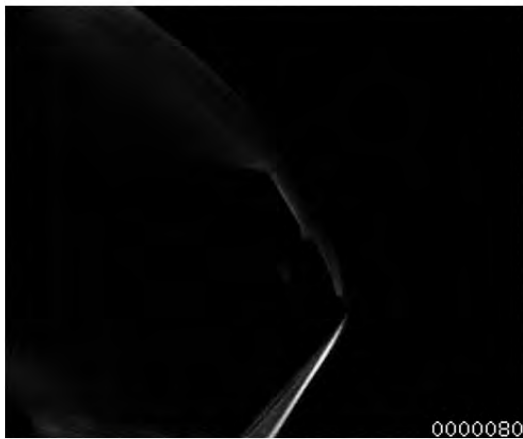
High-speed video footage was captured again during the second experimental campaign. This time, however, bandpass filters were put in front of the camera to isolate specific wavelength regions corresponding to the radiative phenomena of interest. The filters used were Newport 10BPF10-250 for atomic Si, Laser2000 FF01-380/14-25 BrightLine for CN violet, Newport 10BPF10-470 for C₂ Swan, and Edmund Optics



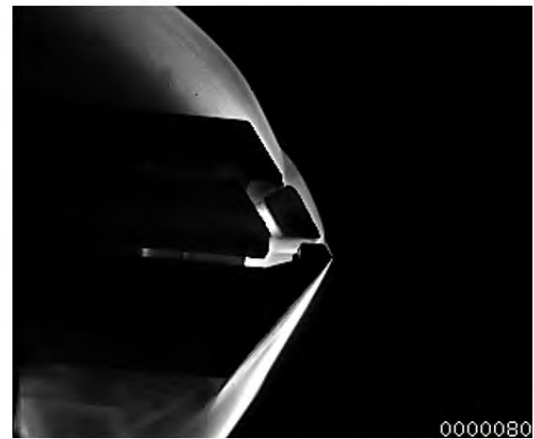
(a) Without a filter



(b) With 380 ± 7 nm filter for CN violet



(c) With 470 ± 5 nm filter for C₂ Swan



(d) With 740 ± 5 nm filter for atomic N

Figure 49. High-speed video image for SiC-coated C-C with and without bandpass filters. All images are from different shots during steady test time $80 \mu s$ from the start of the video.

740nm Stock No. 67-908 for atomic N. Figure 49 shows images taken from high-speed video footage for SiC-coated C-C without a filter and with filters for CN, C₂, and atomic N. Attempts were made to capture high-speed footage with the filter for atomic Si but the camera used has no response in this wavelength region. A figure of this camera's response can be found in Appendix F of Eichmann's PhD Thesis [47]. The same gain setting of 10 was used with all three filters; a gain of 3 was used for the shot without a filter to avoid saturating the camera. C₂ and CN are visible close to the wall of the model. The image with C₂ is visibly dimmer than the image with

CN. The image with the atomic N filter is very similar to the image with no filter. Since the test gas is primarily N_2 , a large portion of which likely dissociates when it contacts the strong shock that forms, this observation is hardly surprising.

UV Spectra.

CN violet.

Figures 50 and 51 show UV spectra of C-C samples targeting CN violet bands averaged across the near-stagnation region and expansion region 0.75 mm above the model, respectively. Similarly, Figures 52 and 53 show UV spectra for SiC-coated C-C targeting CN violet bands averaged across the near-stagnation region and expansion region 0.75 mm above the model, respectively, while Figures 54 and 55 show spectra for SiC-coated C-C and C-C plotted together. For all of these cases, data from the first experimental campaign is included to provide a more complete data set.

As was the case in the first experimental campaign, the averaged spectra were extracted by averaging between the rows depicted by horizontal lines in Figures 33 and 34. For the near-stagnation region, this region was from the shock front to the model edge. For the expansion region, this region was from the shock front to a distance approximately 10 mm downstream of the shock, where radiating species are no longer observed. Temperatures with an asterisk (*) indicate that a temperature measurement was not obtained for that shot and the value shown is the average of all measurements at this condition. Identification of spectra was accomplished using the NIST Atomic Spectra Database [136] and Pearse and Gaydon [145].

The general trend of intensity increasing with surface temperature is again observed. For uncoated C-C in the near-stagnation region, the 2048 K case appears to be the most intense, but it should be noted that this case was the only one where the temperature was measured directly, so it may in fact be the hottest. This same

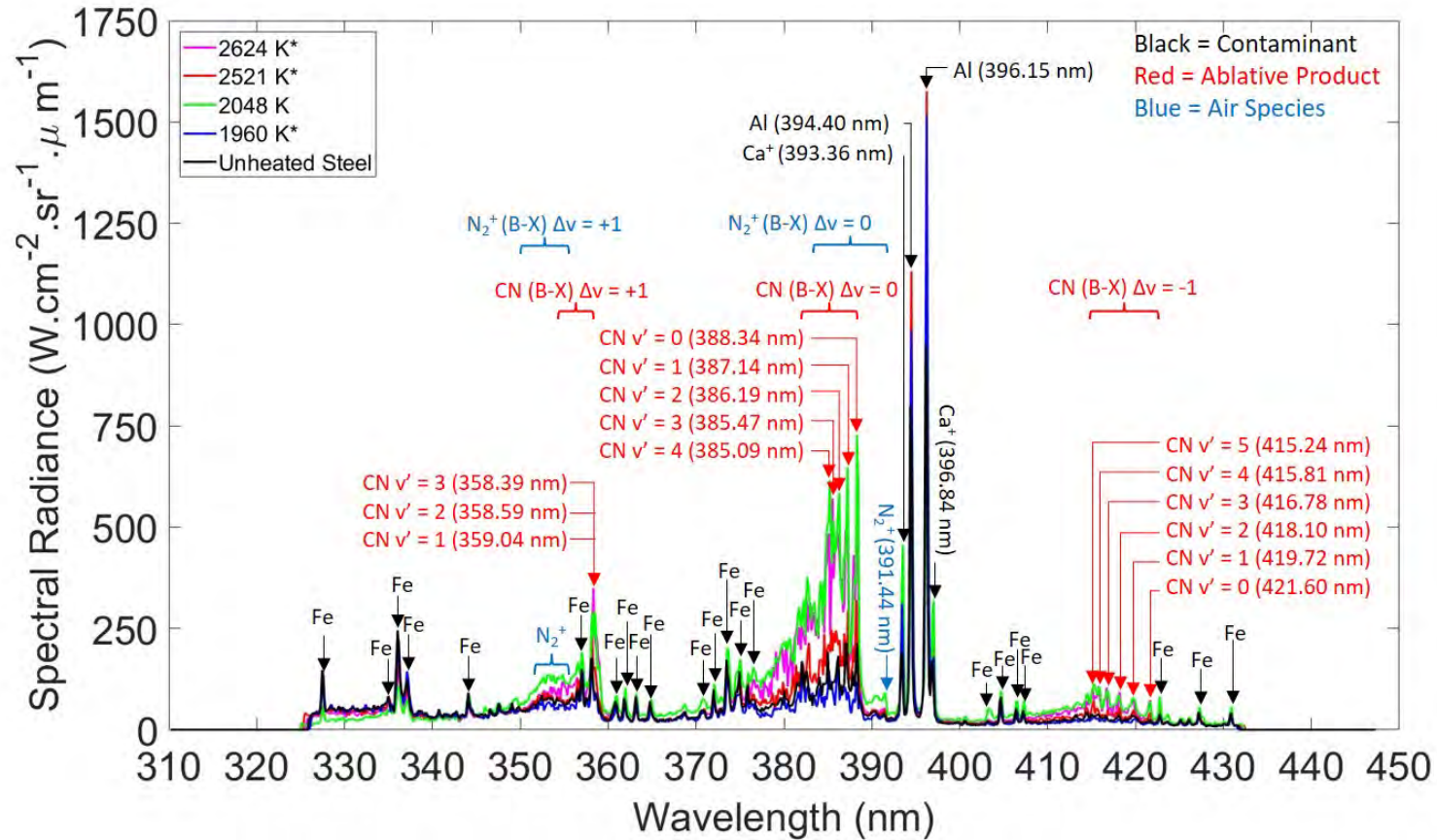


Figure 50. Spectral radiance comparison for C-C at four temperatures with unheated steel. All measurements were taken by averaging in the near-stagnation region targeting CN violet bands.

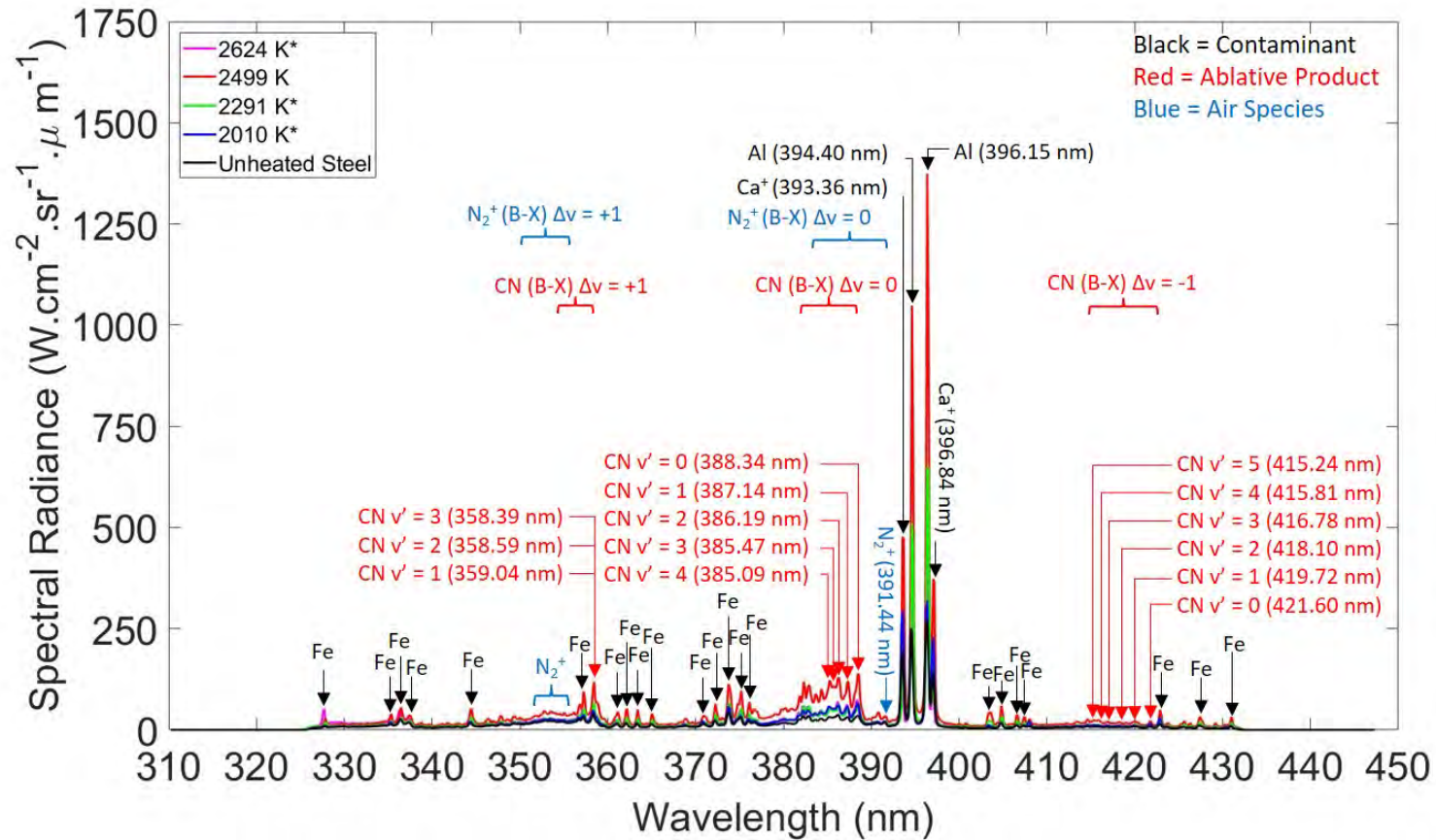


Figure 51. Spectral radiance comparison for C-C in the expansion region at four temperatures with unheated steel. All measurements were taken by averaging in the expansion region 0.75 mm above the model targeting CN violet bands.

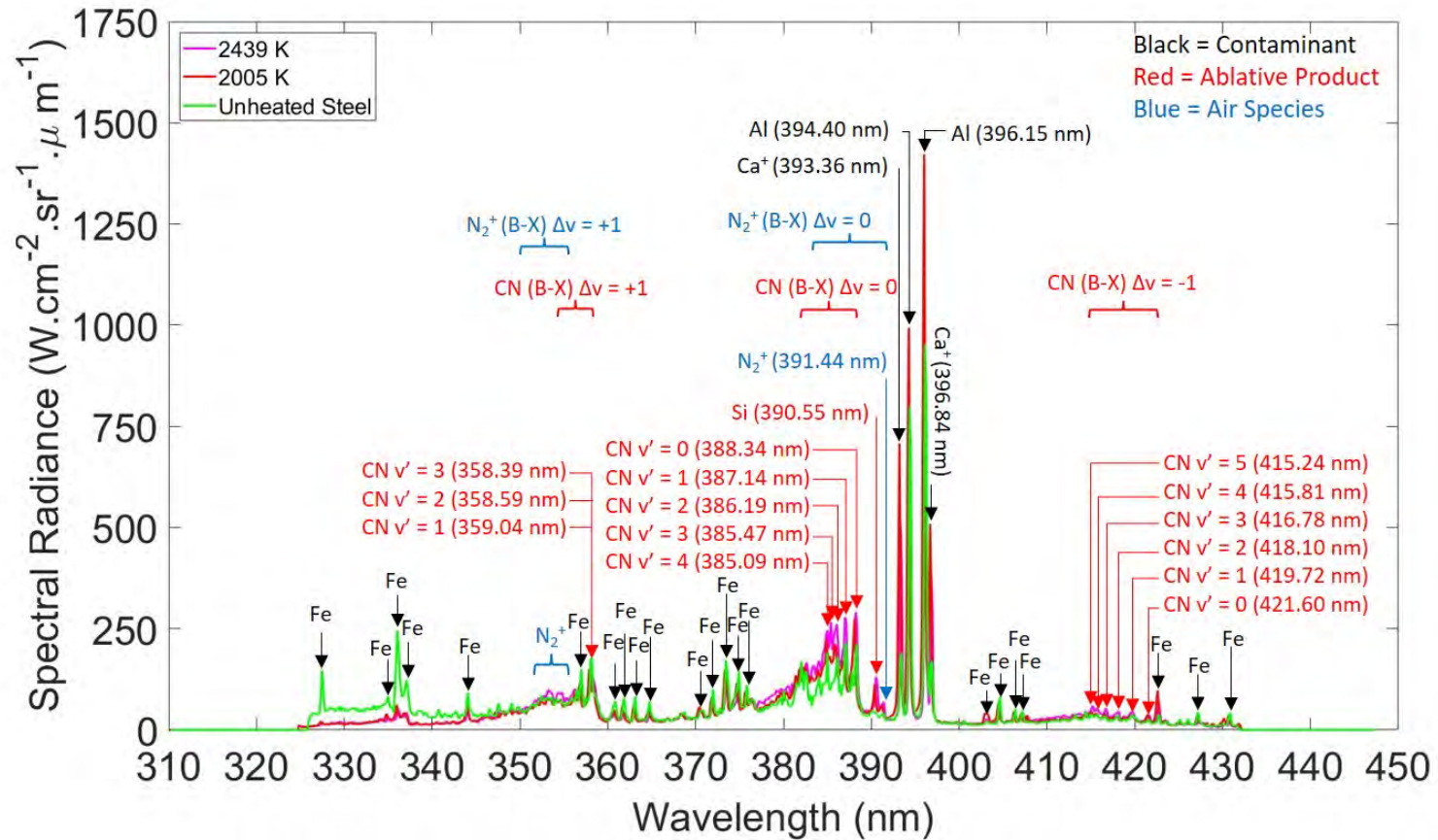


Figure 52. Spectral radiance comparison for SiC-coated C-C at two temperatures with unheated steel. All measurements were taken by averaging in the near-stagnation region targeting CN violet bands.

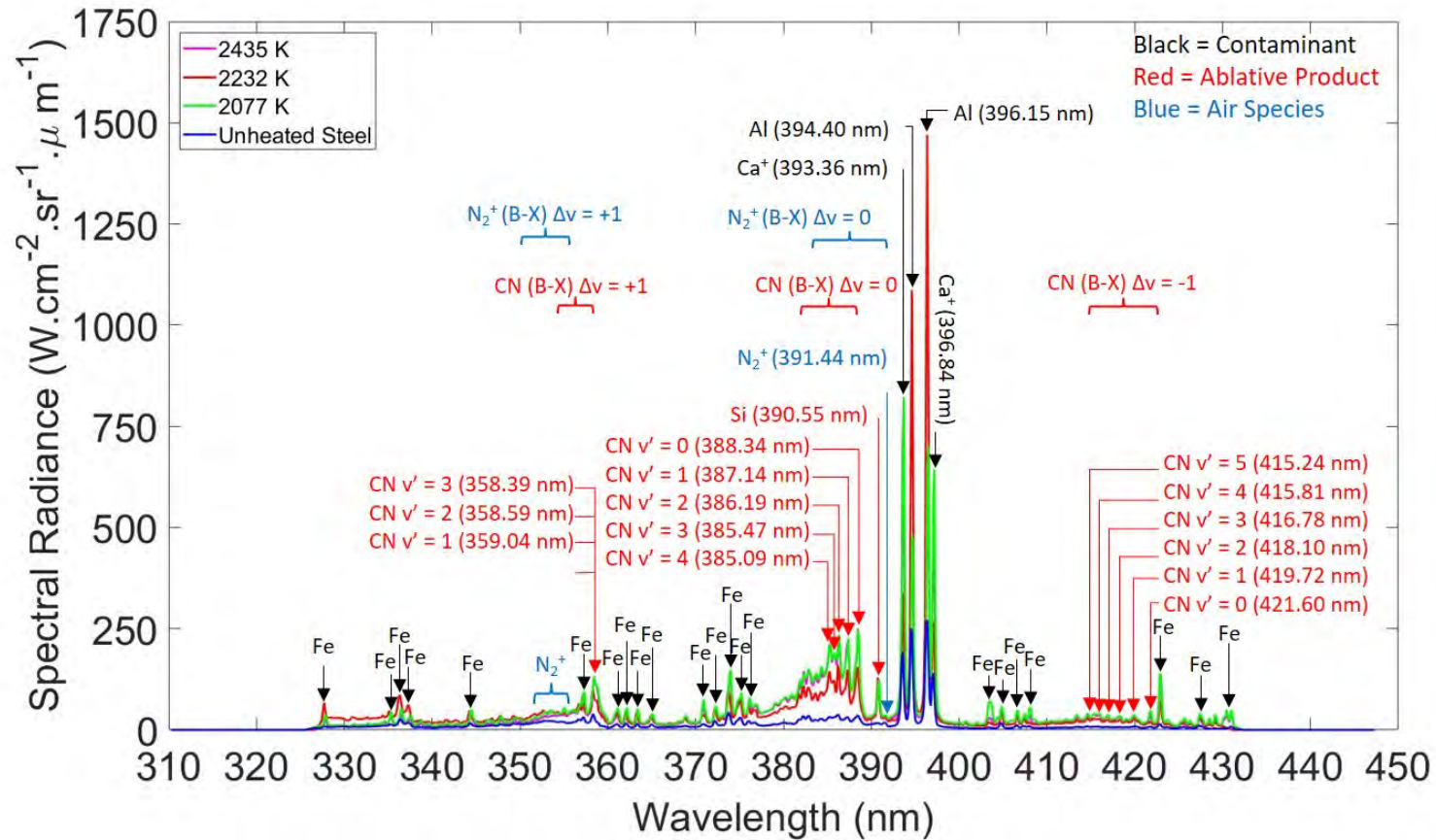


Figure 53. Spectral radiance comparison for SiC-coated C-C in the expansion region at three temperatures with unheated steel. All measurements were taken by averaging in the expansion region 0.75 mm above the model targeting CN violet bands.

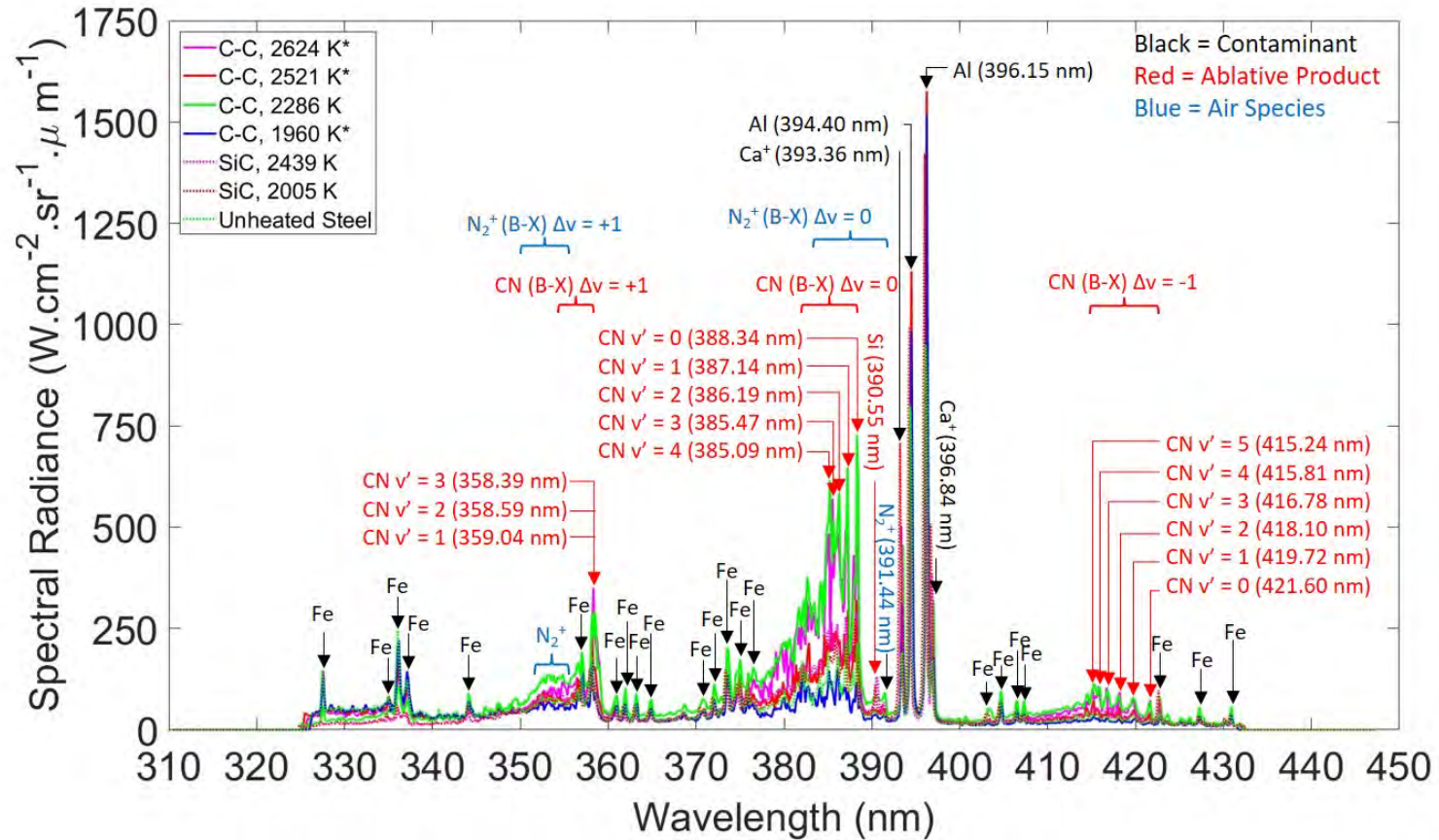


Figure 54. Spectral radiance comparison for C-C and SiC-coated C-C at multiple temperatures with unheated steel. All measurements were taken by averaging in the near-stagnation region targeting CN violet bands.

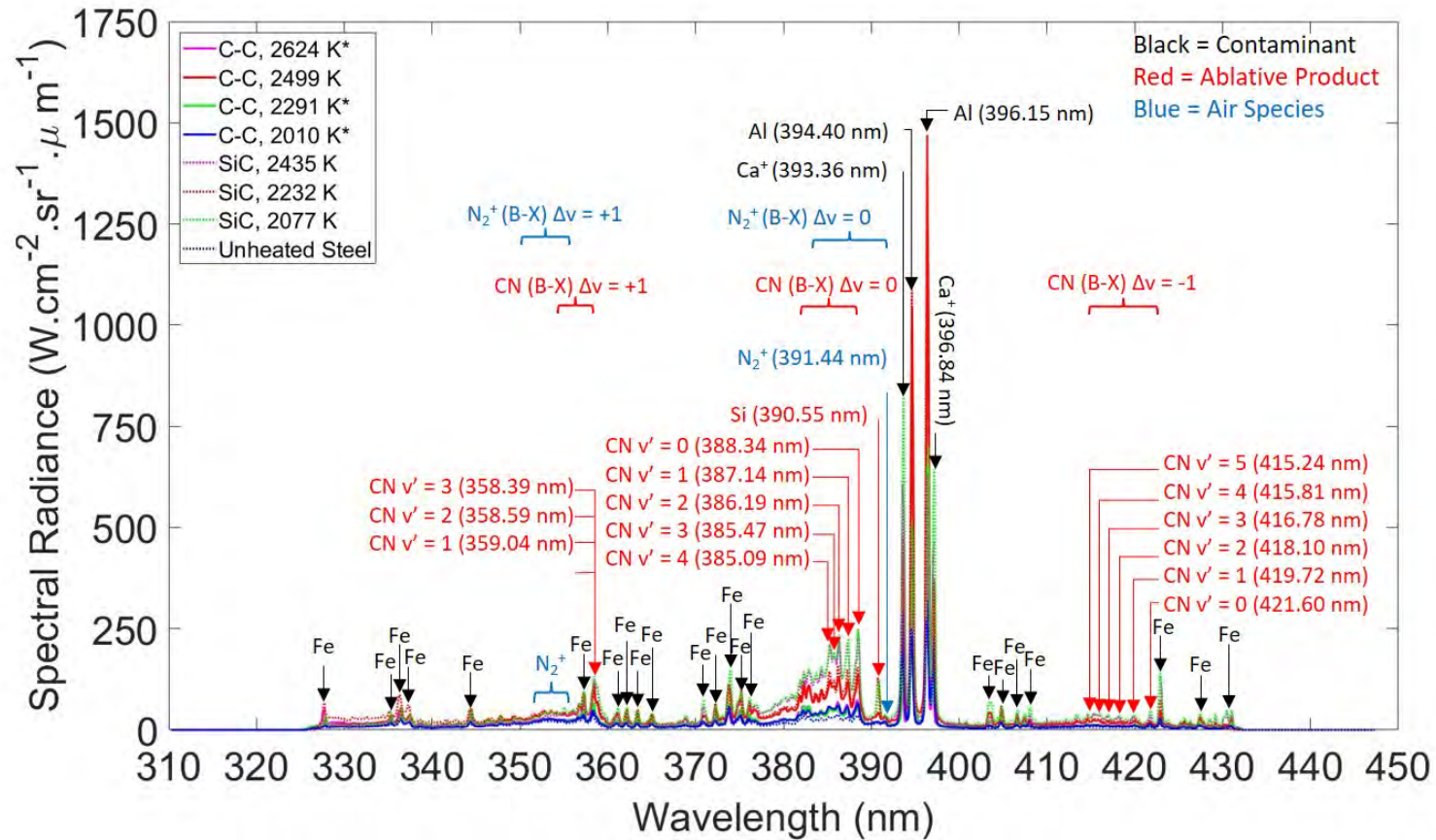


Figure 55. Spectral radiance comparison for C-C and SiC-coated C-C at multiple temperatures with unheated steel. All measurements were taken by averaging in the expansion region 0.75 mm above the model targeting CN violet bands.

scenario applies to the 2499 K case for C-C in the expansion region.

An interesting observation can be made by plotting C-C and SiC-coated C-C together. In the near-stagnation region, intensity is highest for uncoated C-C while the opposite is true in the expansion region. This observation suggests that more ablative products are entering the flowfield for SiC-coated C-C compared to uncoated C-C, which likely means that the SiC coating is ablating at a faster rate than uncoated C-C; this phenomenon will likely result in underprediction of simulated results.

Atomic Si.

Figures 56 and 57 show UV spectra of SiC-coated samples targeting atomic Si lines averaged across the near-stagnation region and expansion region 0.75 mm above the model, respectively. It is immediately obvious that the results averaged in the expansion region are significantly more intense than the near-stagnation region, which is not logical. It was mentioned in the previous chapter that there were issues with data collection during the first experimental campaign, particularly with triggering of the data collection system. The photo diode was used to trigger all of the SiC-coated C-C shots targeting atomic Si lines in the first experimental campaign. Therefore, it can reasonably be concluded that these shots likely missed the steady test time and were collected during the driver gas. If the shots in the expansion region from the first experimental campaign are removed, the results make more sense as shown in Figure 58.

During the first experimental campaign, a number of potential atomic Si lines were identified based on similar experiments conducted by Panerai [26]. Further investigation of these lines has determined that most of the potential atomic Si lines are in fact iron (Fe) contaminants from the primary steel diaphragm. It is believed, however, that the cluster of four lines from 250 to 253 nm, as well as the line at 288.16

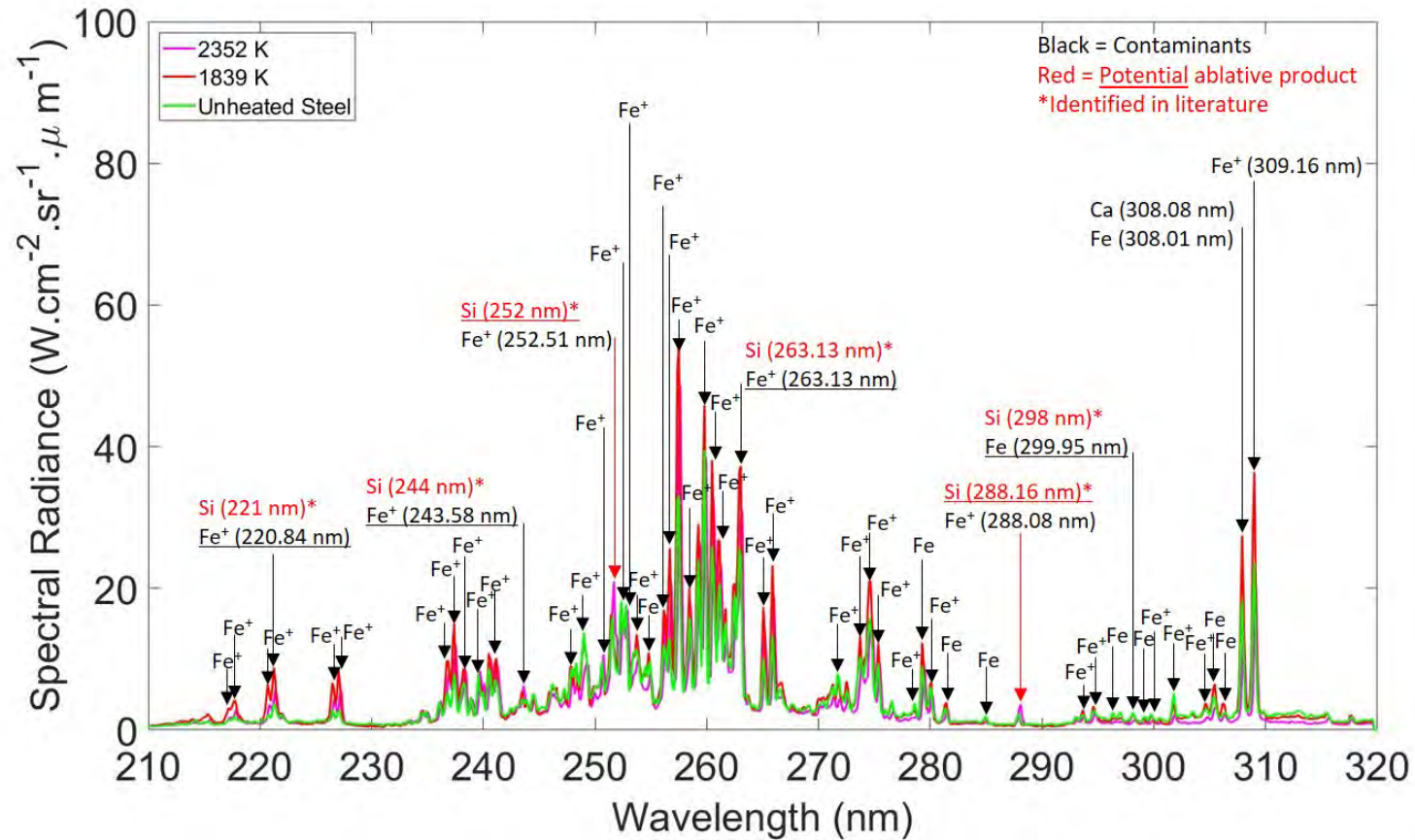


Figure 56. Spectral radiance comparison for SiC-coated C-C at two temperatures with unheated steel. All measurements were taken by averaging in the near-stagnation region targeting region atomic Si lines.

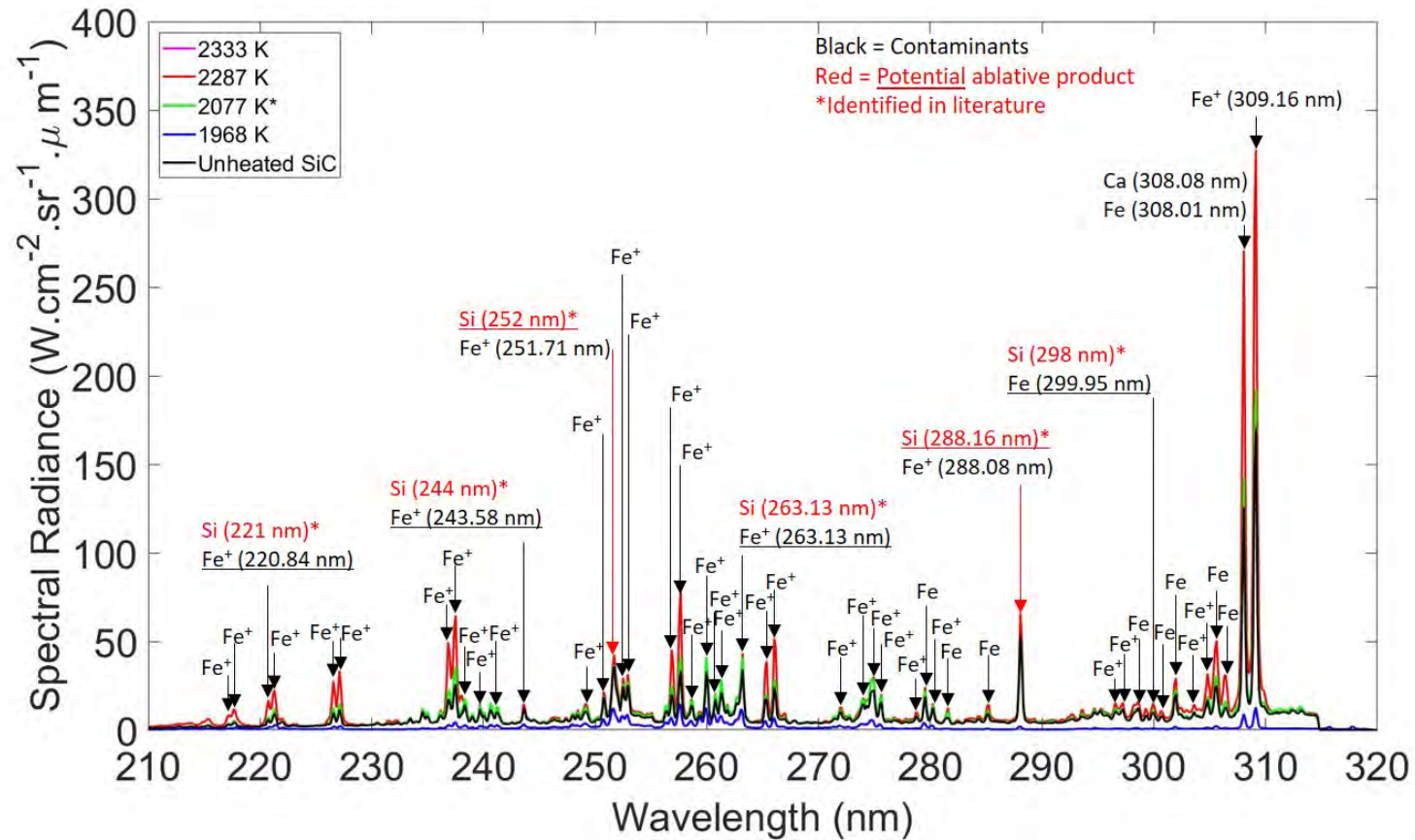


Figure 57. Spectral radiance comparison for SiC-coated C-C at four temperatures with unheated steel. All measurements were taken by averaging in the expansion region 0.75 mm above the model targeting atomic Si lines.

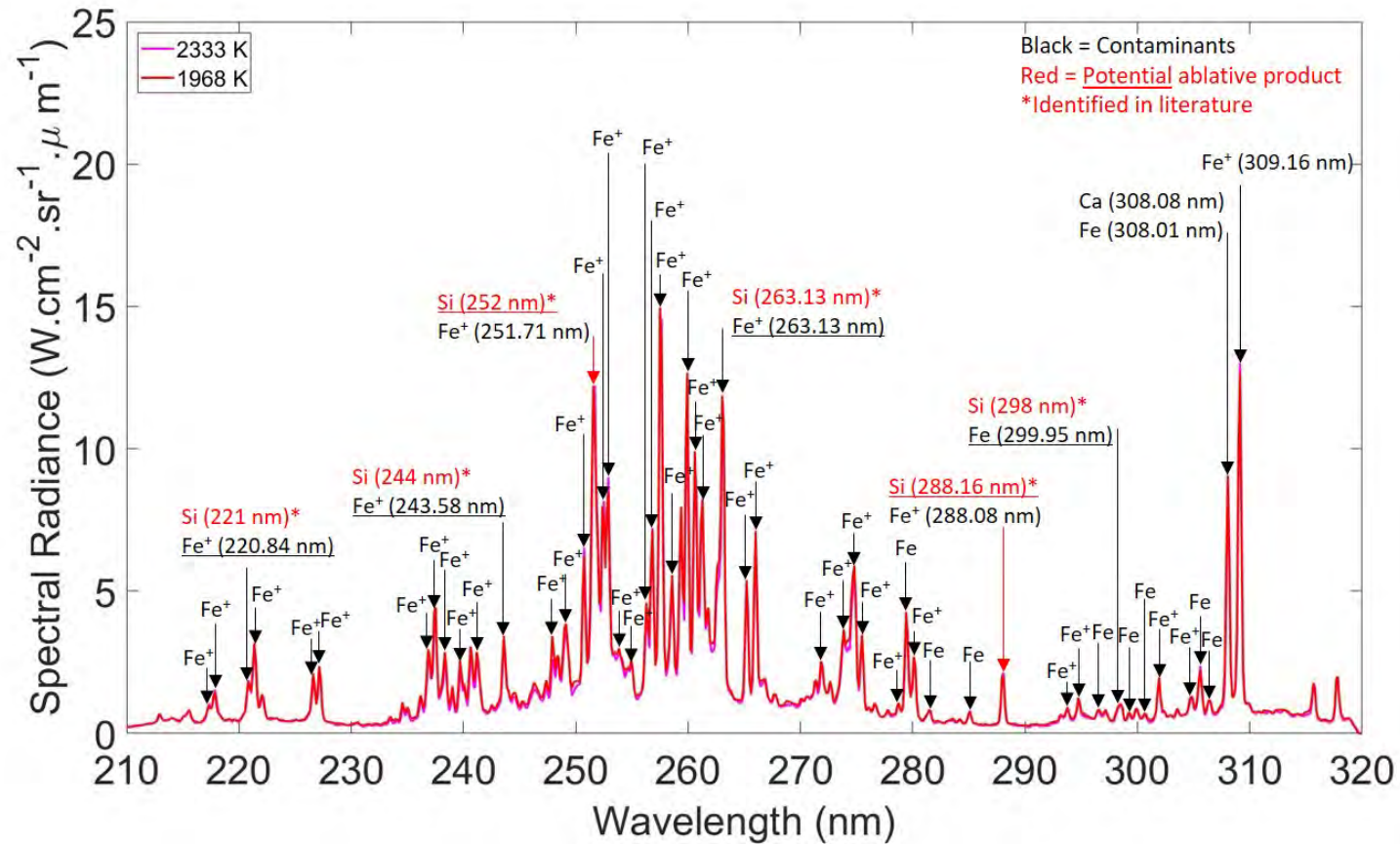


Figure 58. Spectral radiance comparison for SiC-coated C-C at two temperatures. All measurements were taken by averaging in the expansion region 0.75 mm above the model targeting atomic Si lines.

nm, are atomic Si. The details of this claim will be discussed later in this dissertation.

vis/nIR Spectra.

The vis/nIR spectrometer was used during the second experimental campaign in place of the MWIR spectrometer with the goal of investigating to see if C₂ Swan bands could be detected. Past researchers at UQ have had mixed success with detecting C₂ Swan bands. Atomic N and O lines were also investigated.

C₂ Swan.

Figures 59 and 60 show vis/nIR spectra for uncoated C-C targeting C₂ Swan bands averaged across the near-stagnation region and expansion region 0.75 mm above the model, respectively. Likewise, Figures 61 and 62 show vis/nIR spectra for SiC-coated C-C targeting C₂ Swan bands averaged across the near-stagnation region and expansion region 0.75 mm above the model, respectively. Figures 63 and 64 show spectra for uncoated and SiC-coated C-C together.

The averaged spectra were again extracted by averaging between the rows depicted by horizontal lines in Figures 33 and 34. For the near-stagnation region, this region was from the shock front to the model edge. For the expansion region, this region was from the shock front to a distance approximately 10 mm downstream of the shock, where radiating species are no longer observed. Temperatures with an asterisk (*) indicate that a temperature measurement was not obtained for that shot and the value shown is the average of all measurements at this condition. Identification of spectra was accomplished using the NIST Atomic Spectra Database [136] and Pearse and Gaydon [145].

Potential signs of C₂ Swan bands have been observed for both uncoated and SiC-coated C-C, though the peaks are a bit more distinct for uncoated C-C. Any

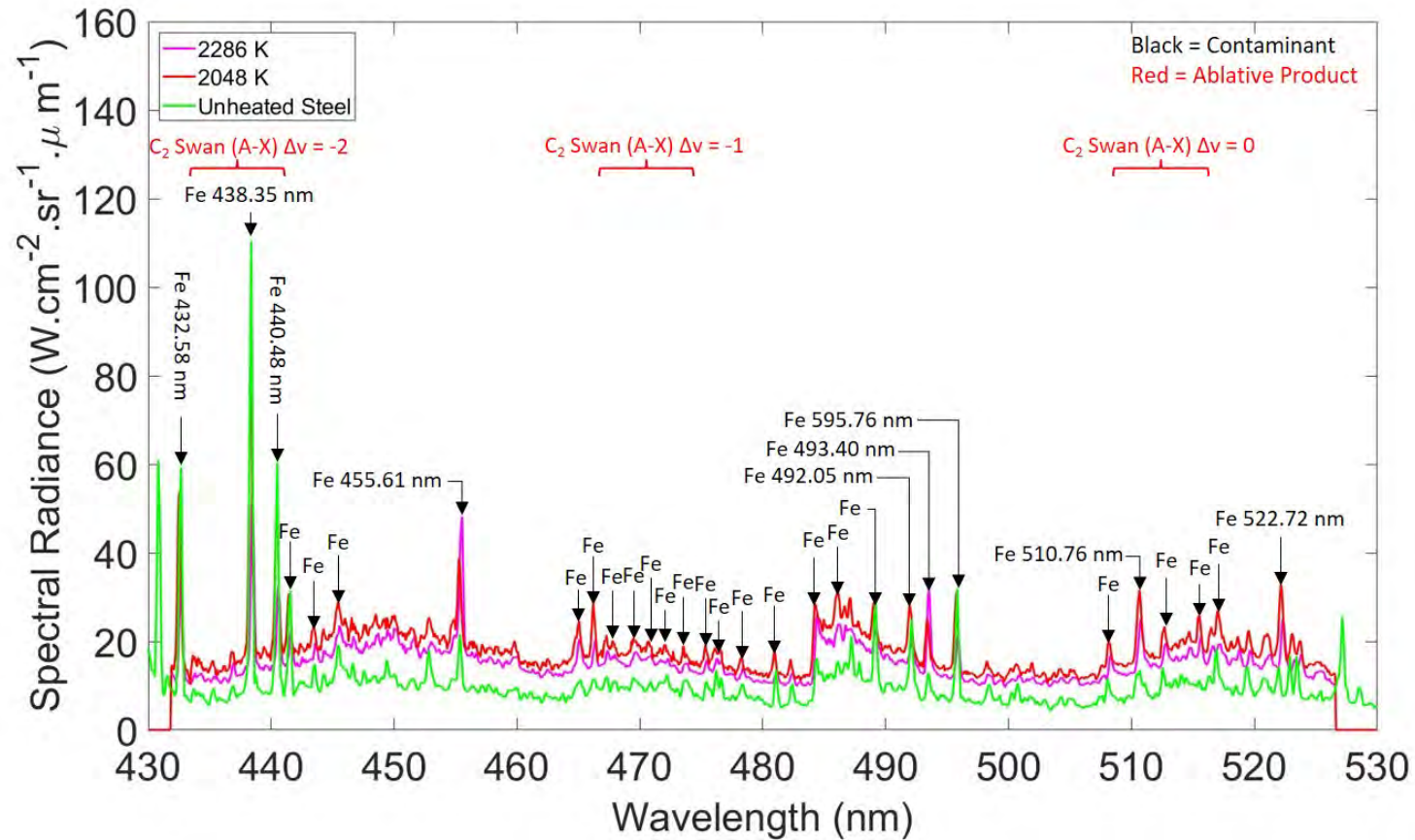


Figure 59. Spectral radiance comparison for C-C at two temperatures with unheated steel. All measurements were taken by averaging in the near-stagnation region targeting C₂ Swan bands.

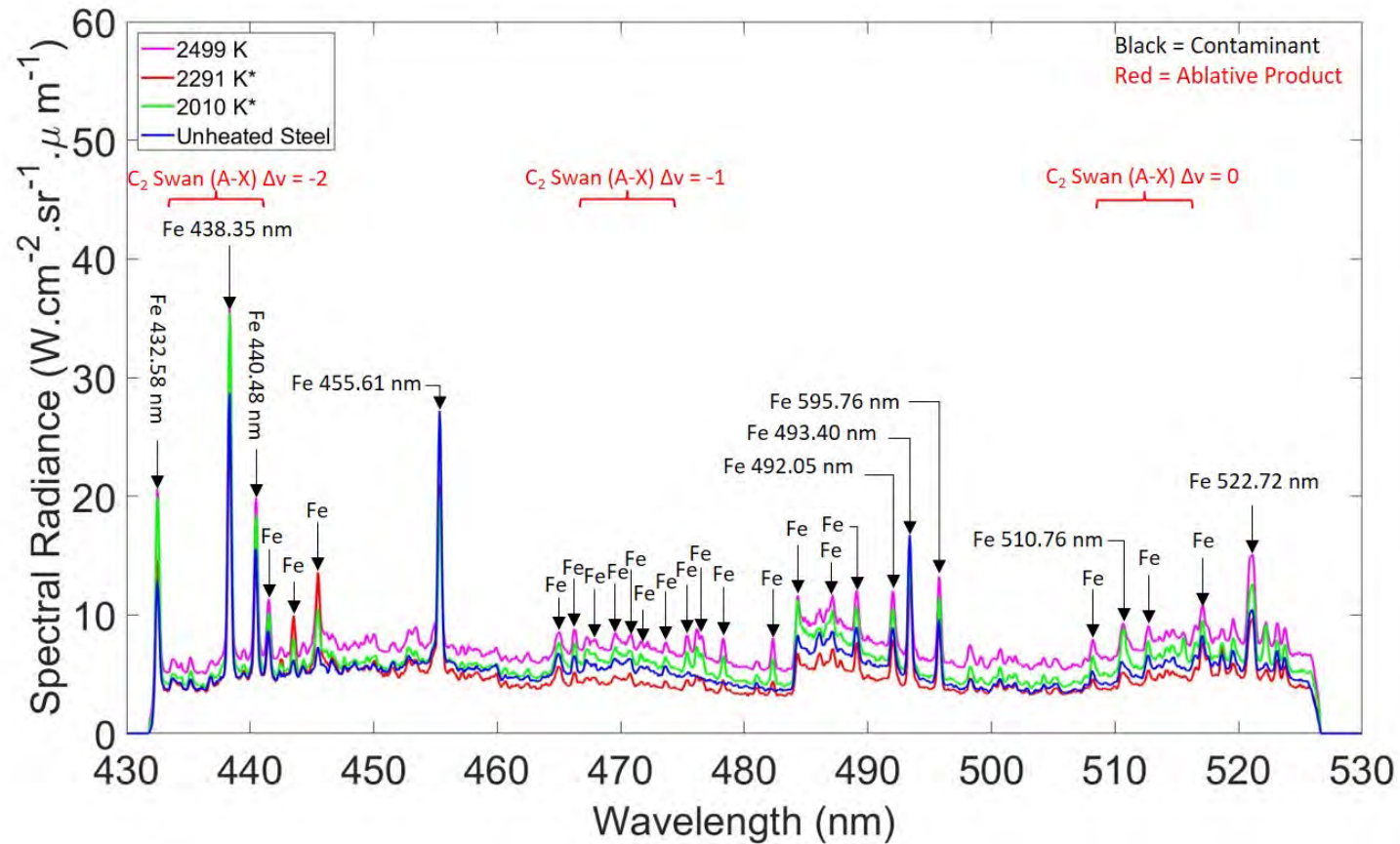


Figure 60. Spectral radiance comparison for C-C in the expansion at three temperatures with unheated steel. All measurements were taken by averaging in the expansion region 0.75 mm above the model targeting C₂ Swan bands.

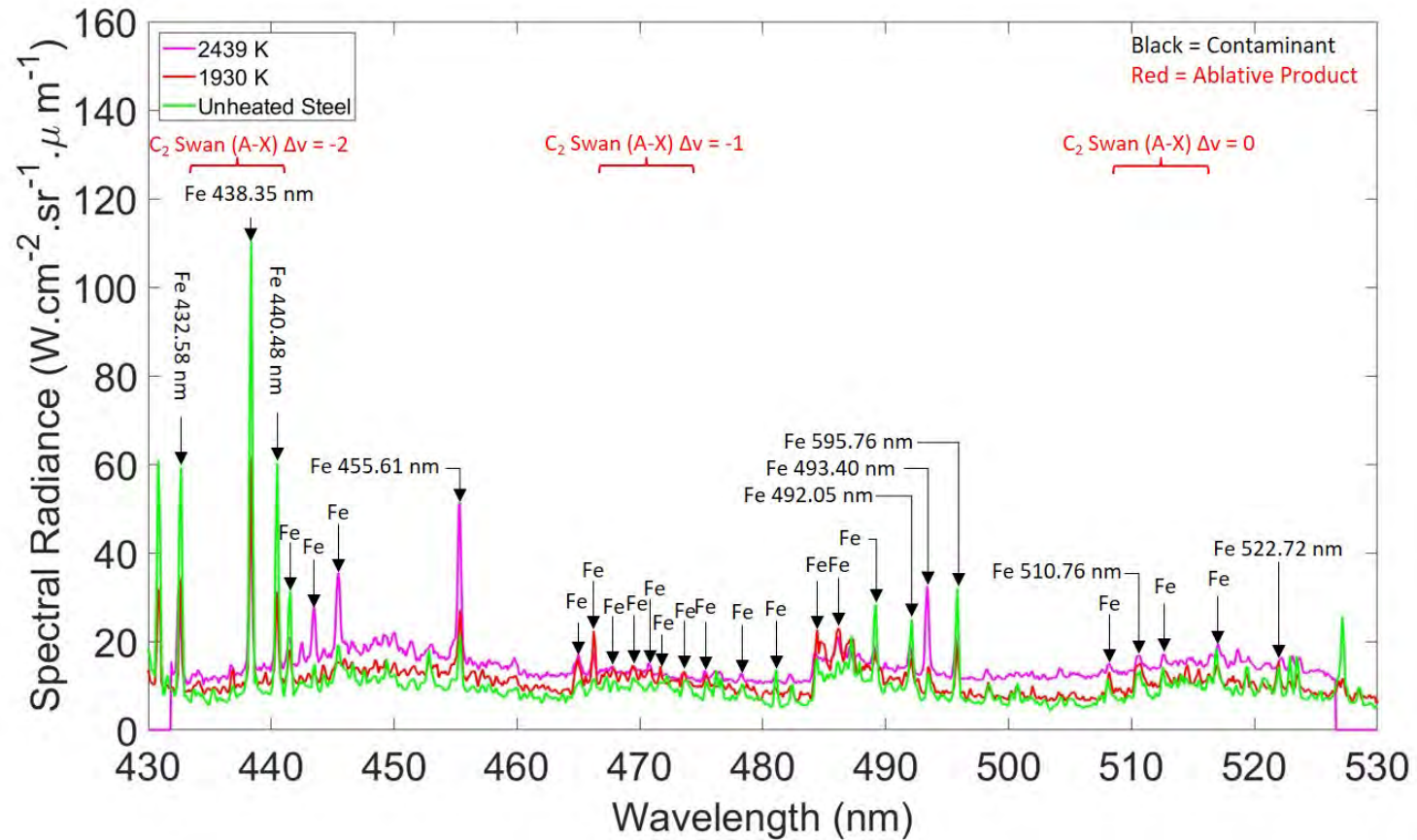


Figure 61. Spectral radiance comparison for SiC-coated C-C at two temperatures with unheated steel. All measurements were taken by averaging in the near-stagnation region targeting C₂ Swan bands.

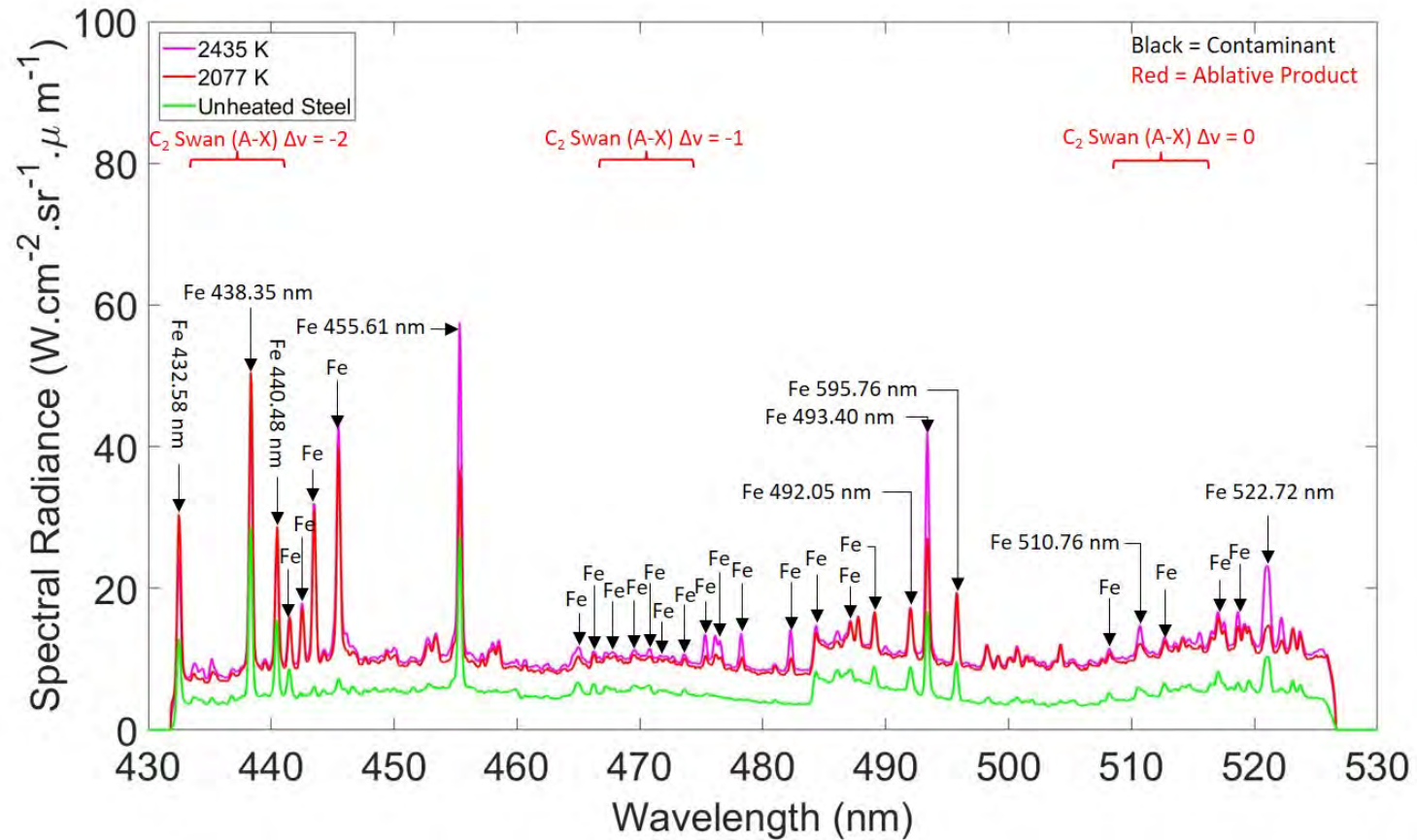


Figure 62. Spectral radiance comparison for SiC-coated C-C in the expansion at two temperatures with unheated steel. All measurements were taken by averaging in the expansion region 0.75 mm above the model targeting C_2 Swan bands.

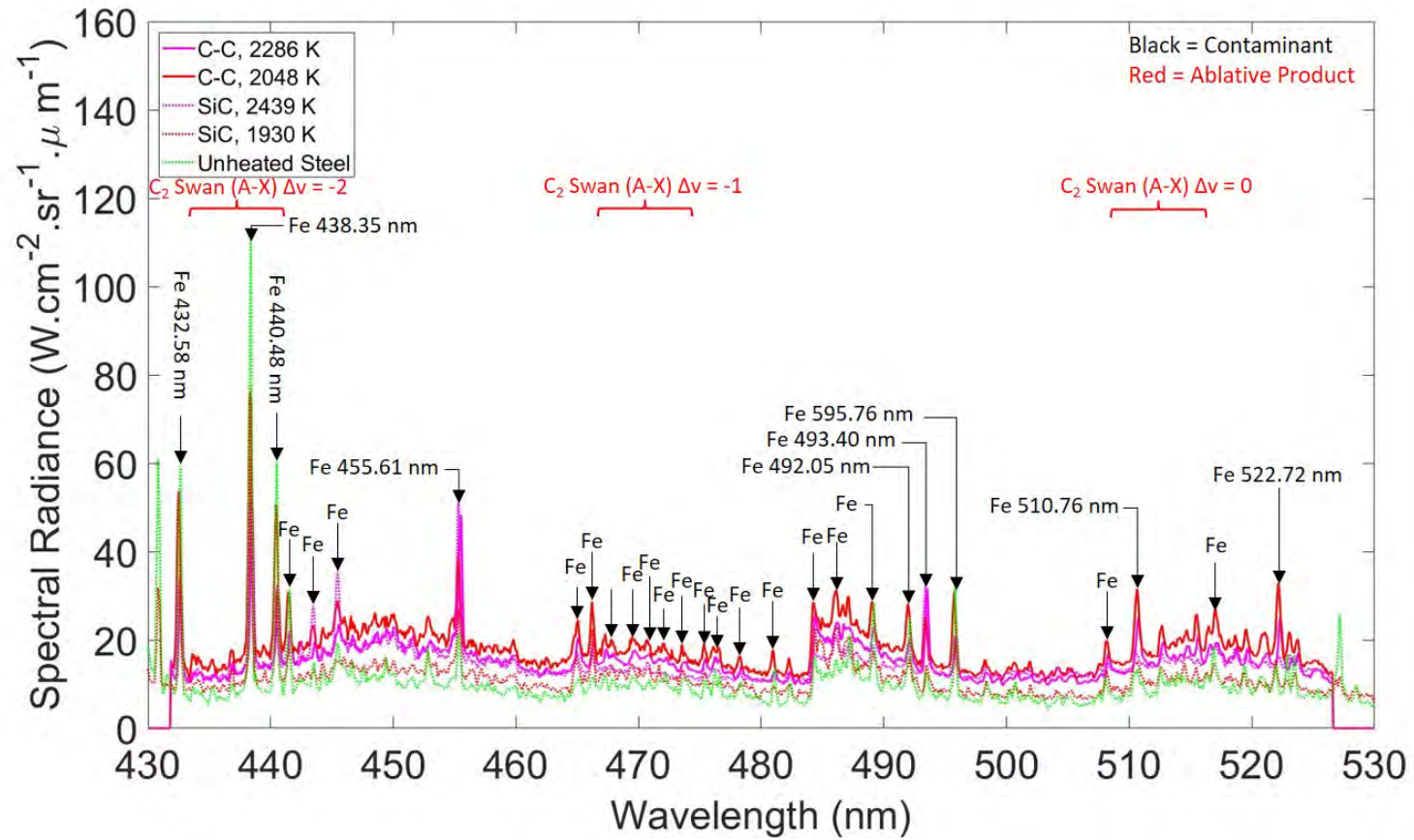


Figure 63. Spectral radiance comparison for C-C and SiC-coated C-C at multiple temperatures with unheated steel. All measurements were taken by averaging in the near-stagnation region targeting C_2 Swan bands.

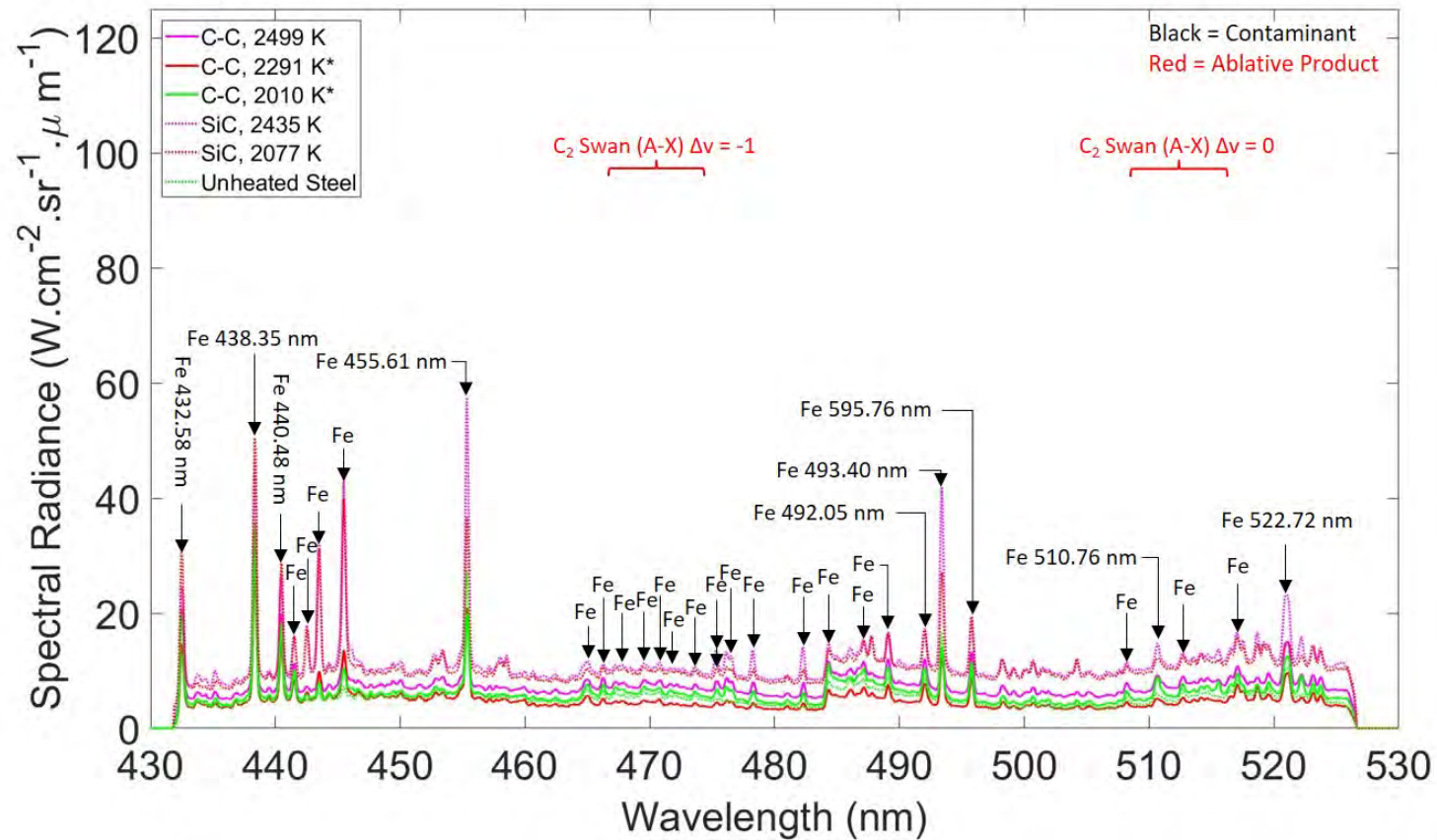


Figure 64. Spectral radiance comparison for C-C and SiC-coated C-C at multiple temperatures with unheated steel. All measurements were taken by averaging in the expansion region 0.75 mm above the model targeting C₂ Swan bands.

potential C₂ Swan bands are of the same intensity as the relatively constant non-zero continuum. Therefore, their significance, if any, should be taken lightly. A significant number of facility contaminants, predominantly Fe from the steel diaphragm, are again present. Some of the Fe lines are labeled while others are not; the Fe lines that are labeled were used to help with the wavelength calibration and identification of other lines.

The general trend of intensity increasing with surface temperature is again present but similar to other cases already discussed, there are exceptions. Most of these inconsistencies can be attributed to the fact that temperature estimates were not obtained for all samples. In these cases, the actual temperature was likely lower than the value used since the DSLR camera underexposed on all of these shots. The trend of spectral radiance being higher for uncoated C-C in the near-stagnation region and higher for SiC-coated C-C in the expansion region is present again, further supporting the theory that the SiC-coated samples are ablating at a higher rate and that the ablation products are entering the flowfield and traveling through the expansion region.

Atomic N and O.

Finally, Figures 65, 66, 67, and 68 show vis/nIR spectra for SiC-coated C-C targeting atomic N and O lines. Figures 65, 66, and 67 show spectra in the near-stagnation region while Figure 68 shows spectra in the expansion region. The dominant features in all of these plots, with the exception of Figure 66, are second-order diffracted UV spectra including CN violet bands, the atomic Si line at 390.55 nm, and the strong Al and Ca lines between 393 and 397 nm.

Although this phenomenon was previously identified by Eichmann [47], most of the shots targeting atomic N and O had been completed before changes to the test

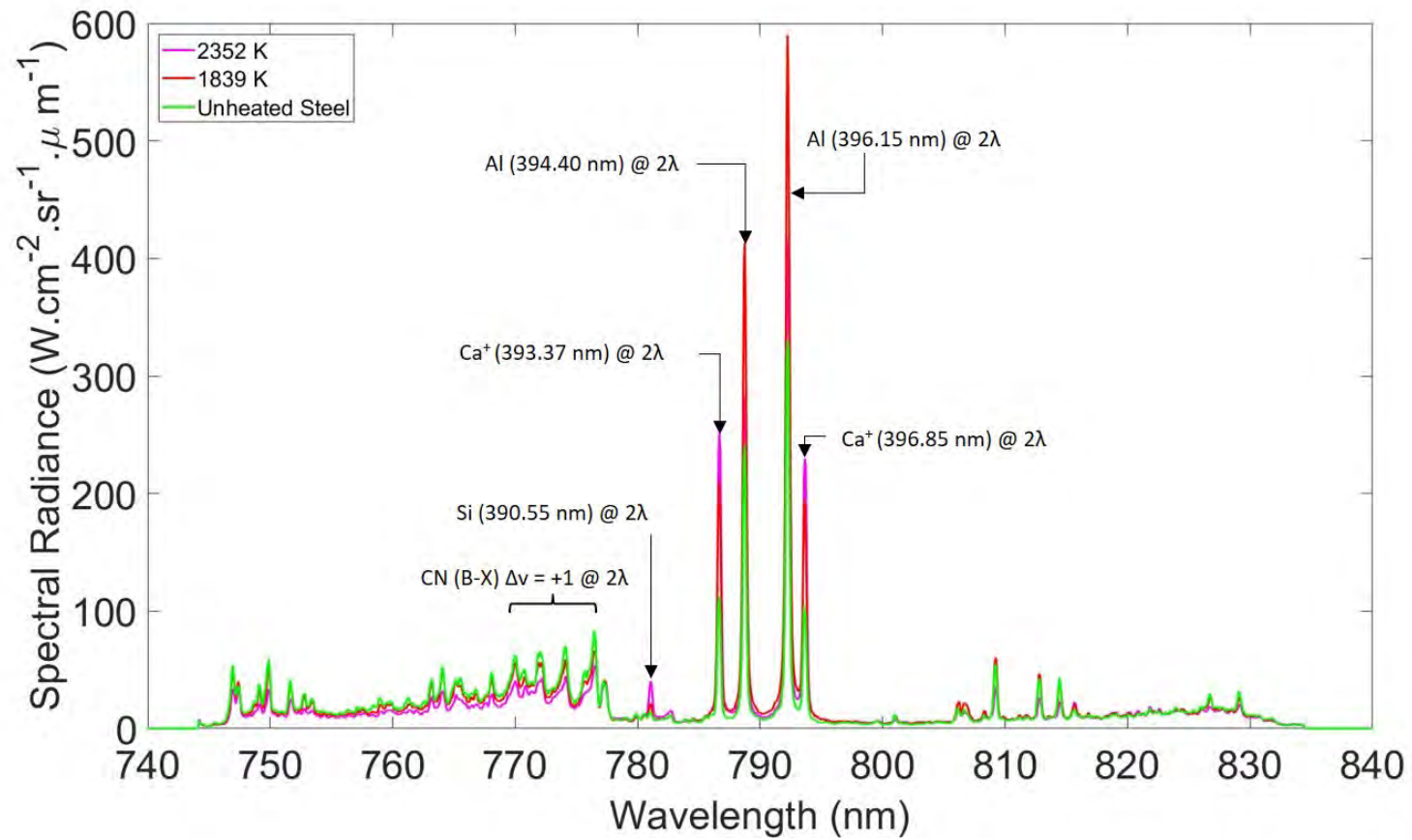


Figure 65. Spectral radiance comparison for SiC-coated C-C in the expansion at two temperatures with unheated steel. All measurements were taken by averaging in the near-stagnation region targeting atomic N and O lines. Results shown are without a filter to block wavelengths below 495 nm.

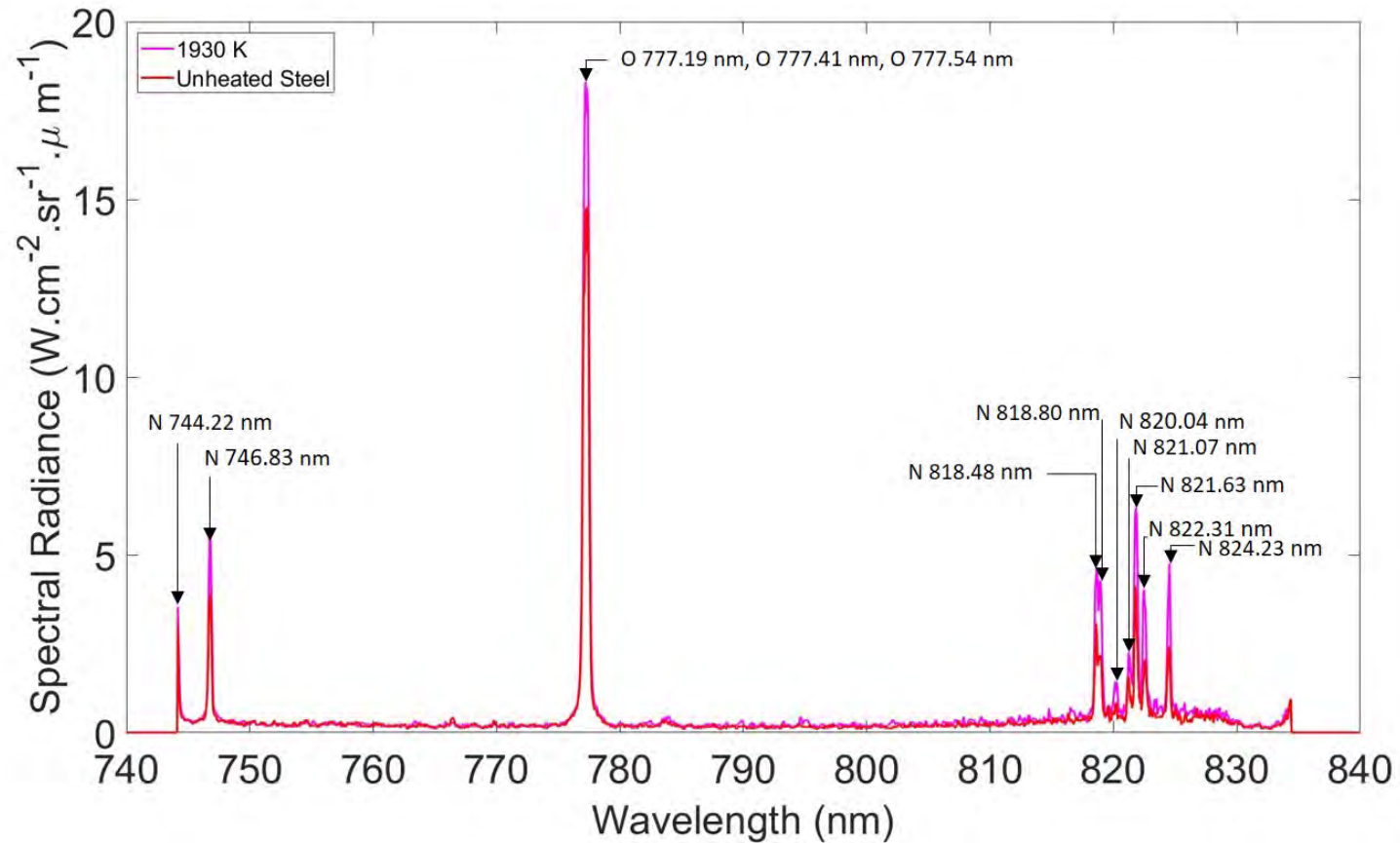


Figure 66. Spectral radiance comparison for SiC-coated C-C in the expansion at two temperatures with unheated steel. All measurements were taken by averaging in the near-stagnation region targeting atomic N and O lines. A filter was used to block wavelengths below 495 nm.

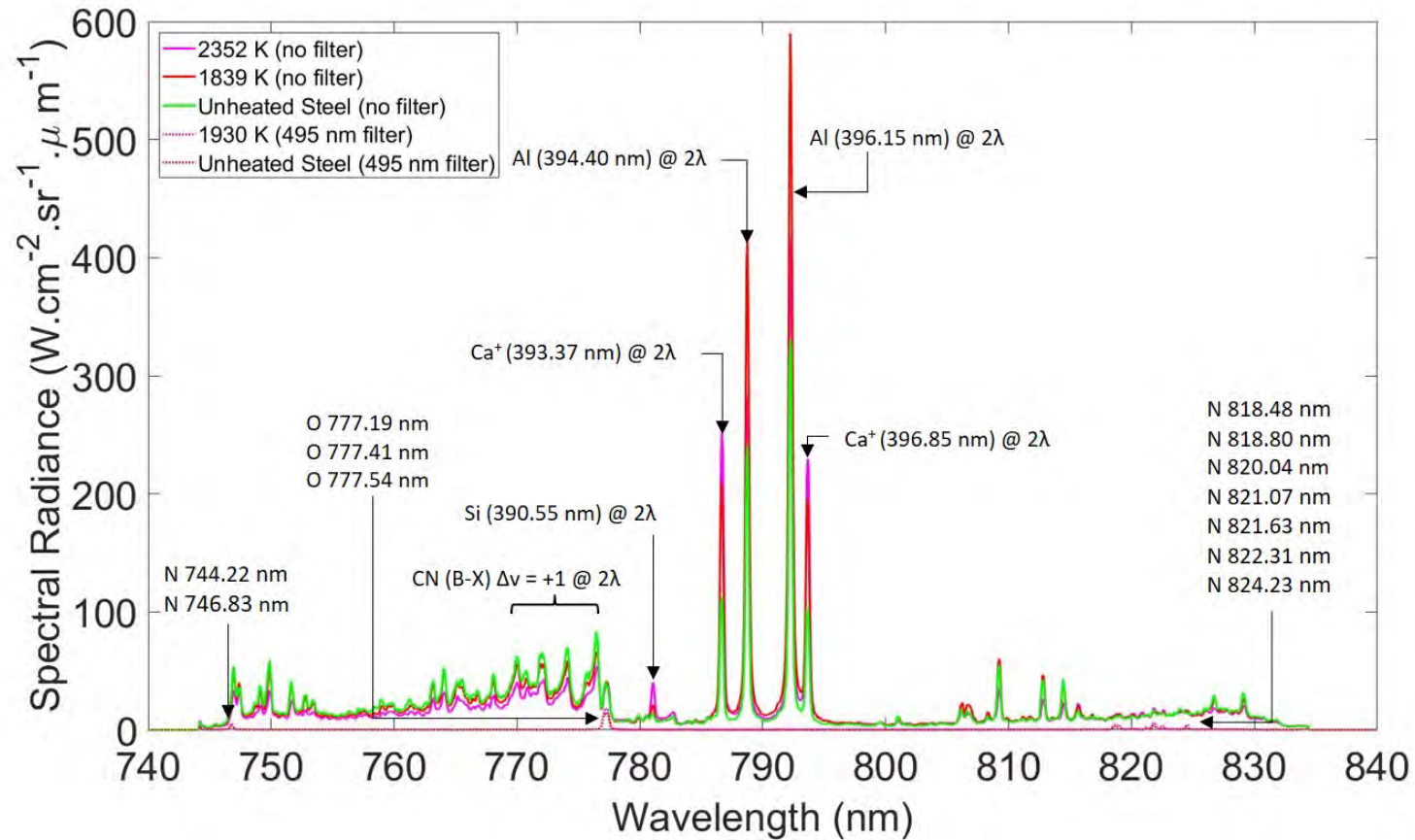


Figure 67. Spectral radiance comparison for SiC-coated C-C in the expansion at multiple temperatures with unheated steel. All measurements were taken by averaging in the near-stagnation region targeting atomic N and O lines. Results shown are with and without a filter to block wavelengths below 495 nm.

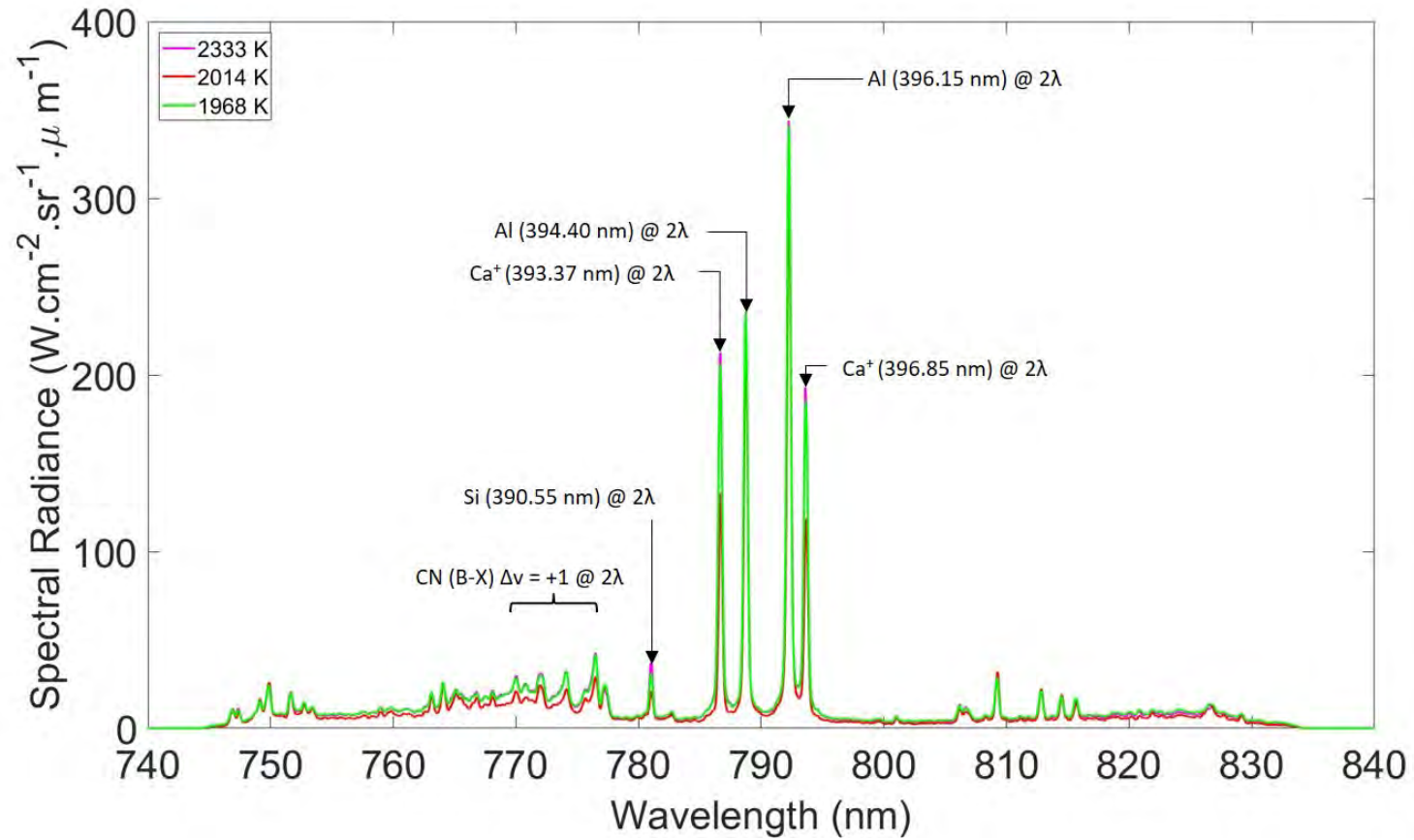


Figure 68. Spectral radiance comparison for SiC-coated C-C in the expansion at two temperatures with unheated steel. All measurements were taken by averaging in the expansion region 0.75 mm above the model targeting atomic N and O lines. Results shown are without a filter to block wavelengths below 495 nm.

setup could be made. Once identified, a filter was used to block wavelengths below 495 nm. The spectra resulting from these shots are shown in Figure 66. From this figure, one can clearly see that only atomic N and O lines are observed. Plotting results in the near-stagnation region obtained with and without a filter, shown in Figure 67, shows that the second-order diffracted spectra will dominate the targeted atomic N and O lines for all shots where a filter is not used to block lower wavelengths. Any future experiments should be planned with a filter to block all wavelengths below 495 nm.

Spatial Profile of Spectra.

Comparing averaged spectra for uncoated C-C and SiC-coated C-C, particularly when plotted together, allows comparisons to be drawn and also allows a means to compare with simulated results. This comparison does not, however, provide any insight into the spatial variation of the spectra. A more detailed study of the spatial profile of the spectra will be conducted in this section.

Figures 69 and 70 show spectral radiance profiles for C-C in the near-stagnation region and Figures 71, 72, and 73 show spectral radiance profiles for SiC-coated C-C in the near-stagnation region. The figures for C-C and SiC-coated C-C appear similar, though the intensity for C-C is visibly higher. For both materials, the intensity between 384 and 389 nm, corresponding to CN violet, is highest just upstream of the model edge. This trend is also true between 250 and 253 nm for SiC-coated C-C, where atomic Si lines are suspected, however the intensity appears highest between 467 and 474 nm, corresponding to C₂ Swan bands, just behind the shock. This observation adds further evidence that radiation of C₂ is not significant, if present at all.

Averaging the spectral radiance over the wavelength regions just mentioned pro-

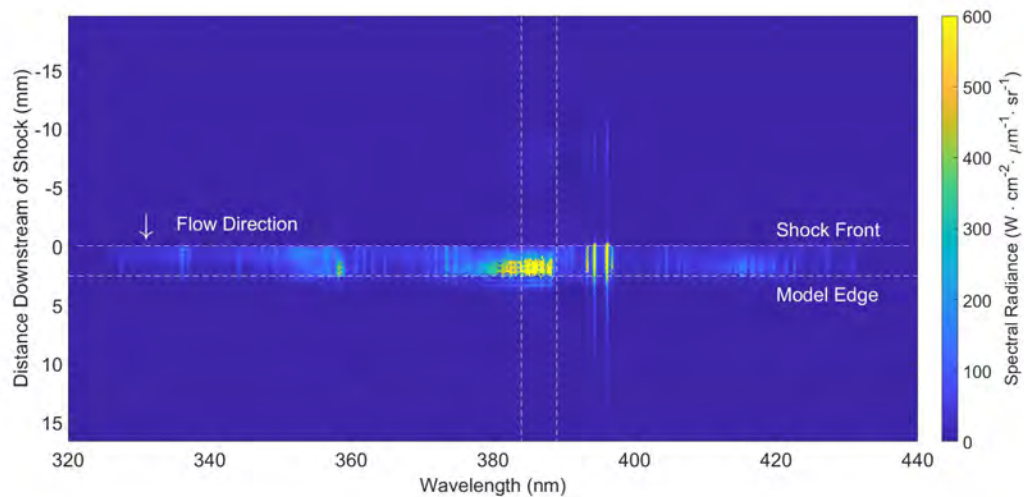


Figure 69. Calibrated UV spectra for C-C in the near-stagnation region targeting CN violet bands.

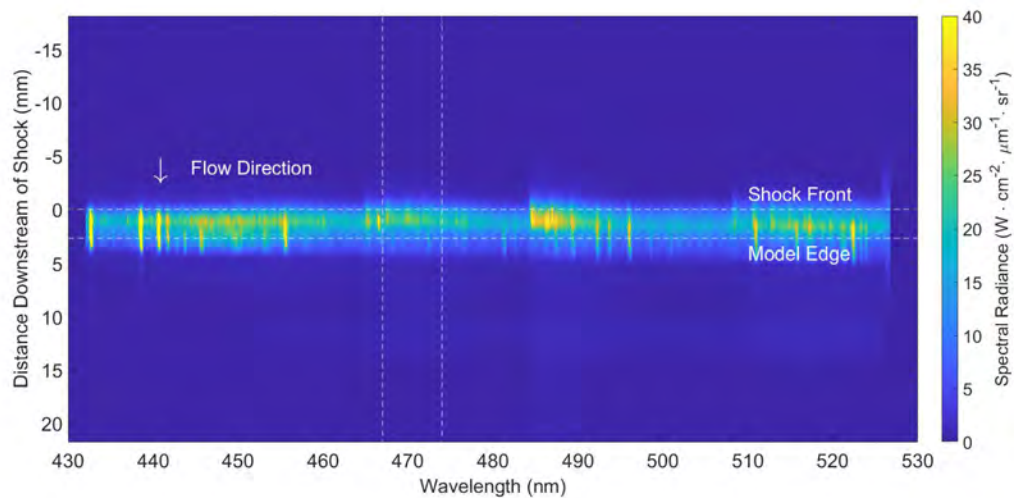


Figure 70. Calibrated UV spectra for C-C in the near-stagnation region targeting C₂ Swan bands.

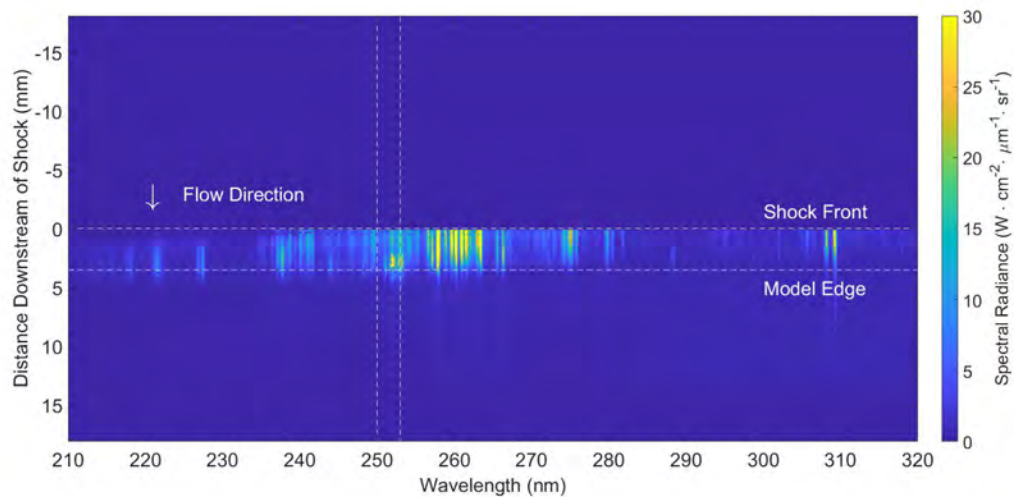


Figure 71. Calibrated UV spectra for SiC-coated C-C in the near-stagnation region targeting atomic Si lines.

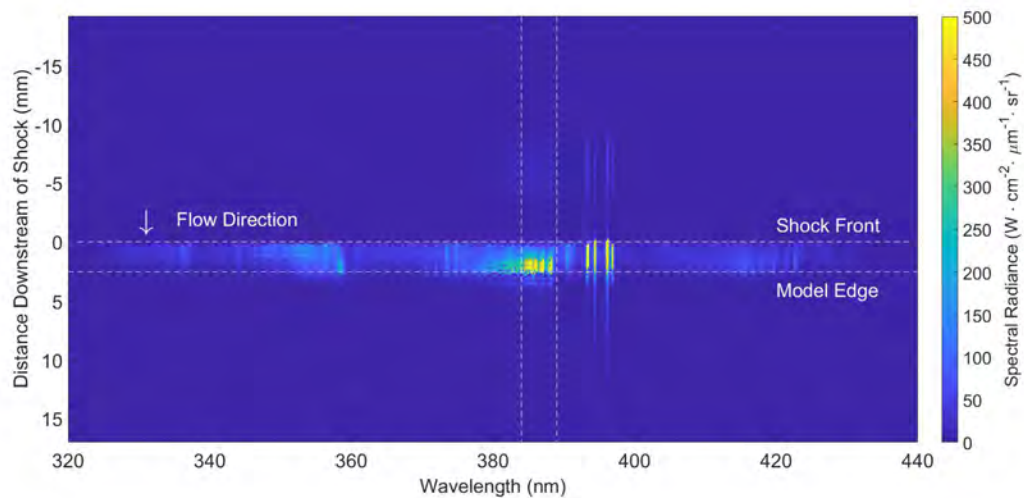


Figure 72. Calibrated UV spectra for SiC-coated C-C in the near-stagnation region targeting CN violet bands.

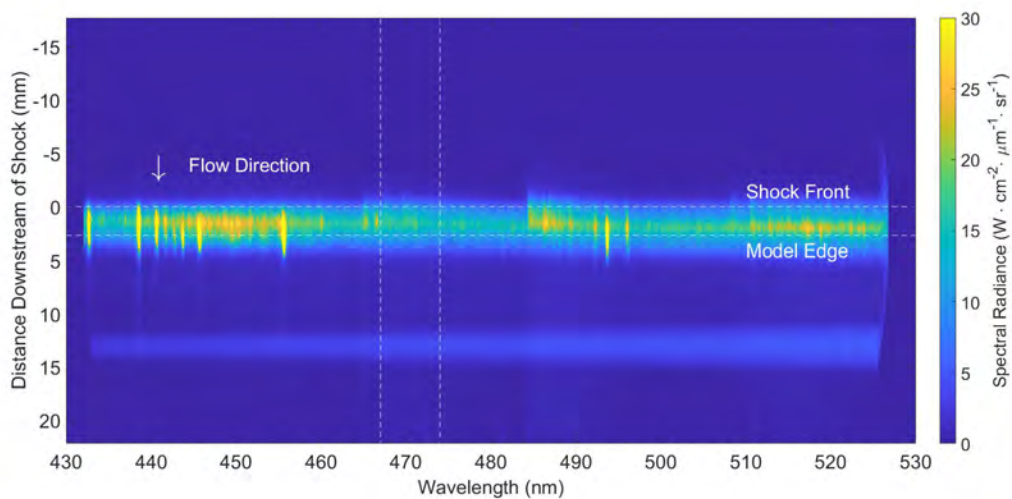


Figure 73. Calibrated UV spectra for SiC-coated C-C in the near-stagnation region targeting C_2 Swan bands.

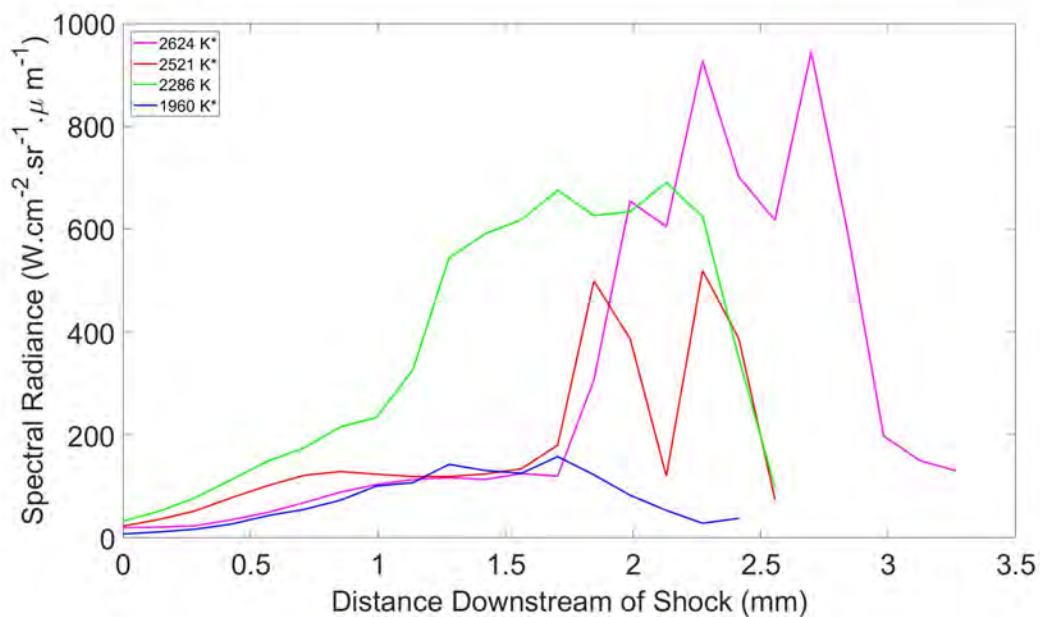


Figure 74. Average spectral radiance for C-C in the near-stagnation region. Values displayed were calculated by averaging between 384 and 389 nm.

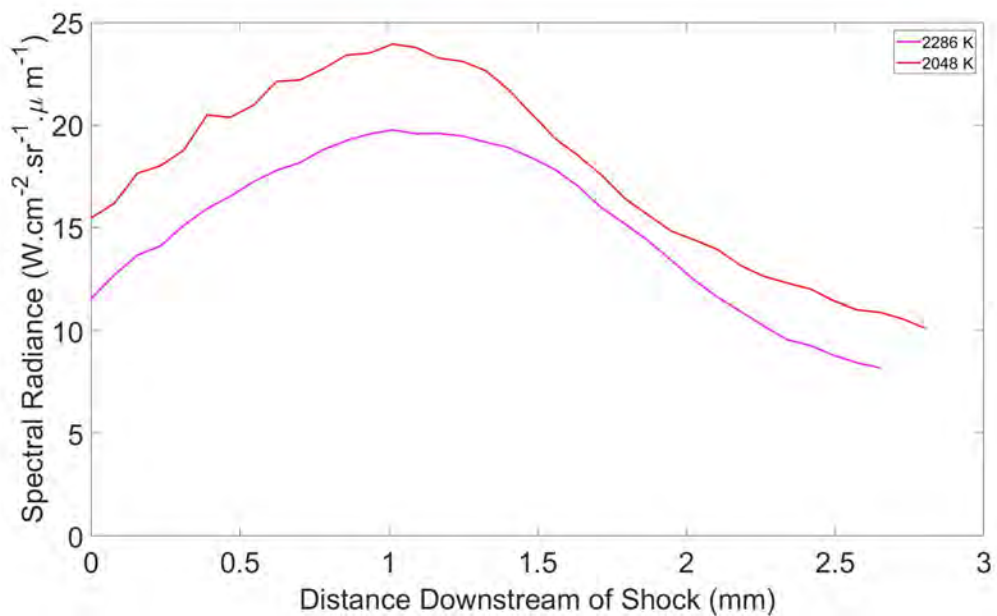


Figure 75. Average spectral radiance for C-C in the near-stagnation region. Values displayed were calculated by averaging between 467 and 474 nm.

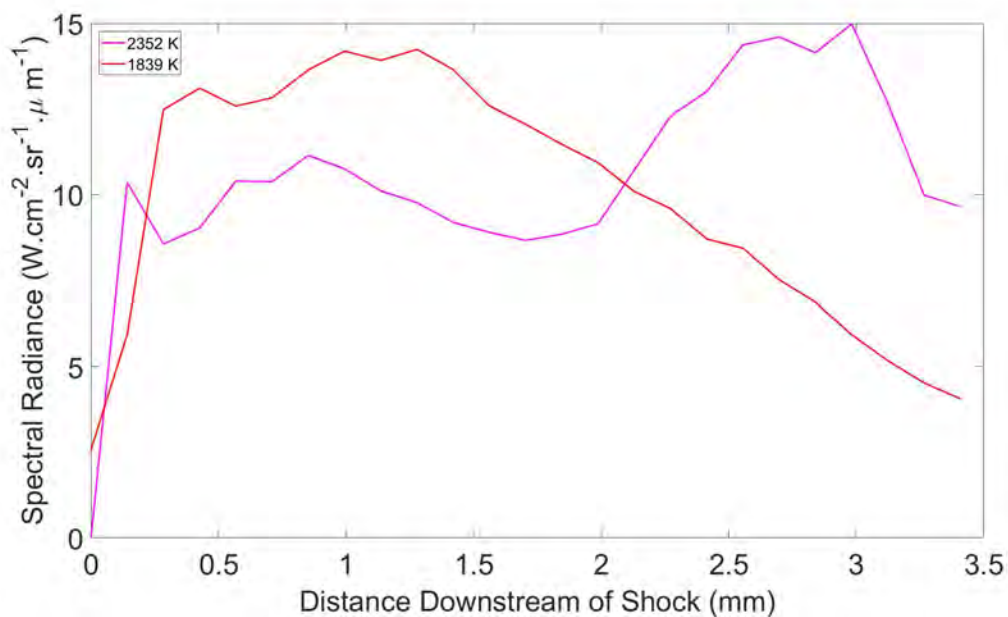


Figure 76. Average spectral radiance for SiC-coated C-C in the near-stagnation region. Values displayed were calculated by averaging between 250 and 253 nm.

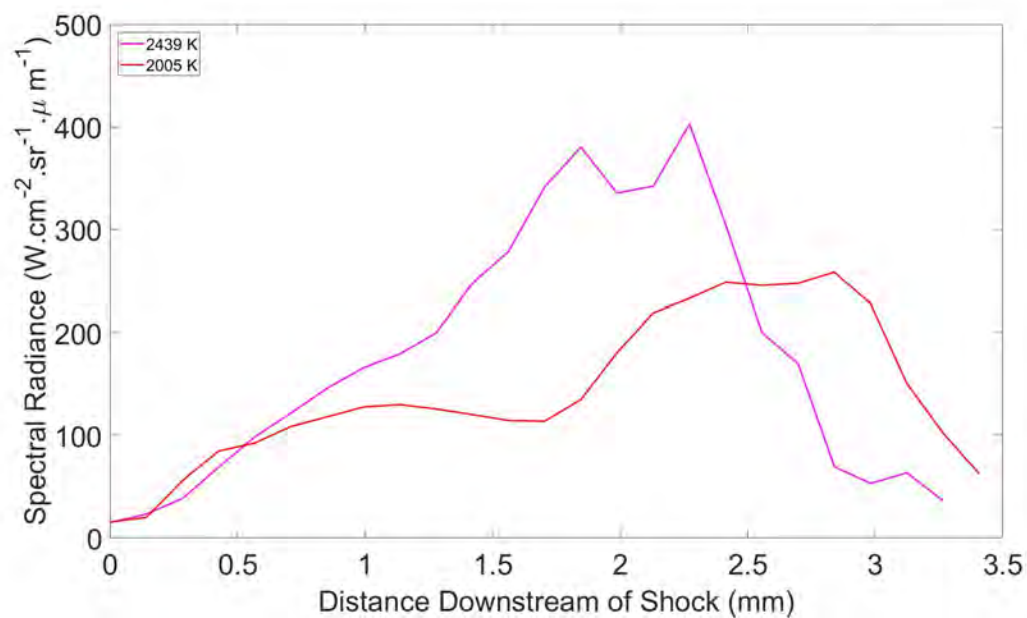


Figure 77. Average spectral radiance for SiC-coated C-C in the near-stagnation region. Values displayed were calculated by averaging between 384 and 389 nm.

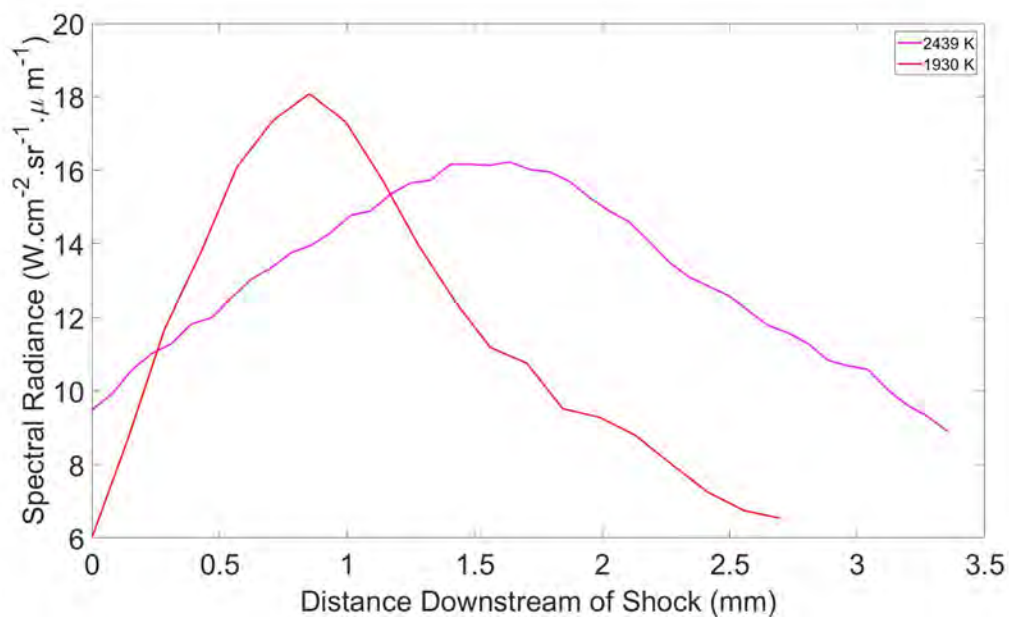


Figure 78. Average spectral radiance for SiC-coated C-C in the near-stagnation. Values displayed were calculated by averaging between 467 and 474 nm.

duces plots that are a bit more intuitive, where the trends discussed earlier can be more easily observed. These results are shown in Figures 74, 75, 76, 77, and 78. One thing that can be observed is that the shock thickness, shown as the distance between the two dashed horizontal lines in the spectral radiance profiles in Figures 69, 70, 71, 72, and 73, varied slightly during some of the shots, within the range of about 2.5 to 3.5 mm. This variation could suggest some shot-to-shot variation in the test conditions. The error bars in Table 6 should account for variation between shots. In order to be consistent with data processing, the averaged spectra in the near-stagnation region were computed from the shock to the model edge rather than a fixed distance. It should also be noted that the 1839 K case for SiC-coated C-C, shown in Figure 76, does not follow the same trend as the 2352 K case. This deviation is likely the result of this sample being heated to a much lower temperature than in other cases investigated and perhaps also indicates that the shot was fired well before the sample reached a steady temperature.

Similarly, Figures 79 and 80 show spectral radiance profiles for C-C in the expansion region while Figures 81, 82, and 83 show spectral radiance profiles for SiC-coated C-C in the expansion region. There is a striking difference in these plots, depending on the material. For uncoated C-C, the intensity of spectra for ablation-related species, between 384 and 389 nm for CN violet and between 467 and 474 nm for C₂ Swan, is highest just behind the shock while it is significantly higher about 5 mm downstream of the shock for SiC-coated C-C, which is approximately where the expansion corner is located. This pattern also holds true between 250 and 253 nm, corresponding to what is believed to be atomic Si. The line at 288.16 nm, as well as the previously-identified line at 390.55 nm, also display this behavior.

The observations just made can be seen in Figures 84, 85, 86, 87, and 88, which show spectral radiance averaged over the same wavelength regions for the expan-

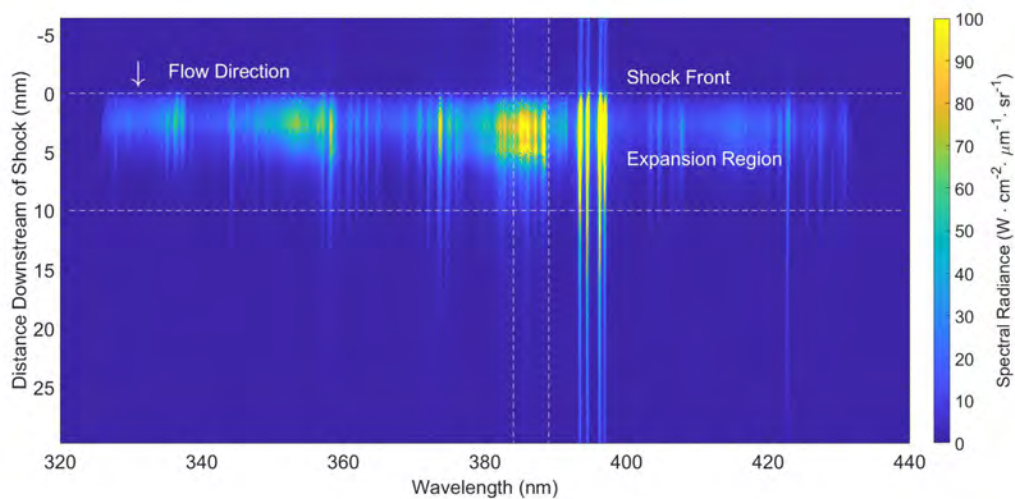


Figure 79. Calibrated UV spectra for C-C in the expansion region targeting CN violet bands.

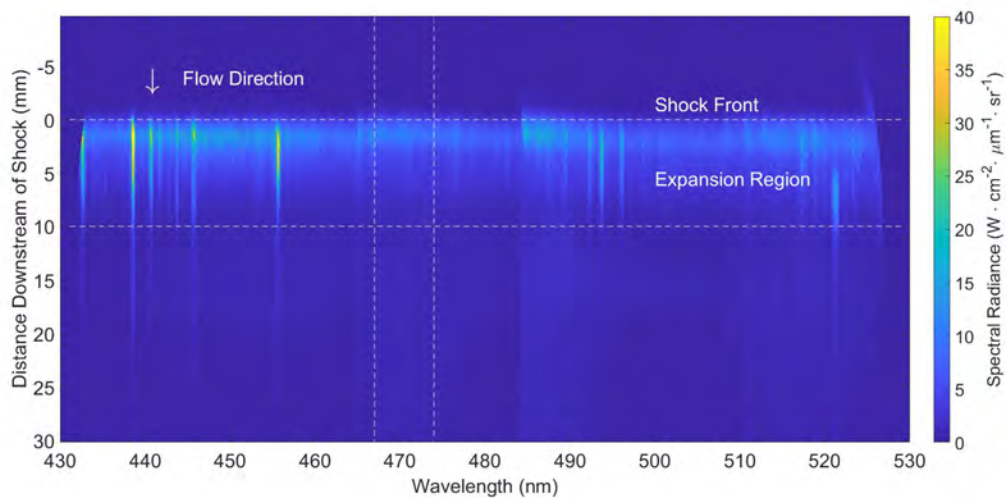


Figure 80. Calibrated UV spectra for C-C in the expansion region targeting C₂ Swan bands.

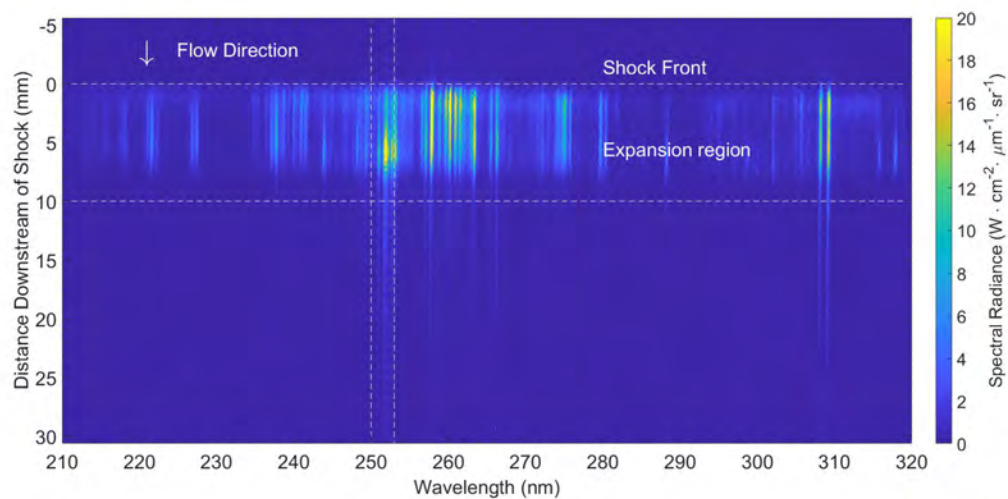


Figure 81. Calibrated UV spectra for SiC-coated C-C in the expansion region targeting atomic Si lines.

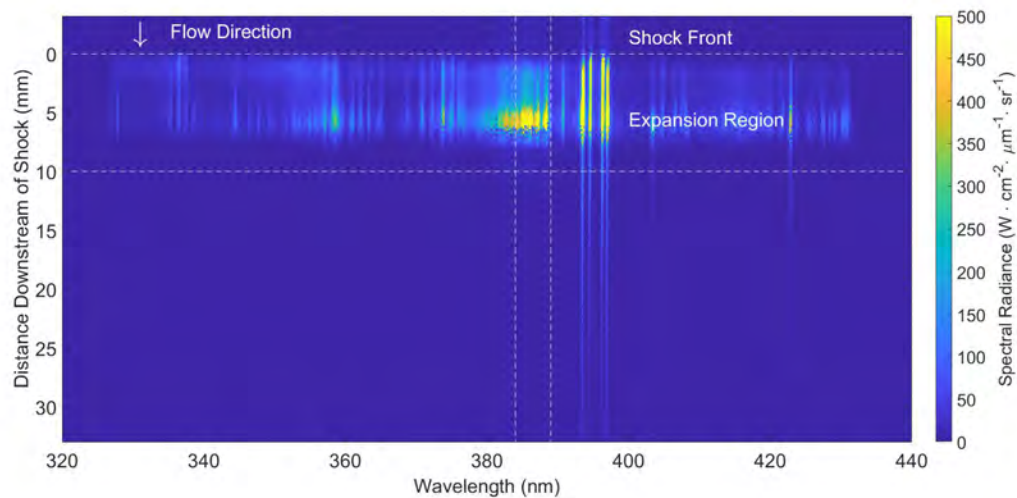


Figure 82. Calibrated UV spectra for SiC-coated C-C in the expansion region targeting CN violet bands.

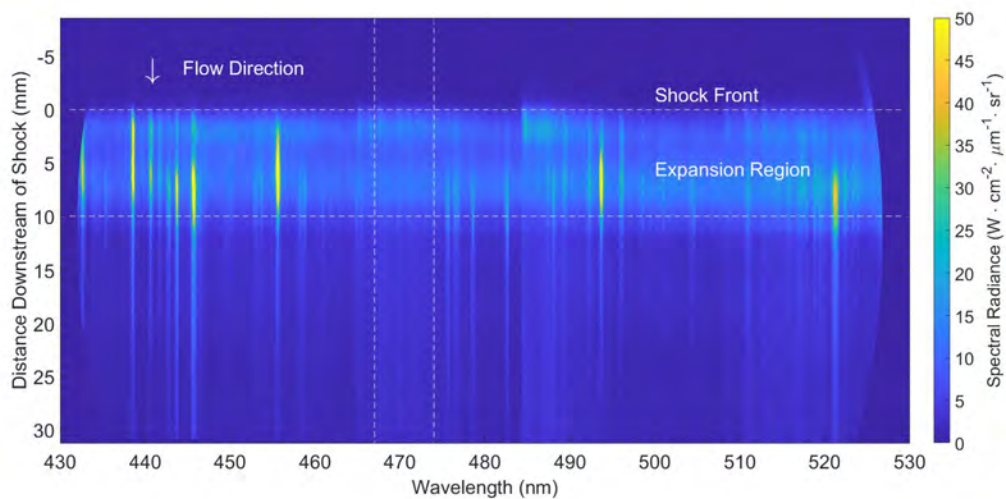


Figure 83. Calibrated UV spectra for SiC-coated C-C in the expansion region targeting C_2 Swan bands.

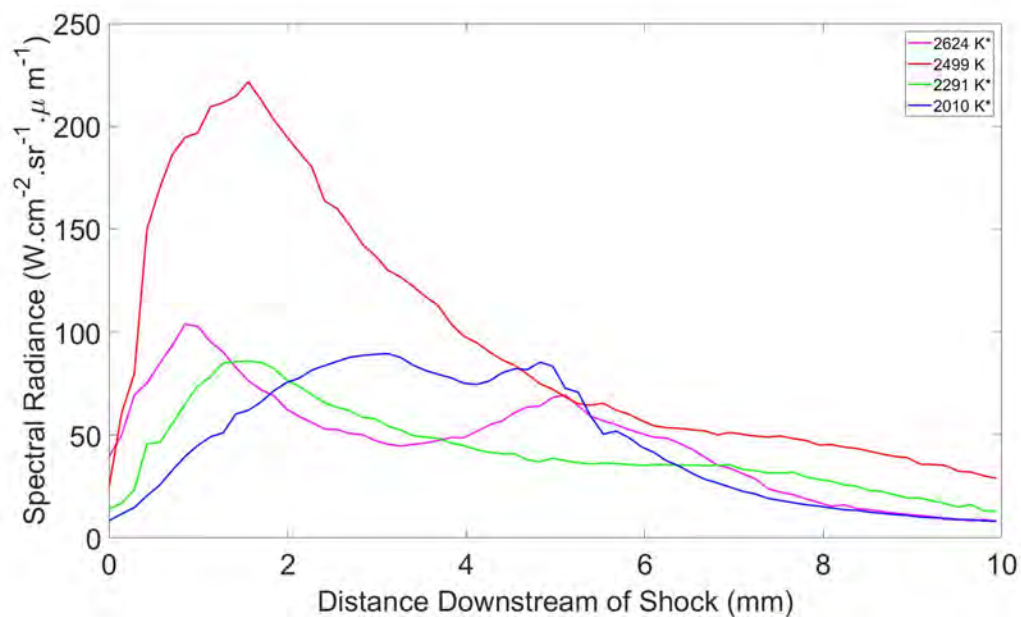


Figure 84. Average spectral radiance for C-C in the expansion region. Values displayed were calculated by averaging between 384 and 389 nm.

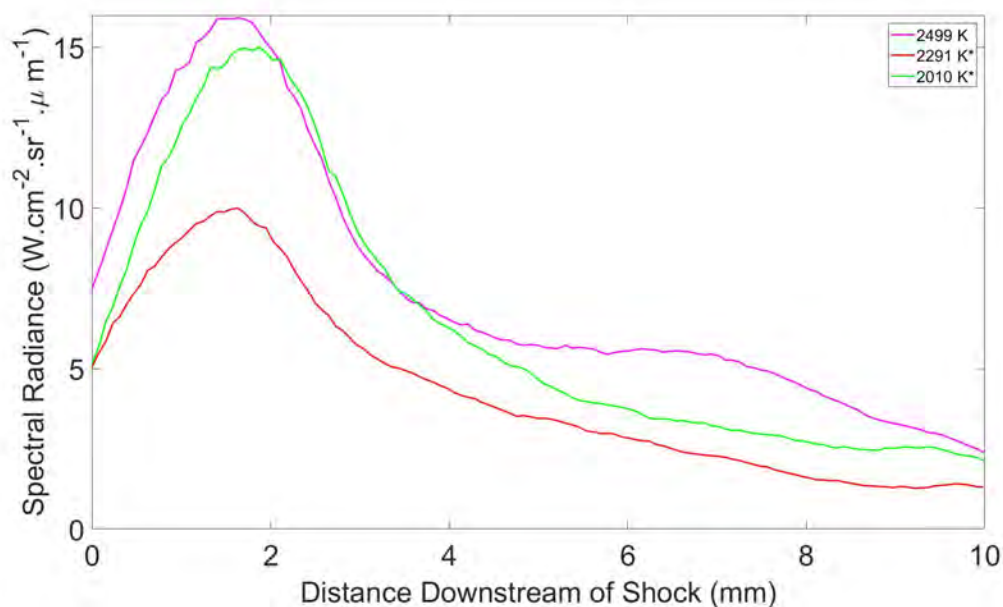


Figure 85. Average spectral radiance for C-C in the expansion region. Values displayed were calculated by averaging between 467 and 474 nm.

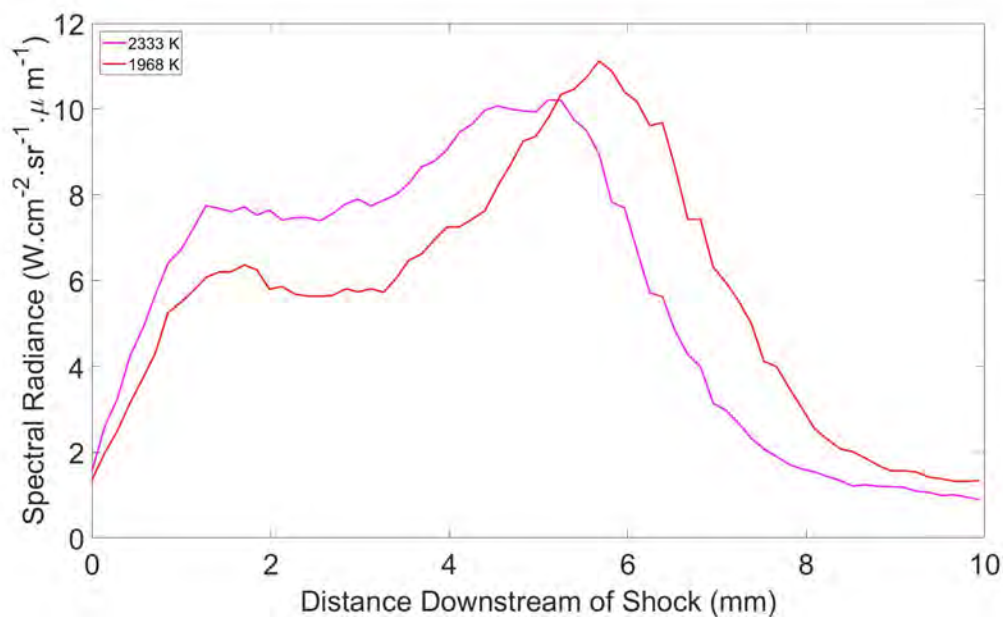


Figure 86. Average spectral radiance for SiC-coated C-C in the expansion region. Values displayed were calculated by averaging between 250 and 253 nm.

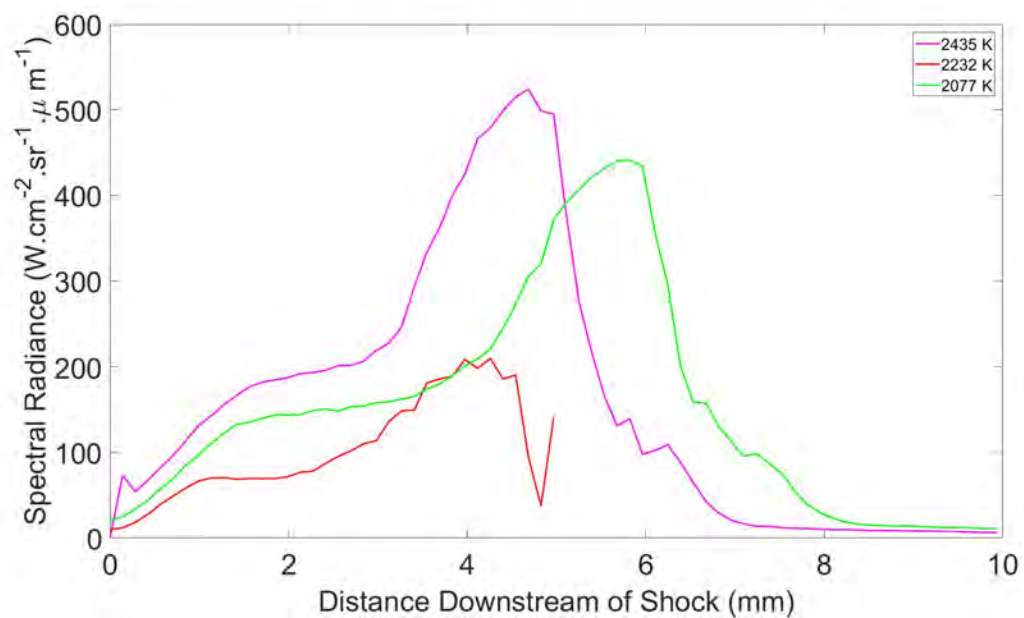


Figure 87. Average spectral radiance for SiC-coated C-C in the expansion region. Values displayed were calculated by averaging between 384 and 389 nm.

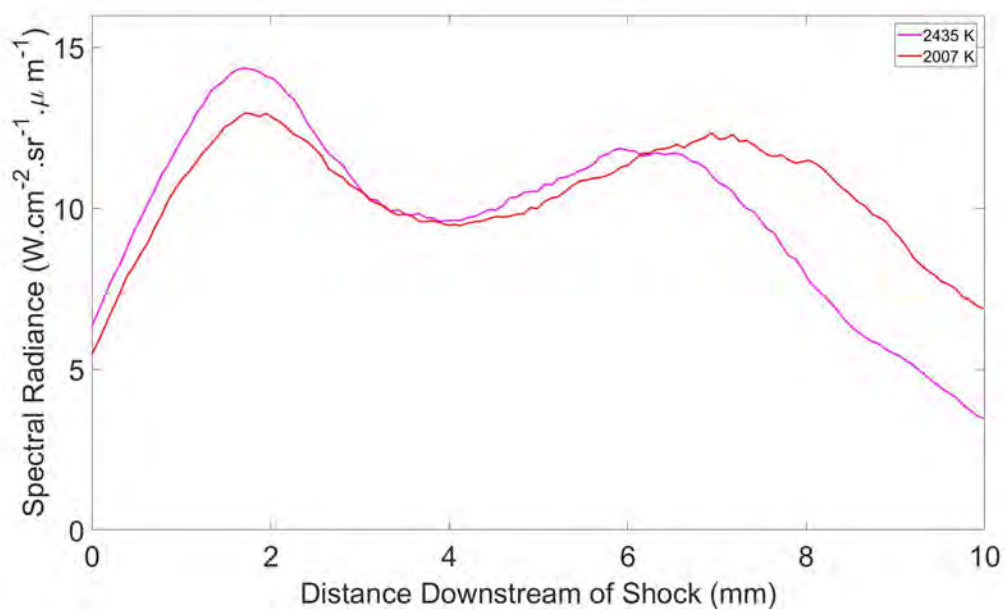


Figure 88. Average spectral radiance for SiC-coated C-C in the expansion region. Values displayed were calculated by averaging between 467 and 474 nm.

sion region. It should be noted that the 2232 K case targeting CN violet bands for SiC-coated C-C, shown in Figure 82, cuts off approximately 5 mm downstream of the shock. These plots clearly show the distinct increase in spectral radiance approximately 5 mm downstream of the shock for the SiC-coated samples. This same increase is present between 467 and 474 nm corresponding to C₂ Swan, however there is a larger increase immediately downstream of the shock, which is also present in the uncoated C-C cases.

Decoupled ICCD Imaging.

At the end of the second experimental campaign, the ICCD cameras were decoupled from the spectrometers and it was attempted to observe emissions in two spatial dimensions. This technique was only attempted on a total of five shots since delays in pumping the tunnel to vacuum during the campaign limited the total number of shots. This imaging technique has been attempted before at UQ but never with this model.

Figures 89, 90, and 91 show images taken for SiC-coated C-C with filters for atomic Si, CN violet, and C₂ Swan, respectively. All of these images are uncalibrated; the spatial axes are in pixels, intensity is in counts. All images show an increase in intensity just upstream of the model but otherwise are not particularly useful. Further investigation in future experiments, particularly adjusting gain settings, might provide more useful images.

5.3 Summary

The second experimental campaign built on the lessons learned during the first experimental campaign and continued investing atomic Si and CN violet while expanding to include investigation of C₂ Swan, atomic N, and atomic O with the vis/nIR

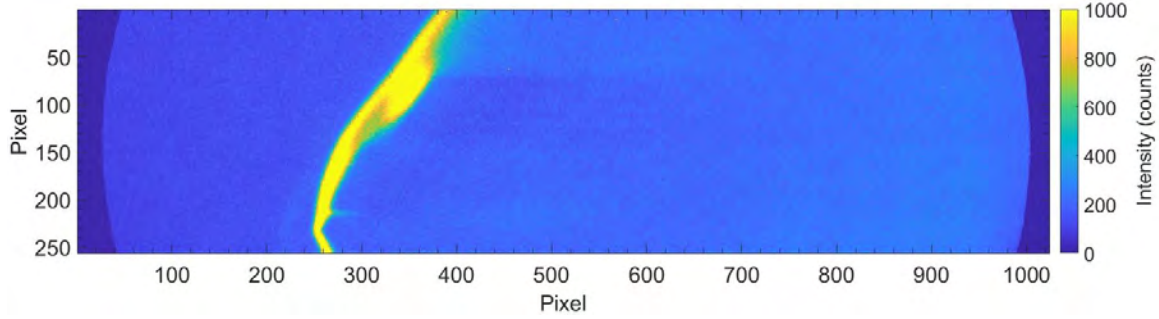


Figure 89. Two-dimensional image taken with stand-alone ICCD camera for SiC-coated C-C. A filter restricting all wavelengths except 250 ± 5 nm, corresponding to suspected atomic Si lines, was used.

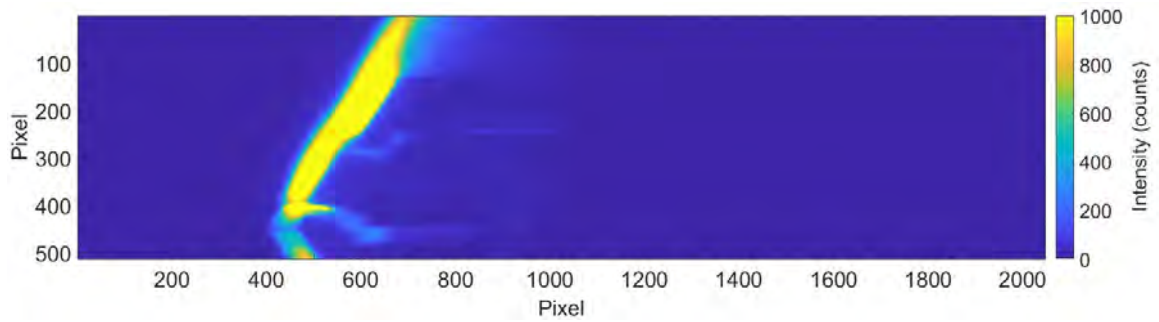


Figure 90. Two-dimensional image taken with stand-alone ICCD camera for SiC-coated C-C. A filter restricting all wavelengths except 380 ± 7 nm, corresponding to CN violet bands, was used.

spectrometer. The improvements made to the test specimens proved successful as none broke and the coating of all SiC-coated samples was more than adequate even when reusing a sample for multiple shots, which had never been done at the X2 facility before; the time and cost savings provided by reusing test articles could be significant. Bandpass filters were used in conjunction with the high-speed video camera and decoupled ICCD cameras to produce images isolating specific wavelength ranges.

CN violet emissions were the dominant feature, continuing to display an increase with surface temperature. Atomic N and O lines were clearly observed at a significantly lower intensity level than CN violet, however only two shots displaying these lines were conducted as the lack of a filter to block wavelengths lower than 495 nm clouded the results with second-order UV spectral lines. Similarly, a number of

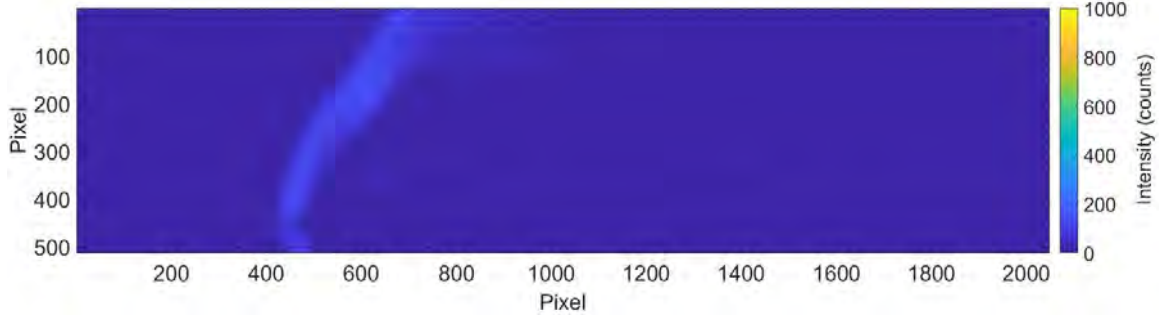


Figure 91. Two-dimensional image taken with stand-alone ICCD camera for SiC-coated C-C. A filter restricting all wavelengths except 470 ± 5 nm, corresponding to C_2 Swan bands, was used.

atomic Si lines were observed, particularly between 250 and 253 nm and 288.16 nm, with approximately the same intensity as and atomic N and O. Although potential signs of C_2 Swan emissions may have been observed, their significance, if any, should be taken lightly. The constant non-zero continuum across that wavelength region make it difficult to draw concrete conclusions.

Plotting spectral radiance results for uncoated C-C and SiC-coated C-C together produced interesting results. In the near-stagnation region, intensity is higher for uncoated C-C while intensity is higher for SiC-coated C-C in the expansion region, regardless of the wavelength region investigated. This observation suggests that the ablation rate for SiC-coated C-C is higher than uncoated C-C, which likely will not be captured by existing ablation models. A distinct increase in spectral radiance averaged between 250 and 253 nm and 384 and 389 nm, corresponding to atomic Si and CN violet, was clearly observed for SiC-coated C-C, likely the result of more of these species entering the flowfield and traveling downstream.

Over 50 shots were conducted in the X2 facility during the two experimental campaigns providing a significant amount of data to compare with simulated results. The test conditions used at the X2 facility were well characterized and will provide a basis for simulations that were conducted using the LAURA code. Running of the simulations will be discussed in the next chapter, as will comparisons between

experimental and simulated results.

VI. Computational Results

The following sections detail the process developed to use the LAURA and HARA simulation codes to replicate shock tube experiments and the results obtained using this technique. The simulations were conducted using a two-dimensional (2D) structured grid with 27,880 cells. The grid was divided into four blocks in order to specify different solid surface boundary conditions, corresponding to the ablative strip and the model (which is made out of stainless steel). The simulations were run in 2D to reduce computational cost, which can be quite expensive with the technique used for these simulations. The initial grid used for all simulations is shown in Figure 92; Figure 93 shows the grid after adaptation. Displaying each of the grids as a contour plot of temperature, which shows temperatures characteristic of hypersonic flows [46], allows the shock to be visualized.

The grid was adapted to capture the shock 75% of the arc length distance between the wall and domain boundary and also to cluster cells around the shock. This value was suggested by the LAURA code developers in order to focus cells on features of interest inside the shock layer. A value of 5.0 for the “ep0_grd” flag, which sets a coefficient in a function that specifies grid clustering around the shock, was used for these simulations. A variety of values were examined and any further increase (leading to tighter clustering around the shock) resulted in poorer resolution elsewhere in the flowfield with no improvement near the shock. Only the top half of the wedge was modeled since the model was symmetric and data was only collected on the top half of the model during experiments. Additionally, the grid extended 10 mm downstream of the expansion corner since this distance adequately covered the line of sight of the spectrometers used during the experiment.

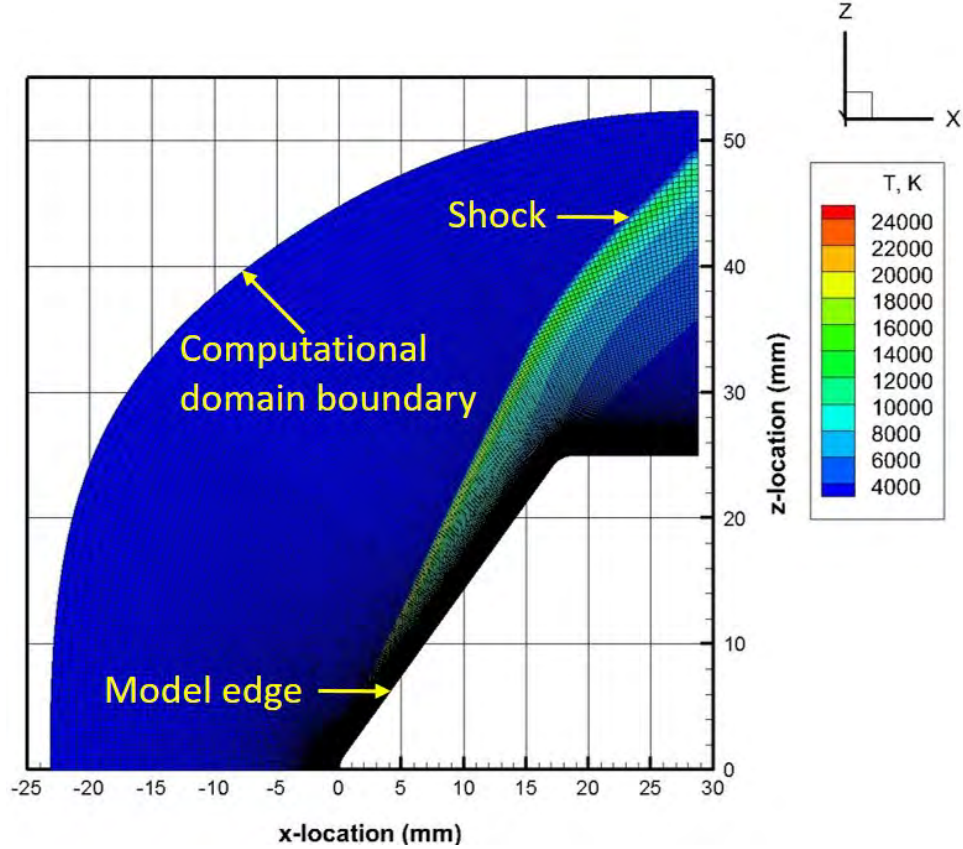


Figure 92. Initial grid used in LAURA simulations.

6.1 Grid Independence Study

Before commencing with running the various cases used to compare to experiments, a grid independence study was conducted to ensure that the grid had an adequate number of cells. The grid independence study consisted of a coarse grid with 6,970 cells, a medium grid with 27,880 cells, and a fine grid with 111,520 cells corresponding to a refinement factor of two. A non-ablating flowfield simulation was run to convergence for each grid. Data was extracted from these solutions along $z = 8$ mm and $z = 25.75$ mm slices, corresponding to the near-stagnation and expansion region 0.75 mm above the wall, respectively, using Tecplot[®]. All other data processing was done using Matlab[®]. The slice 0.75 mm above the model can be seen in Figure 93. Plots of temperature along these slices are shown in Figures 94 and 95.

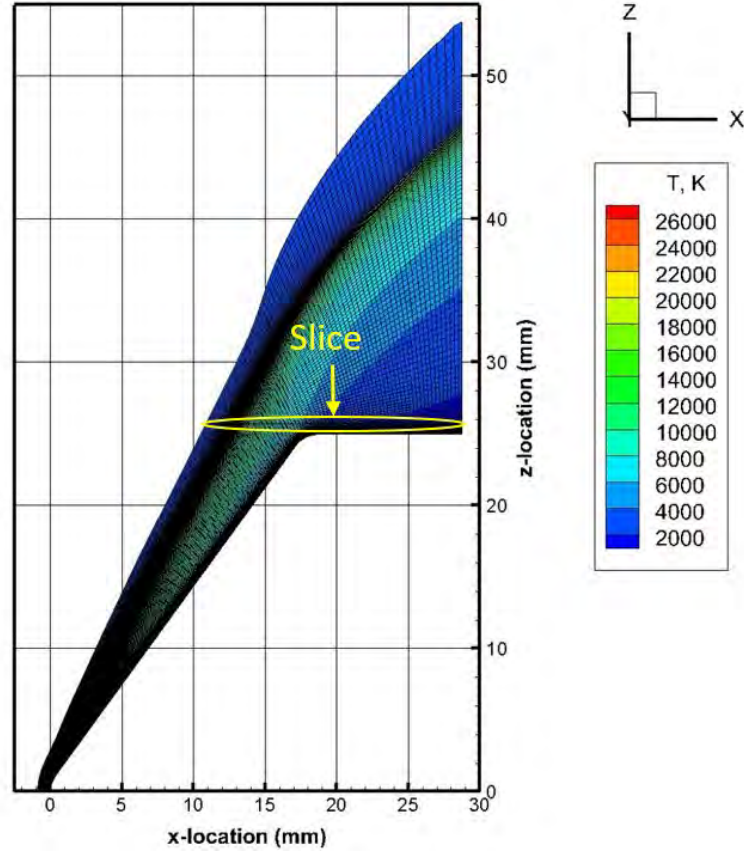


Figure 93. Grid used in LAURA simulations adapted to capture shock 75% between wall and domain boundary.

The solution obtained with the coarse grid does not appear to match the other two grids, especially near the shock and in the expansion region. There appears to be much better agreement between the medium and fine grids. A point-by-point comparison between the grids confirms these observations. The largest difference between the coarse and medium grids occurs at an x-location of 3.2 mm along the $z = 8$ mm slice, with a difference of 18.04%. The largest difference between the medium and fine grids, which is 5.13%, occurs at an x-location of 12.35 mm along the $z = 25.75$ mm slice. Both of these discrepancies occur in the vicinity of the shock where gradients are highest. Averaging the difference between grids for all points shows much better results with an average difference between the coarse and medium grids of 1.55% while the average difference between the medium and fine grids is 0.35%.

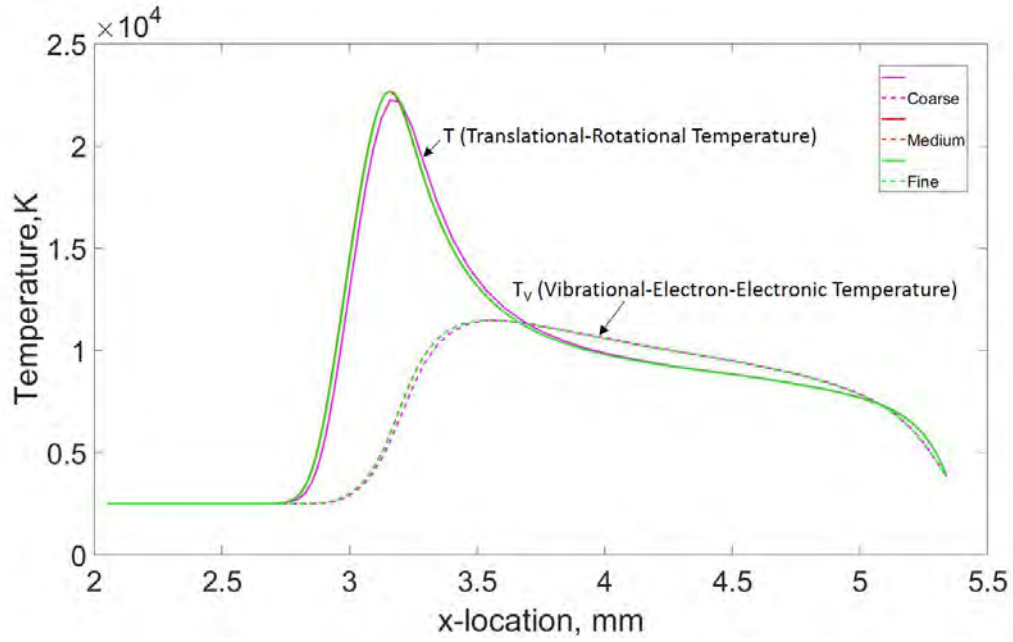


Figure 94. Temperature along $z = 8$ mm slice, corresponding to the near-stagnation region.

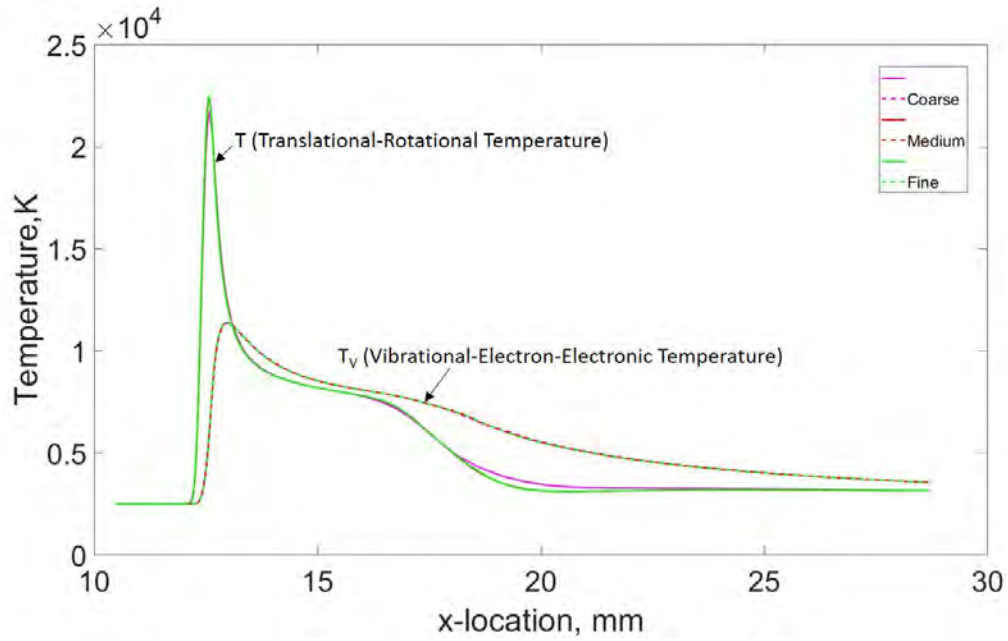


Figure 95. Temperature along $z = 25.75$ mm slice, corresponding to the expansion region 0.75 mm above the model.

Therefore, the medium grid with 27,880 cells was used for all simulations conducted in this dissertation.

6.2 Simulation Technique

The process developed to use the LAURA and HARA codes to simulate shock tube experiments is discussed in the following subsections.

If running the coupled version of the HARA code, one change must be made to the source code in order to replicate shock tube experiments. In the `src/relax_laura.f90` file, the “`radiation_coupling_type`” flag must be changed from “`laura coupled`” to “`shock tube`”. This change is required since shock tube experiments require intensity directed parallel to the surface rather than towards the surface, which is normally how the radiation solver operates. This change is not required if running the stand-alone version of the HARA code since it is hard-coded into the code.

Flowfield Solution Technique.

A four-step processes was developed to obtain a fully-converged flowfield solution using the LAURA code. The steps of this process are as follows:

Step 1: Run LAURA using the test conditions from the X2 experiments, shown in Table 6, until the shock is well established. For these simulations, this step took approximately 7,500 iterations.

Step 2: Take the solution from Step 1, turn on grid adaptation, and run to convergence. This step took about 52,000 iterations. Adapting the grid every 2,000 iterations a total of 10 times was found to work well for this step. When grid adaptation was attempted in the first step, LAURA grew unstable and eventually crashed. For these simulations, a solution was considered converged when the L2 norm dropped below a value of $1.0E - 10$.

Step 3: Set surface temperatures to constant values and repeat Step 2. This action was done by setting the “`surface_temperature_type`” flag to “`constant`” and specifying the corresponding surface temperature; room temperature, taken as 300 K

for the unheated/non-ablating parts of the model and the heated surface temperature, as measured during the X2 experiments, for the ablative surface. This step took about 93,000 iterations. The grid does not need to be adapted as often during this step since the grid shape is well established. Adapting every 5,000 iterations a total of 10 times was found to work well with this step. Attempts to set the surface temperature to a constant value during Step 1 or 2 resulted in the solution crashing.

Step 4: Turn on ablation and run to convergence. For finite-rate, a converged solution was obtained in roughly 300,000 to 400,000 iterations depending on the surface temperature. For equilibrium-char, it took approximately 1,200,000 to 1,400,000 iterations to achieve a converged solution, depending on the surface temperature. For both ablation models, it took longer to achieve a converged solution for higher surface temperatures. A solution was considered converged during this step when the L2 norm dropped below a value of $1.0E - 10$ and the $\dot{m}$ (massflow) residual fell below a value of $1.0E - 2$; an $\dot{m}$ residual of less than $1.0E - 2$ indicates that the ablation rate has converged within 1%.

This step is significant as holding the surface temperature constant while running ablation greatly increases the time it takes to achieve a converged solution. Fully converged solutions can be obtained in approximately 65,000 iterations for finite-rate and 110,000 iterations for equilibrium-char. However, all simulations, regardless of the initial surface temperature, converge to the same solution if the surface temperature is not held constant. Not running simulations with the surface temperature held as constant would yield results entirely inconsistent with the experimental results, where the general trend of intensity increasing with temperature was observed. Given that the heating occurs immediately before the shot, while the test section is under vacuum, and the duration of the test time is extremely short, holding surface temperature as constant will yield results that are in much better agreement with ex-

perimental results. It should also be noted that the number of processors used must be the same as the number of blocks. Attempts were made to run simulations with more processors than blocks. These attempts failed as LAURA is unable to enforce the constant wall temperature boundary condition, likely due to the way tasks are assigned to processors. As a result, this step can take an extremely long time to complete; several weeks in some cases.

Maintaining a constant surface temperature is done differently depending on the ablation model used. For the equilibrium-char model, maintaining a constant surface temperature is accomplished by manually overriding the temperature values in the “ablation_from_laura” file that is produced from running this ablation model. If the user does not already have this file to update, they may need to run this step twice: once to produce that file, and another to run it with overridden values. For the finite-rate ablation model, the surface temperature is kept constant by setting the “freq_mdot” flag to a value larger than the total number of iterations. For the equilibrium-char model, this flag determines how often the ablation rate is updated; however, for the finite-rate model, the ablation rate is updated based on the “nexch” flag.

It was discovered, as the simulations were nearing completion, that the “freq_mdot” flag also specifies how often the mdot (massflow) residual is output. As a result, convergence of the ablation rate was confirmed by extracting the massflow values from each surface cell of two consecutive solution files and manually computing the massflow residual. Doing this task showed that the massflow residual had dropped below a value of $1.0E - 10$ after approximately 200,000 iterations for all cases. Future researchers should consider modifying the LAURA source code to enable writing of the massflow residual based on different namelist parameter.

For the four steps listed above, the following files were required:

1. `laura.g`, which is the Plot3D grid file.
2. `laura_bound.data`, which specifies the grid block face boundary conditions.
3. `laura_namelist.data`, which contains the simulation configuration input parameters.
4. `tdata`, which specifies the gas model and starting test gas composition.
5. `surface_property.data`, which specifies solid surface properties when there are more than one solid surface type.

The first four files are always required when running LAURA but the last file is only required when there are multiple different solid surface boundaries. In this case, the ablative strip was one solid surface type while the other non-ablating parts of the model were another. After the first step, the `laura.rst` file, which contains the flowfield solution for simulation restart, is also required.

Radiation Solver Technique.

Simulated radiation results were obtained by using a stand-alone version of the HARA code provide by the code developers. The stand-alone version of HARA provides the same functionality as the HARA version contained in LAURA releases. The main benefit of using the stand-alone version is that the user can specify each of the points of a line-of-sight using the cell *i*- and *k*-index. This specification is done in the “main.90” file; if running the standard version of HARA, the points of a line-of-sight would be specified in the `hara_matlab_loc` file, which only allows radiation to be computed in one cell at a time. Additionally, the user must specify “shock tube” as the radiation mode in this file. Doing so is required since shock tube experiments require intensity directed parallel to the surface rather than towards the surface, which is normally how the radiation solver operates. This specification would take place in the `src/relax_laura.f90` file if running the standard version of HARA contained with

LAURA.

The file that governs how the simulated radiation is computed is the `hara_namelist_data` file. Normally, if the `hara_namelist_data` file is not provided, HARA will determine which radiative mechanisms to include based on species present in the flowfield [83]. The user can also manually turn on and off specific radiative mechanisms. Doing so can be potentially beneficial in determining the contribution of a specific radiative mechanism if several are being modeled simultaneously. Note that even if the `hara_namelist_data` is provided, HARA will turn on radiative mechanisms not specifically turned off by the user if it determines that there are adequate species present.

The choice of model for the population of the electric state is also controlled in this file; if not specified by the user, atomic electric states will be populated using the “CR” model while molecular electronic states will be populated using the “CR Park” model. If these models do not exist for a species, a Boltzmann distribution of the population will be used.

For simulations run in “shock tube” mode, a number of additional flags must be specified. These flags are:

1. `tube_z = 10.0`
2. `use_triangle_slit = .true.`
3. `slit_width = 0.3`

The first flag is the length of the radiating gas, which is the width of the model for 2D simulations. The next two flags define the instrument function, which assumes a triangular function. The following subsection will describe the instrument function in more detail.

Instrument Function.

The instrument function was not measured during the experimental campaigns. Therefore, determination of an appropriate slit width was accomplished by producing simulated results and comparing the Full-Width at Half-Maximum (FWHM) for a number of lines, shown in Figures 96, 97, 98, 99, 100, and 101. For the UV spectrometer, the 2048 K C-C case targeting CN violet in the near-stagnation region was used. The lines used for this case were 387.21 nm, 388.42 nm, 418.18 nm, and 419.80 nm, all of which correspond to CN violet emissions. For the vis/nIR spectrometer, it was the 1930 K case for SiC-coated C-C targeting atomic N and O in the near-stagnation region. The lines used for this case were 746.83 nm, 821.63 nm, and 824.24 nm, all of which correspond to atomic N emissions. Each of the lines examined were chosen as they were as free of contaminants as possible, enabling the best possible comparison between experimental and simulated results.

Table 14. Comparison of experimental and simulated lines for UV spectrometer. The case examined was 2048 K surface temperature for C-C targeting CN violet in the near-stagnation region.

CN violet, 387.21 nm line						CN violet, 388.42 nm line					
slit width	Max	Min	$\frac{1}{2}(\text{Max} - \text{Min})$	FWHM	$\Delta X2$	slit width	Max	Min	$\frac{1}{2}(\text{Max} - \text{Min})$	FWHM	$\Delta X2$
X2	648.23	185.61	416.92	0.54	0.00	X2	727.91	61.42	394.67	0.50	0.00
0.1 nm	843.37	218.37	530.87	0.22	-0.32	0.1 nm	921.12	97.92	509.52	0.52	0.02
0.2 nm	643.15	233.08	438.12	0.54	0.00	0.2 nm	679.66	105.76	392.71	0.52	0.02
0.25 nm	618.36	238.14	428.25	0.50	-0.04	0.25 nm	638.12	104.87	371.50	0.56	0.06
0.3 nm	577.97	243.88	410.93	0.56	0.02	0.3 nm	703.34	106.13	404.74	0.48	-0.02
0.4 nm	558.37	267.38	412.88	0.58	0.04	0.4 nm	641.27	104.37	372.82	0.60	0.10
CN violet, 418.18 nm line						CN violet, 419.80 nm line					
slit width	Max	Min	$\frac{1}{2}(\text{Max} - \text{Min})$	FWHM	$\Delta X2$	slit width	Max	Min	$\frac{1}{2}(\text{Max} - \text{Min})$	FWHM	$\Delta X2$
X2	87.17	47.27	67.22	0.52	0.00	X2	78.69	35.50	57.10	0.74	0.00
0.1 nm	129.35	54.52	91.94	0.32	-0.20	0.1 nm	104.51	34.42	69.47	0.42	-0.32
0.2 nm	111.49	53.79	82.64	0.46	-0.06	0.2 nm	91.25	40.05	65.65	0.56	-0.18
0.25 nm	104.72	55.60	80.16	0.50	-0.02	0.25 nm	90.37	39.76	65.07	0.60	-0.14
0.3 nm	99.37	55.09	77.23	0.54	0.02	0.3 nm	81.82	40.17	61.00	0.78	0.04
0.4 nm	97.61	55.31	76.46	0.68	0.16	0.4 nm	76.01	41.97	58.99	0.86	0.12

Table 15. Comparison of experimental and simulated lines for vis/nIR spectrometer. The case examined was 1930 K surface temperature for SiC-coated C-C targeting atomic N and O in the near-stagnation region.

Atomic N, 746.83 nm line					Atomic N, 821.63 nm line					Atomic N, 824.24 nm line				
slit width	Max	$\frac{1}{2} \text{Max}$	FWHM	$\Delta X2$	slit width	Max	$\frac{1}{2} \text{Max}$	FWHM	$\Delta X2$	slit width	Max	$\frac{1}{2} \text{Max}$	FWHM	$\Delta X2$
X2	6.00	3.00	0.26	0.00	X2	5.62	2.81	0.33	0.00	X2	4.06	2.03	0.26	0
0.1 nm	9.64	4.82	0.12	-0.14	0.1 nm	18.07	9.035	0.11	-0.15	0.1 nm	7.57	3.785	0.11	-0.15
0.2 nm	4.96	2.48	0.21	-0.05	0.2 nm	9.3	4.65	0.2	-0.06	0.2 nm	3.9	1.95	0.22	-0.04
0.25 nm	3.99	1.995	0.26	0.00	0.25 nm	7.47	3.735	0.26	0.00	0.25 nm	3.14	1.57	0.25	-0.01
0.3 nm	3.34	1.67	0.32	0.06	0.3 nm	6.26	3.13	0.3	0.04	0.3 nm	2.63	1.315	0.31	0.05
0.4 nm	2.53	1.265	0.44	0.18	0.4 nm	4.72	2.36	0.41	0.15	0.4 nm	1.99	0.995	0.42	0.16

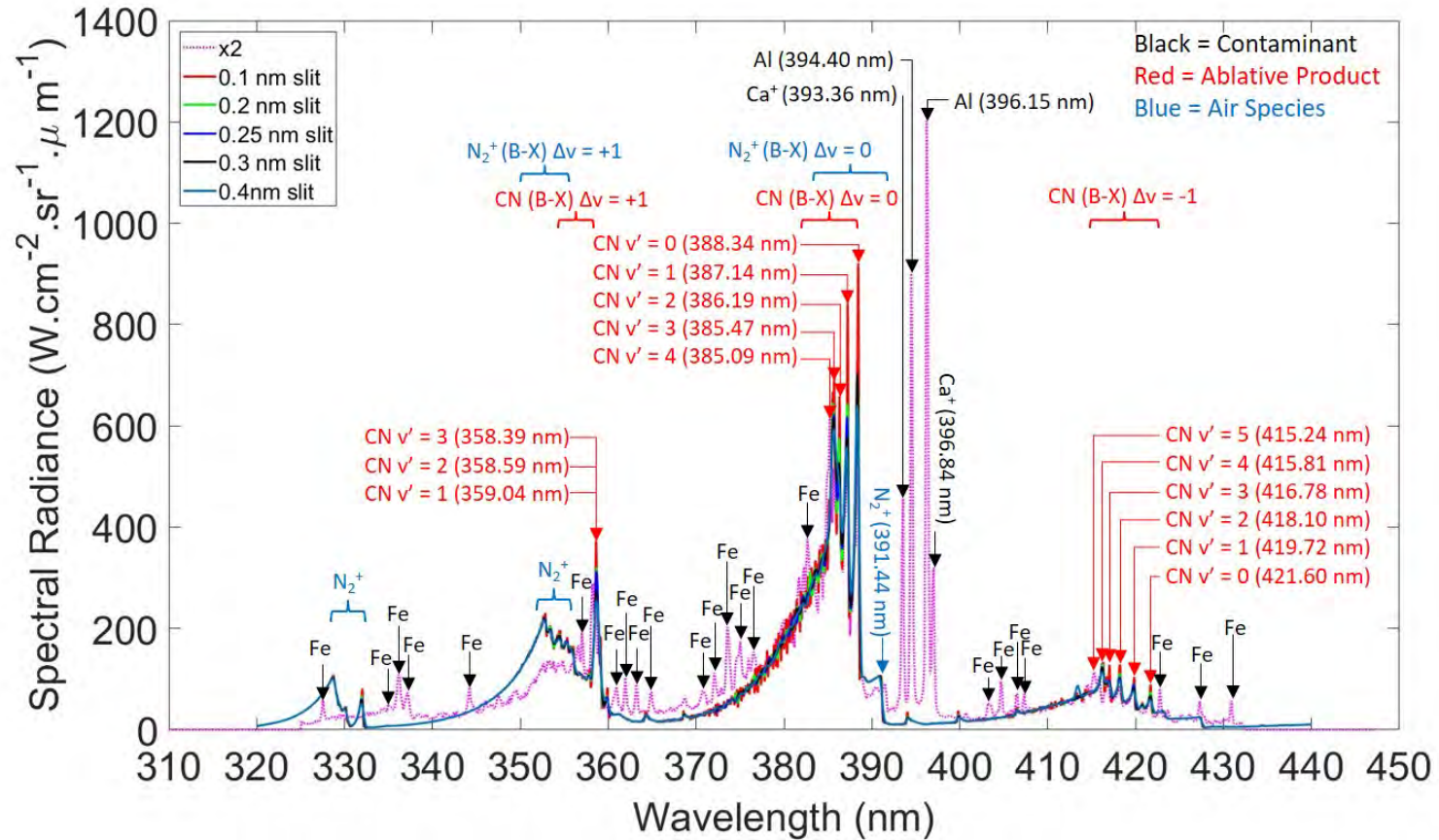


Figure 96. Comparison of experimental and simulated results for various slit widths, UV spectrometer. The case used for this study was the 2048 K case for C-C in the near-stagnation region targeting CN violet. All simulated results were computed using the CR Park model to populate the electronic states.

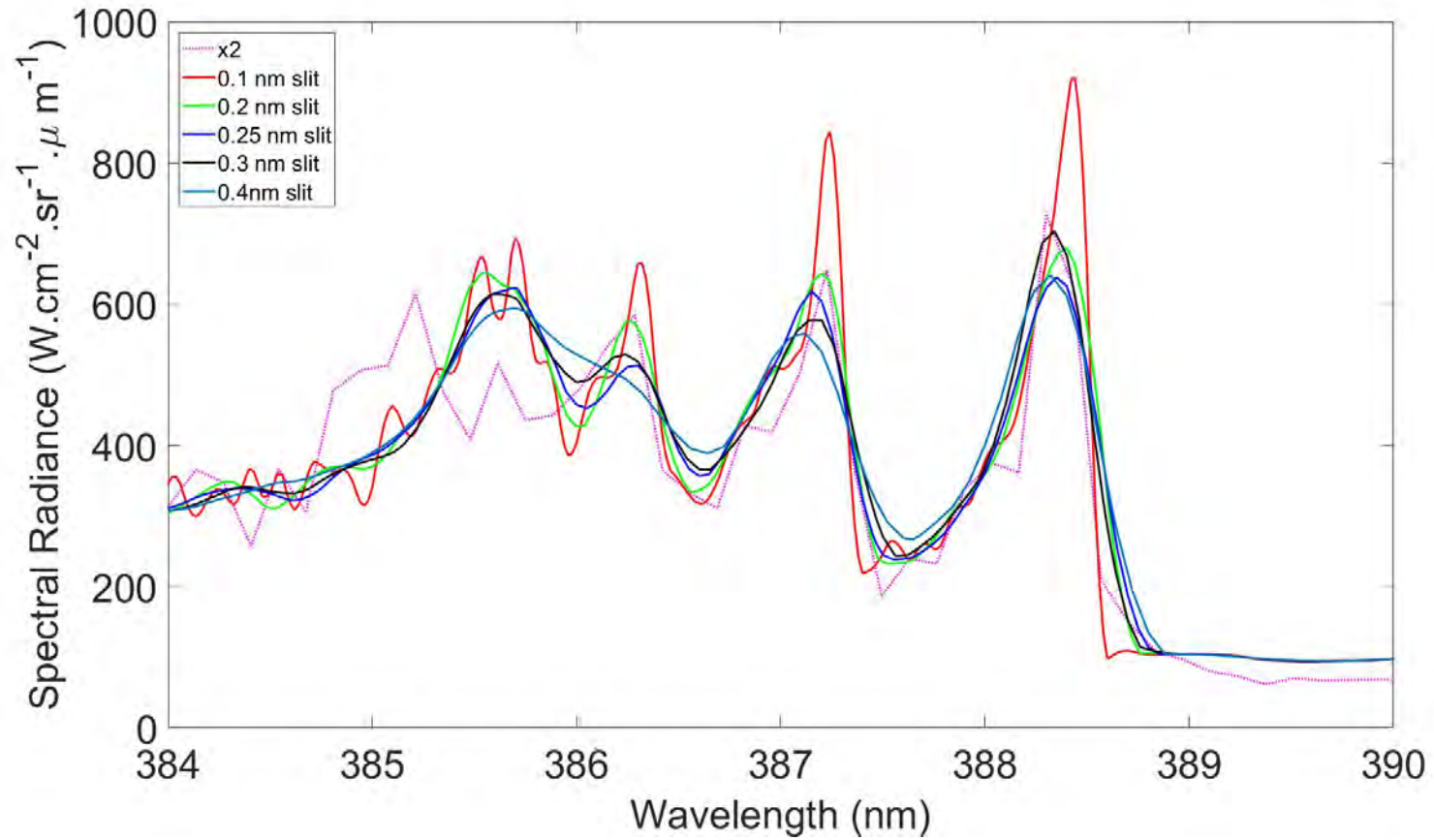


Figure 97. Comparison of experimental and simulated results for various slit widths, UV spectrometer, zoomed in on 384 to 390 nm. The case used for this study was the 2048 K case for C-C in the near-stagnation region targeting CN violet. All simulated results were computed using the CR Park model to populate the electronic states.

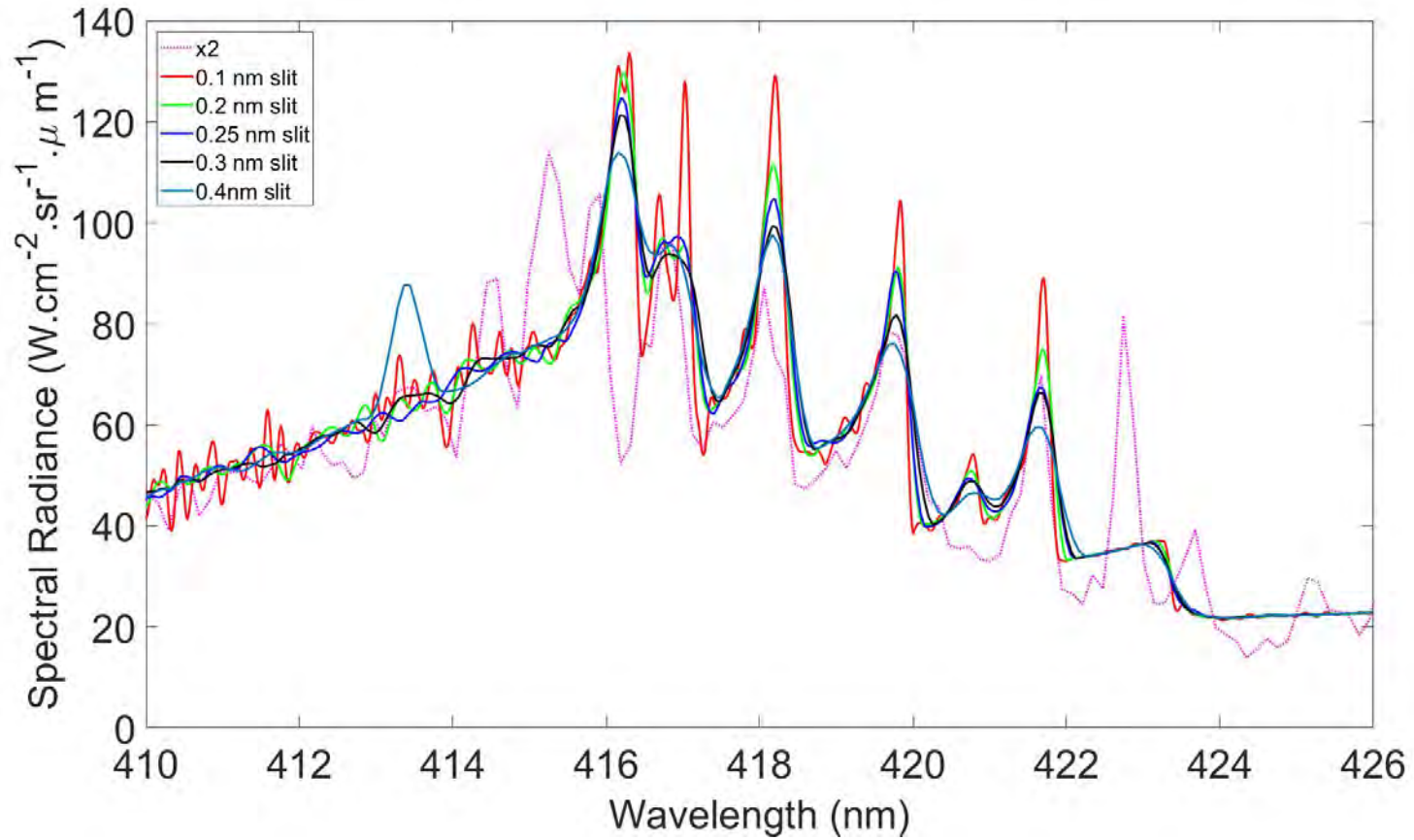


Figure 98. Comparison of experimental and simulated results for various slit widths, UV spectrometer, zoomed in on 410 to 426 nm. The case used for this study was the 2048 K case for C-C in the near-stagnation region targeting CN violet. All simulated results were computed using the CR Park model to populate the electronic states.

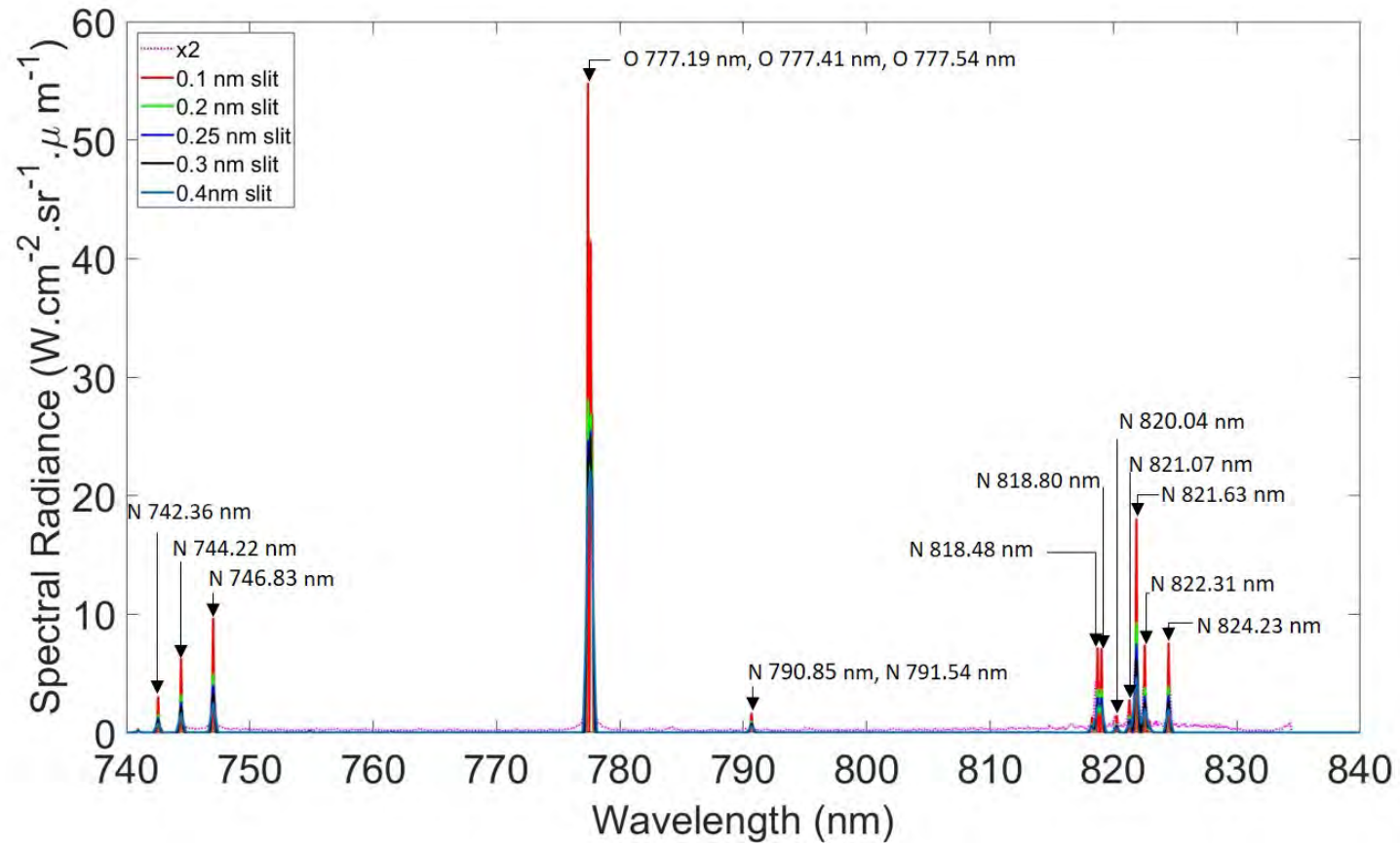


Figure 99. Comparison of experimental and simulated results for various slit widths, vis/nIR spectrometer. The case used for this study was the 1930 K case for SiC-coated C-C in the near-stagnation region targeting atomic N and O. All simulated results were computed using the Gally model to populate the electronic states.

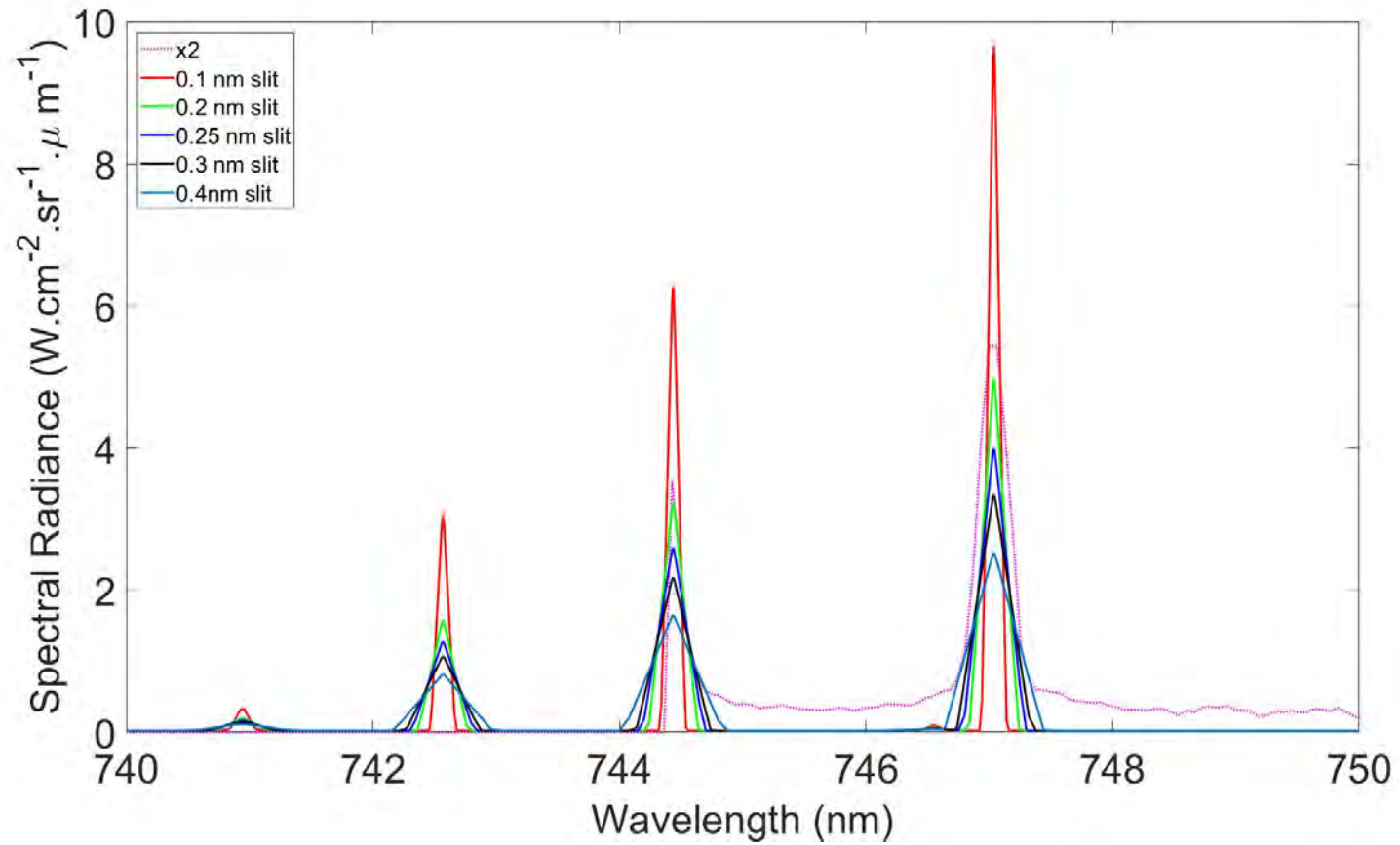


Figure 100. Comparison of experimental and simulated results for various slit widths, vis/nIR spectrometer, zoomed in to 740 to 750 nm. The case used for this study was the 1930 K case for SiC-coated C-C in the near-stagnation region targeting atomic N and O. All simulated results were computed using the Gally model to populate the electronic states.

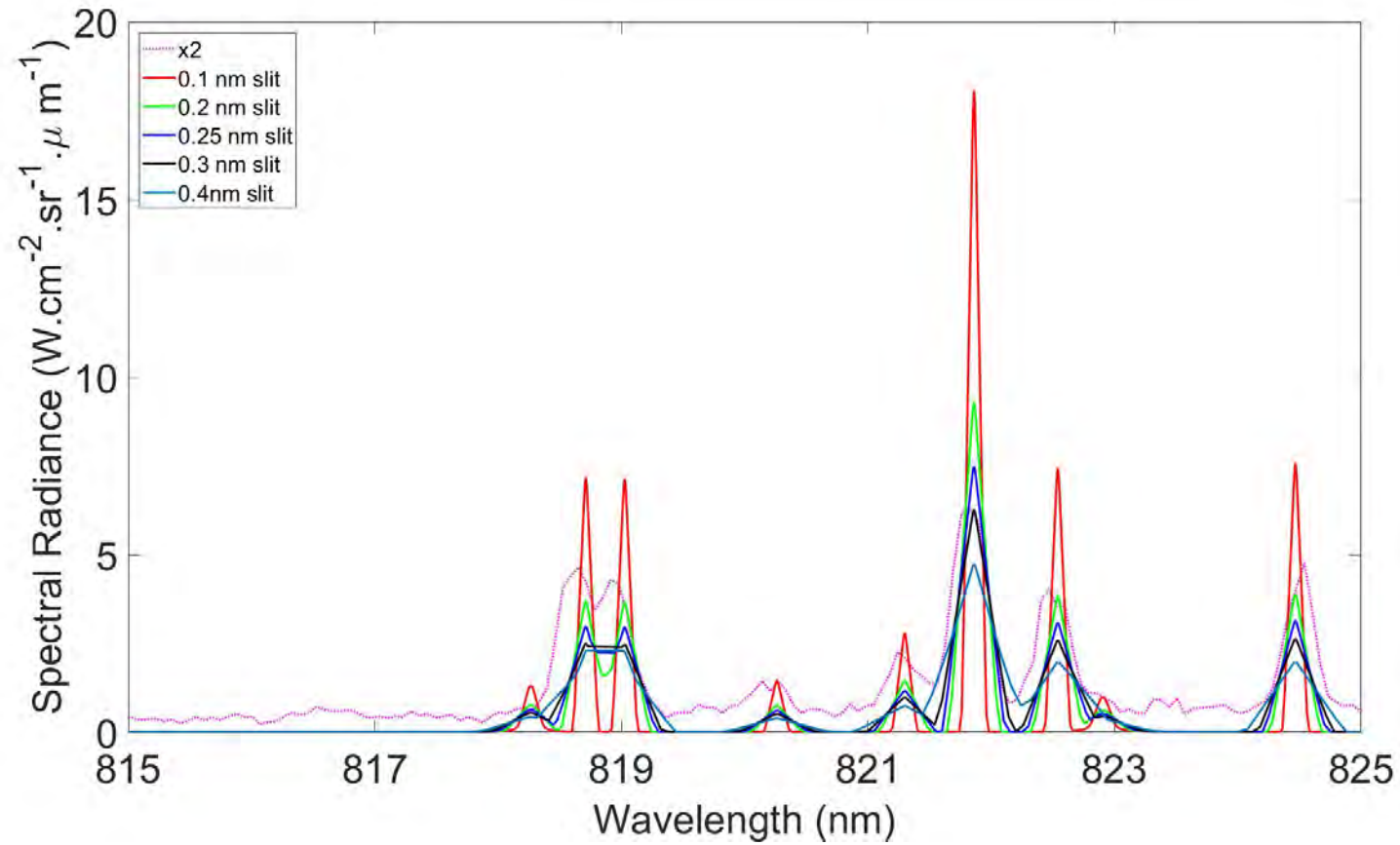


Figure 101. Comparison of experimental and simulated results for various slit widths, vis/nIR spectrometer, zoomed in to 815 to 825 nm. The case used for this study was the 1930 K case for SiC-coated C-C in the near-stagnation region targeting atomic N and O. All simulated results were computed using the Gally model to populate the electronic states.

Comparison of experimental and simulated results obtained using different slit widths, shown in Tables 14 and 15, indicate that a 0.3 nm slit with for a triangular function agrees fairly well with experimental results for the UV spectrometer while a 0.25 nm slit provides the best comparison for the vis/nIR spectrometer. These results are consistent with past researchers [46, 146]. Lewis found that the instrument function could be reproduced by a 0.3 nm Gaussian function [146]. These experimental results were obtained using the UV spectrometer with a 600 g/mm grating and an entrance slit width of 50 μm ; these same parameters were used during both experimental campaigns.

In addition to allowing the user to specify which radiative mechanisms to include, a lower and upper wavelength limit can also be specified in this input file. For these simulations, each radiative mechanism was modeled individually over the wavelength regions corresponding to those of the experiments. This approach significantly reduced the time required for the radiation simulation; most simulations were complete within a few minutes. Additionally, this input file allows the user to specify whether to model the radiation using the Smeared Rotational Band (SRB) approach or the line-by-line (LBL) approach. For this work, all radiation simulations were conducted using the LBL approach in order to provide the best possible comparison between simulated and experimental results.

To replicate the line-of-sight in the near-stagnation region, the radiation calculations were run at 13 points. In the expansion region 0.75 mm above the model, they were run at 21 points. A summary of these points is shown in Tables 16 and 17. The spacing between the points is higher in the expansion region but the cells are significantly larger compared to the near-stagnation region. The first point in each case corresponds to the shock and is referenced to the stagnation point of the model. The values shown in these tables were found using the “probe” feature in Tecplot[®],

Table 16. Points used to replicate spectrometer line-of-sight in the near-stagnation region.

Point	x-location (mm)	Block	i-index	j-index	k-index
1	2.8	2	20	1	150
2	3.0	2	20	1	131
3	3.2	2	21	1	118
4	3.4	2	21	1	111
5	3.6	2	22	1	105
6	3.8	2	22	1	101
7	4.0	2	23	1	97
8	4.2	2	23	1	93
9	4.4	2	23	1	90
10	4.6	2	24	1	86
11	4.8	2	24	1	83
12	5.0	2	25	1	78
13	5.2	2	25	1	69

Table 17. Points used to replicate spectrometer line-of-sight in the expansion region.

Point	x-location (mm)	Block	i-index	j-index	k-index
1	12.5	3	44	1	137
2	13	3	45	1	119
3	13.5	3	46	1	111
4	14	3	48	1	105
5	14.5	3	50	1	101
6	15	3	51	1	96
7	15.5	3	53	1	93
8	16	3	54	1	89
9	16.5	3	56	1	86
10	17	3	58	1	83
11	17.5	3	60	1	80
12	18	3	62	1	77
13	18.5	3	64	1	75
14	19	4	2	1	74
15	19.5	4	4	1	73
16	20	4	6	1	73
17	20.5	4	8	1	72
18	21	4	10	1	71
19	21.5	4	12	1	71
20	22	4	14	1	70
21	22.5	4	16	1	70

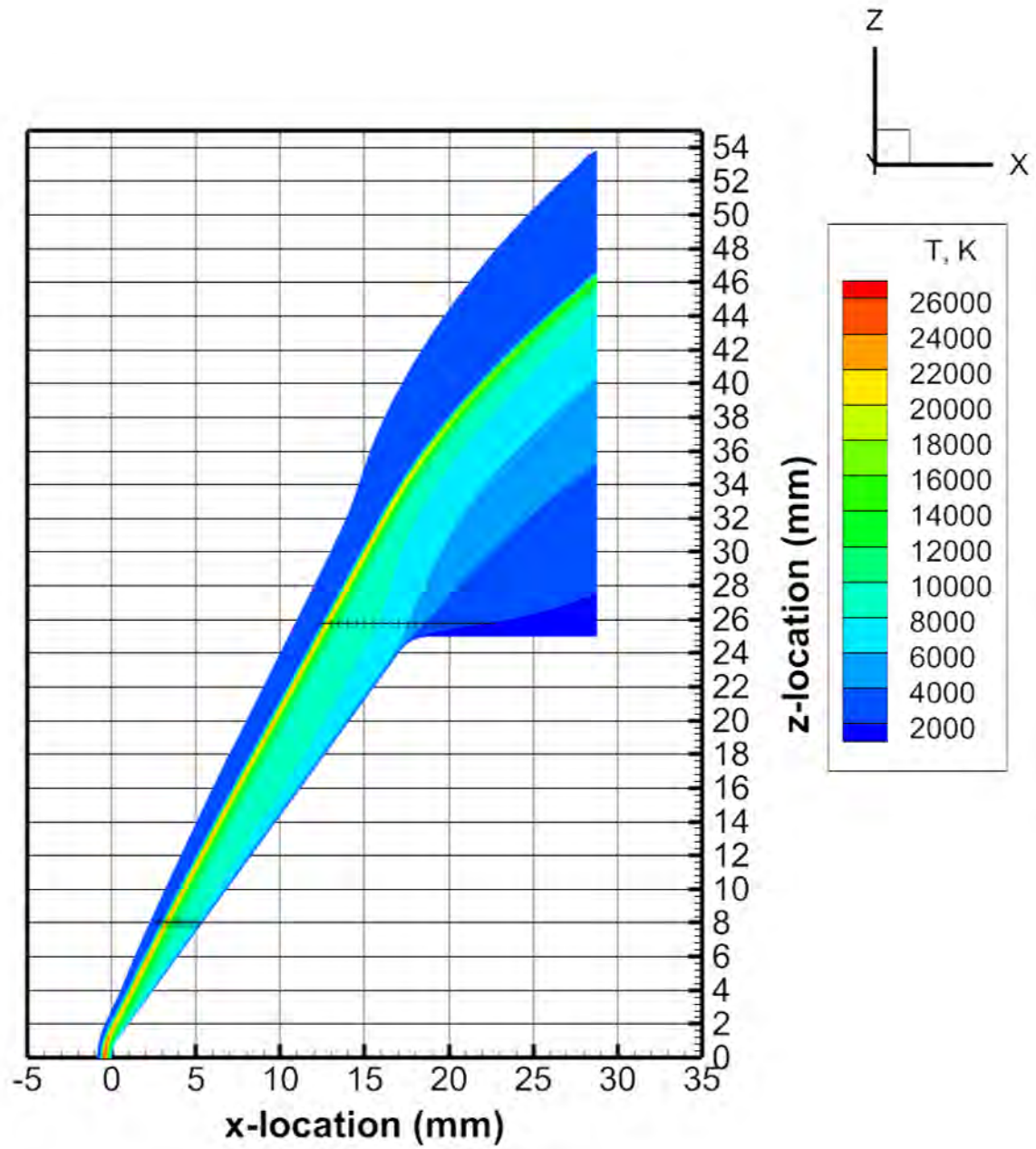


Figure 102. Cell index mapping in Tecplot. Cells used to replicate spectrometer line-of-sight are indicated with a black cross.

shown in Figure 102.

6.3 Results

The following subsections will present comparisons between simulated and experimental results. Note that only cases that had surface temperatures measured during the X2 experiments were simulated. Throughout this chapter, results obtained with the finite-rate ablation model for C-C will be referred to as “FR-CC”, results obtained with the equilibrium-char ablation model for C-C will be referred to as “EC-CC”, and results obtained with the equilibrium-char ablation model for SiC-coated C-C will be referred to as “EC-SiC”. Similarly, experimental results will be denoted by “X2” along with the surface temperature.

CN violet.

Figure 103 shows experimental and simulated radiation results for the 2048 K case for C-C targeting CN violet in the near-stagnation region. The results obtained from flowfield solutions using the finite-rate ablation model are in excellent agreement with experimental results. Simulated CN violet emissions are within about 5% of experimental values while results obtained using the equilibrium-char ablation model are about 40% less intense than the experimental results.

The only difference between the two sets of simulated results is the ablation model, therefore it is likely that the equilibrium-char ablation model is underpredicting the production of CN. This claim can be confirmed by plotting the mass fraction of CN along the $z = 8$ mm slice, corresponding to the near-stagnation line-of-sight, for results obtained with both ablation models, shown in Figure 105. For this case, the equilibrium-char ablation model is predicting up to 50% less CN than the finite-rate model. Since simulated results for SiC-coated C-C can be obtained using only the equilibrium-char ablation model, it is possible that simulated results may underpredict intensity by a similar value.

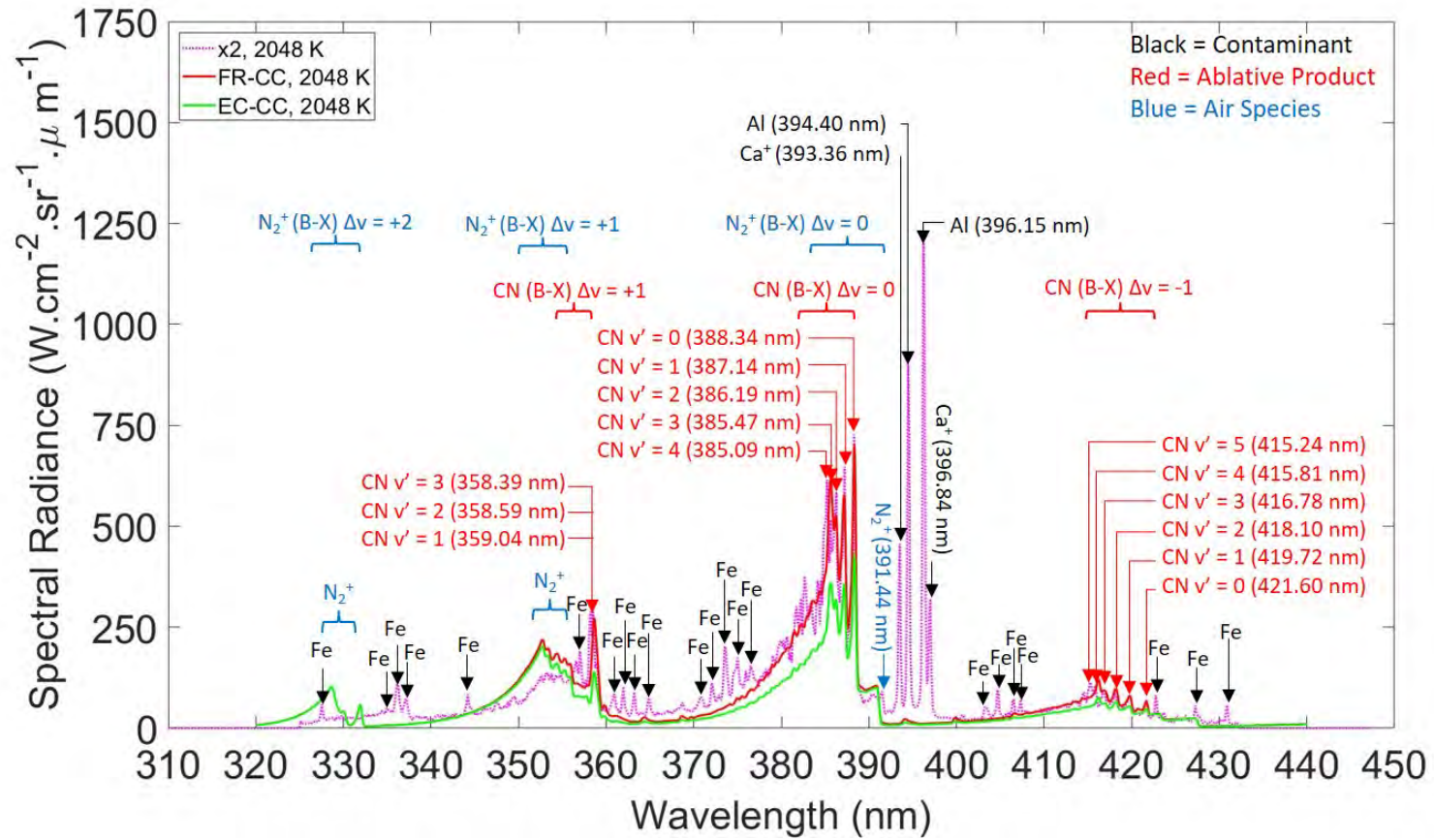


Figure 103. Experimental and simulated results for the 2048 K case for C-C targeting CN violet in the near-stagnation region.

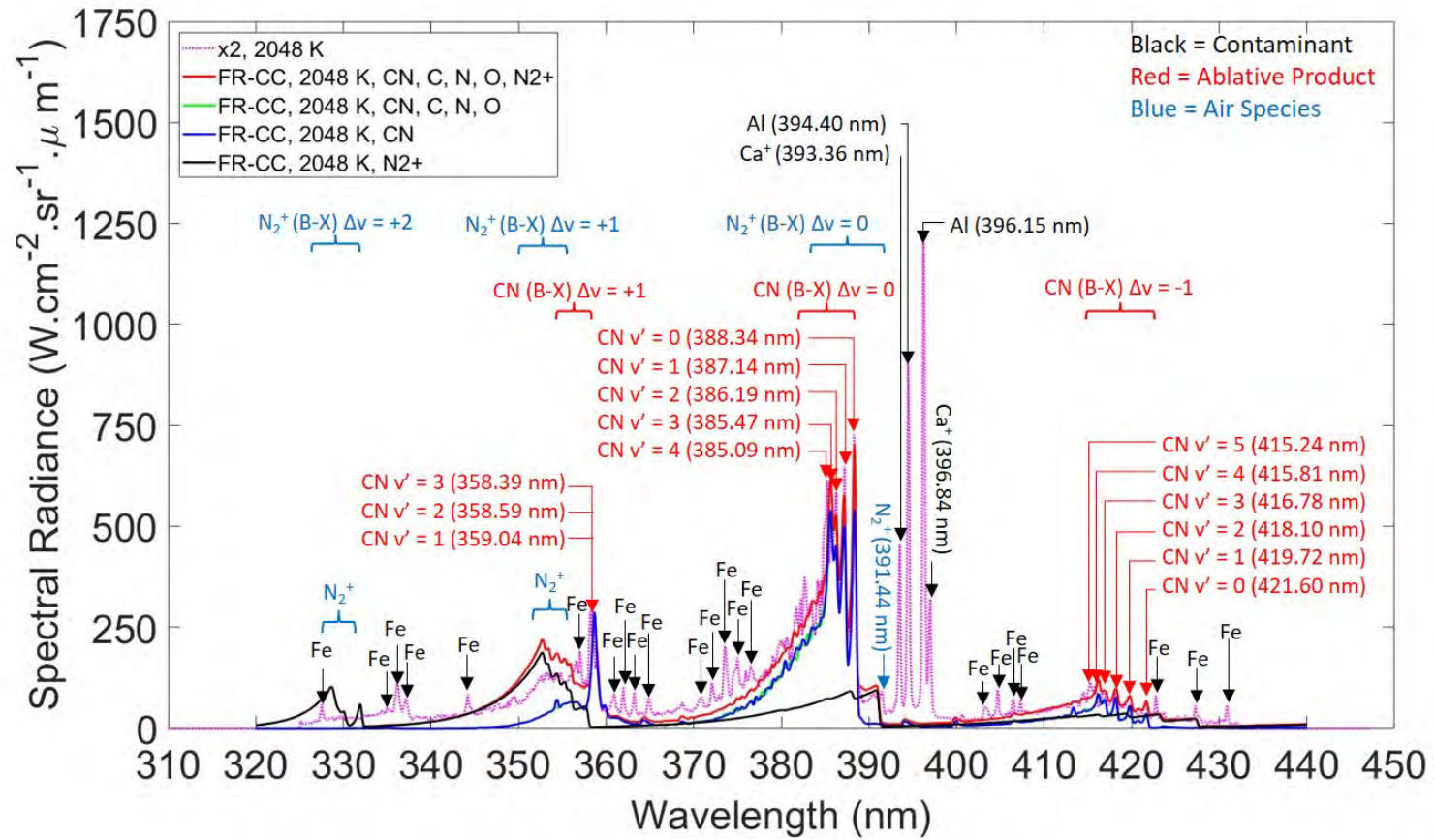


Figure 104. Experimental and simulated results for the 2048 K case for C-C targeting CN violet in the near-stagnation region broken down by species.

Both sets of simulated results are showing intensity values significantly higher than experimental values between 320 and 330 nm and 350 and 360 nm. These overpredictions are believed to be the result of the radiation solver overpredicting radiation of N_2^+ ; this theory can be confirmed in Figure 104 where the various species contributing to radiation are modeled individually, which is one the benefits of running simulated radiation results. The overprediction of N_2^+ radiation suggests that the radiation code is overpopulating the excited state of this transition. Another possibility is that the LAURA code is overpredicting the production of N_2^+ , which in turn leads to higher population in the excited states; the fact that experimental and simulated N_2^+ radiation agree in some wavelength regions but not others suggest that this is less likely.

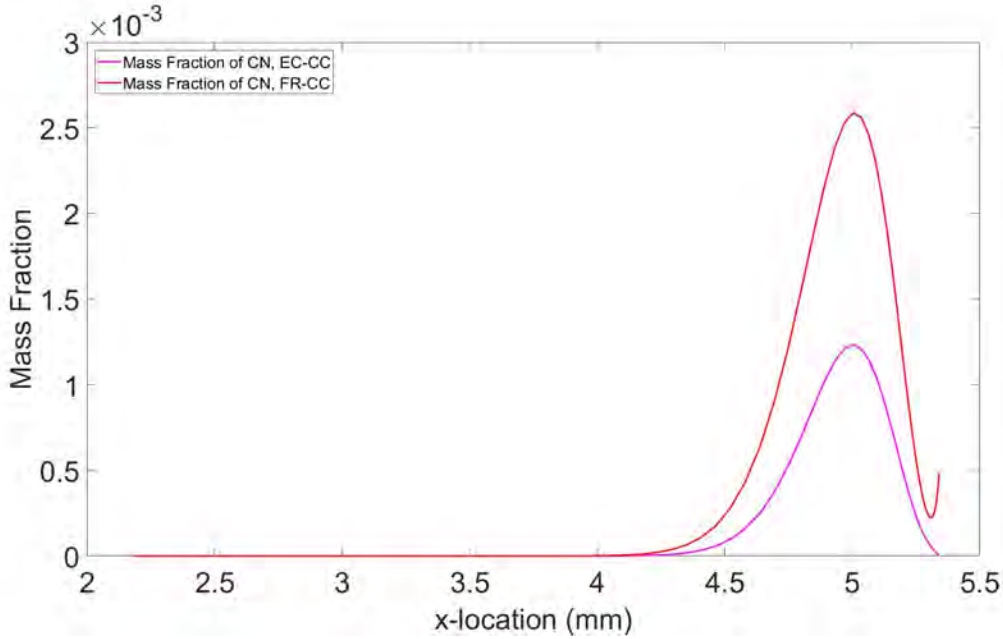


Figure 105. Mass Fraction of CN along the $z = 8$ mm slice, corresponding to the near-stagnation line-of-sight, for the equilibrium-char and finite-rate ablation models for the 2048 K case for C-C.

Figure 106 shows experimental and simulated radiation results for the 2499 K case for C-C targeting CN violet in the expansion region. Similar to the last case, simulated results were obtained using both the finite-rate and equilibrium-char ablation models.

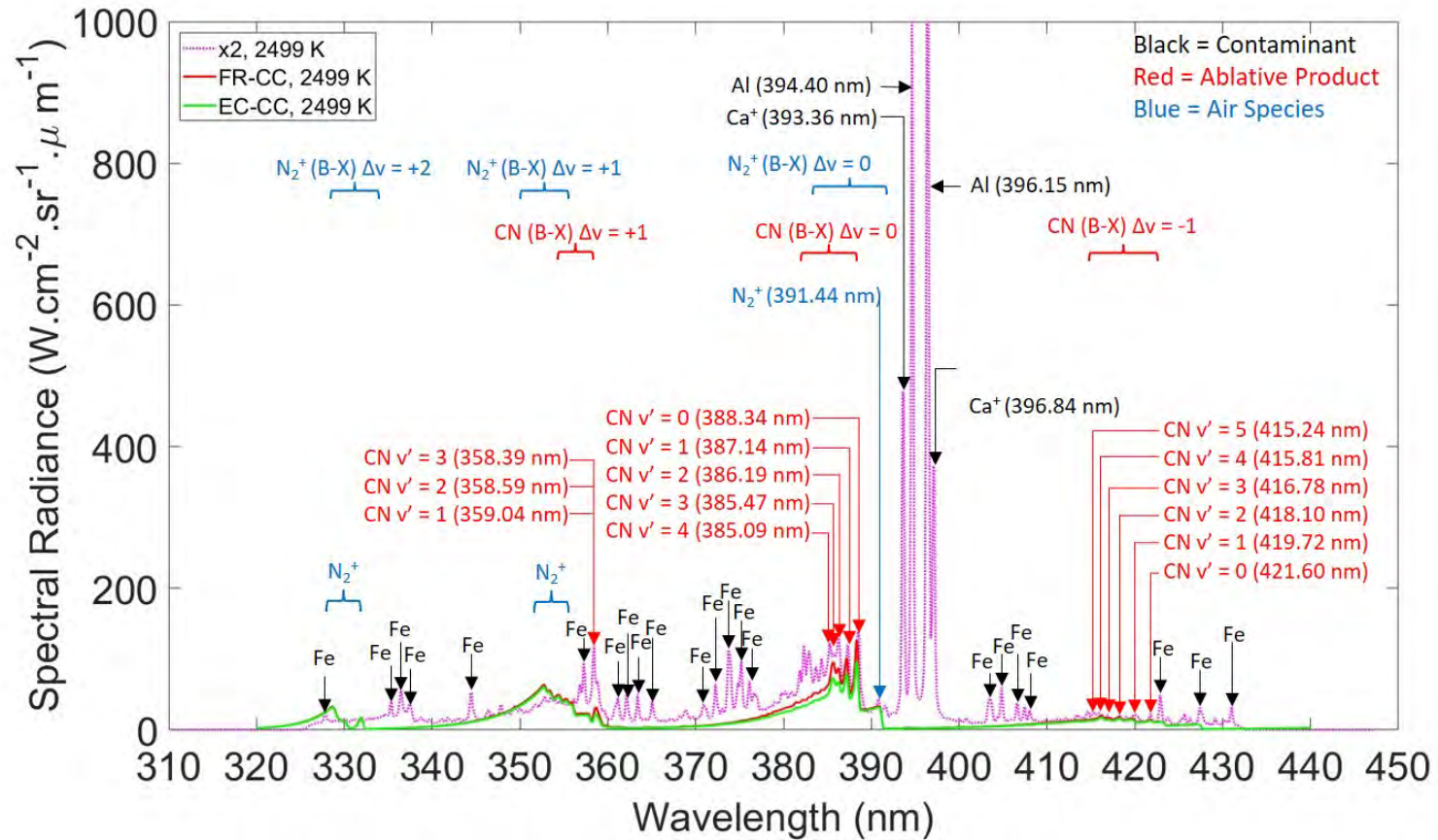


Figure 106. Experimental and simulated results for the 2499 K case for C-C targeting CN violet in the expansion region.

The finite-rate model again yield better results, underestimating experimental results by approximately 25% compared to 40% for the equilibrium-char model. The difference in CN mass fraction is not as drastic in this case, as shown in Figure 107, however the equilibrium-char ablation model is still leading to approximately 30% less CN. There again appears to be an overestimate of N_2^+ radiation, although it is not as pronounced as in the near-stagnation region.

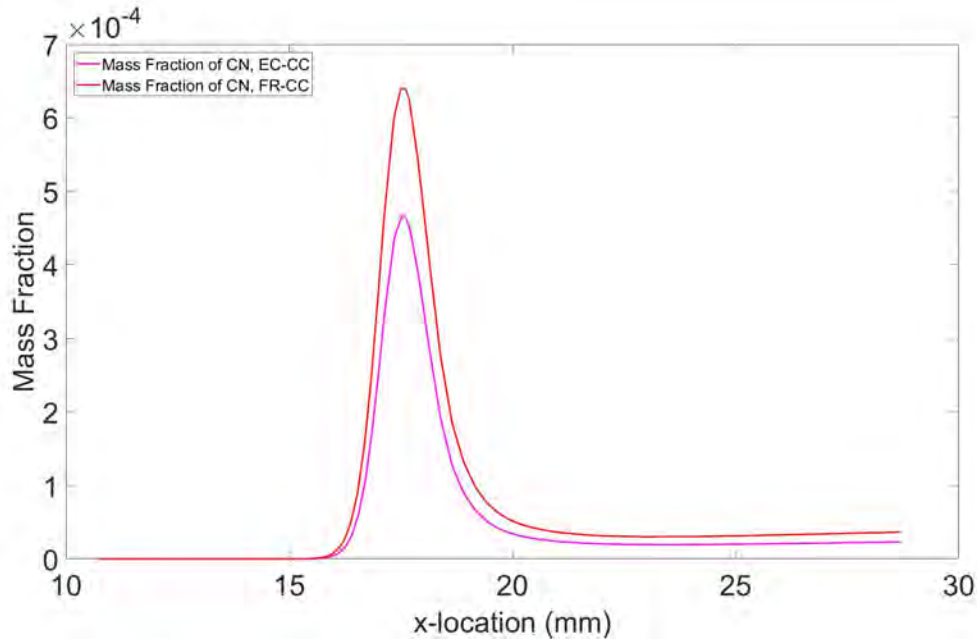


Figure 107. Mass Fraction of CN along the $z = 25.75$ mm slice, corresponding to the expansion region line-of-sight, for the equilibrium-char and finite-rate ablation models for the 2499 K case for C-C.

Figure 108 and 109 show experimental and simulated radiation results for the 2005 K and 2439 K cases, respectively, for SiC-coated C-C targeting CN violet in the near-stagnation region. The simulated results compare surprisingly well to the experimental results. The simulated results for CN violet for the 2005 K case actually overpredict experimental values by about 15% while the 2439 K case overpredicts by 5%. This overprediction is potentially explained by the fact that simulated N_2^+ radiation has repeatedly been overpredicted. The contribution of N_2^+ radiation in the 370 to 390 nm was observed in Figure 104, although the intensity of CN radiation was

far greater. In this case, the intensity in this wavelength region is about 1/3 that of the 2048 K case for C-C in the near-stagnation region, making the overprediction of N_2^+ radiation much more profound. If N_2^+ is not considered in the simulated radiation results, the result is an underprediction of approximately 40% in both cases, shown in Figures 110 and 111. Note that this result is in line with the difference between the finite-rate and equilibrium-char results for C-C.

Figure 108 also offers insight into the modeling of atomic Si using Boltzmann and non-Boltzmann (in this case, “Gally”) models. The Boltzmann model significantly overpredicts the intensity of the 390.55 nm Si line, which is to be expected, while this line is not discernible over the overprediction of the 391.44 nm N_2^+ line using the Gally model.

Similarly, Figures 112 and 113 show experimental and simulated radiation results for the 2077 K and 2435 K cases, respectively, for SiC-coated C-C targeting CN violet in the expansion region. In both cases, the simulated results drastically underpredict experimental results; the underprediction is roughly an order of magnitude for the 2077 K case while it is closer to 70% for the 2435 K. One clear observation from these images is that simulated N_2^+ radiation is significantly lower than in the stagnation region, which may be a main reason why the CN radiation, particularly in the 384 to 389 nm region, is so much lower; the potential underprediction of CN by the equilibrium-char ablation model is another.

It was thought that perhaps using a Boltzmann distribution to populate the electronic states for the molecular species (i.e. CN and N_2^+) may yield results that are more in line with experimental results for these two cases. Figure 114 shows such results for the 2435 K case. Simulated radiation results computed using a Boltzmann distribution to populate the electronic state of the molecular species improves the comparison between experimental and simulated results slightly; rather than under-

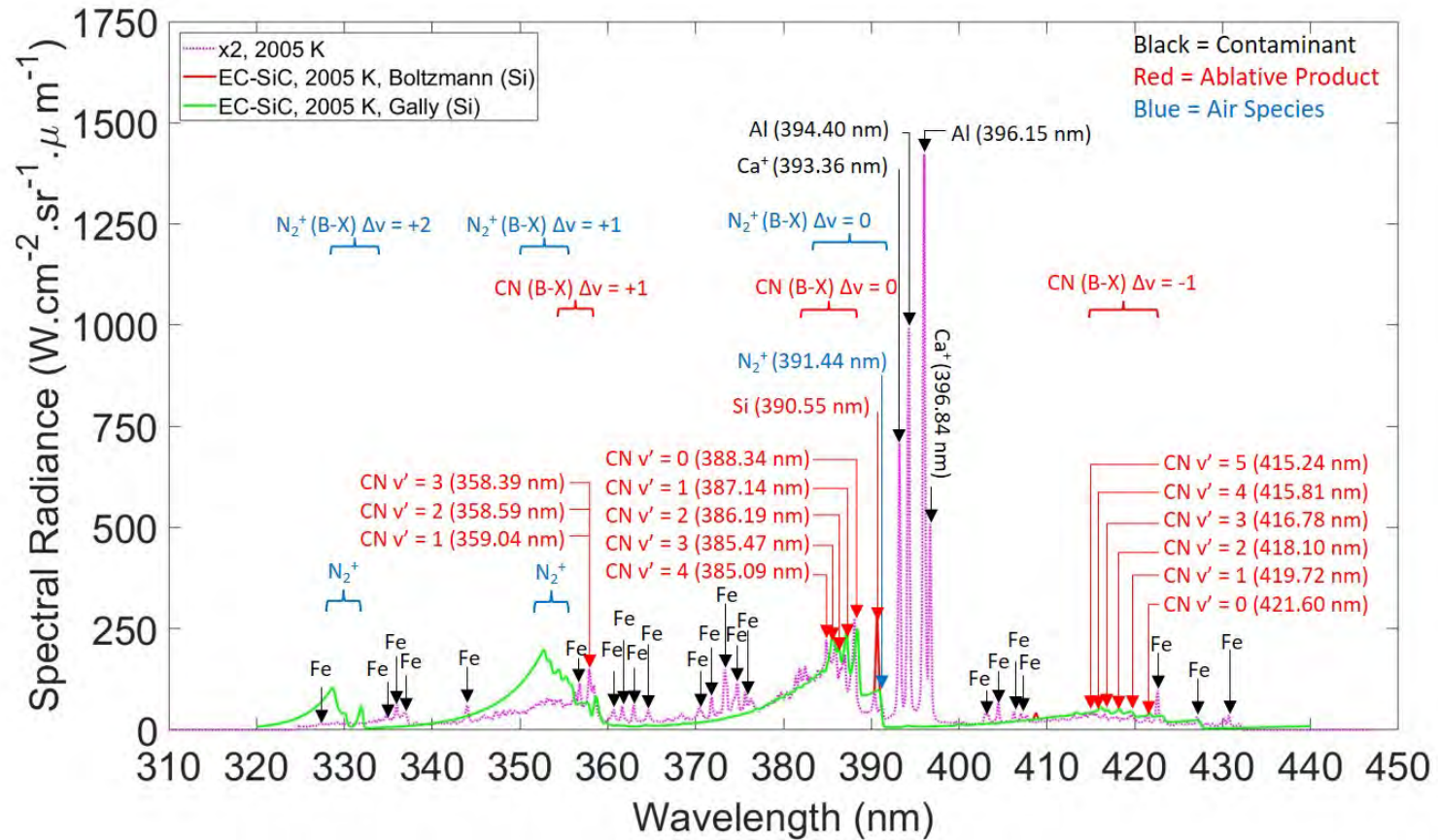


Figure 108. Experimental and simulated results for the 2005 K case for SiC-coated C-C targeting CN violet in the near-stagnation region.

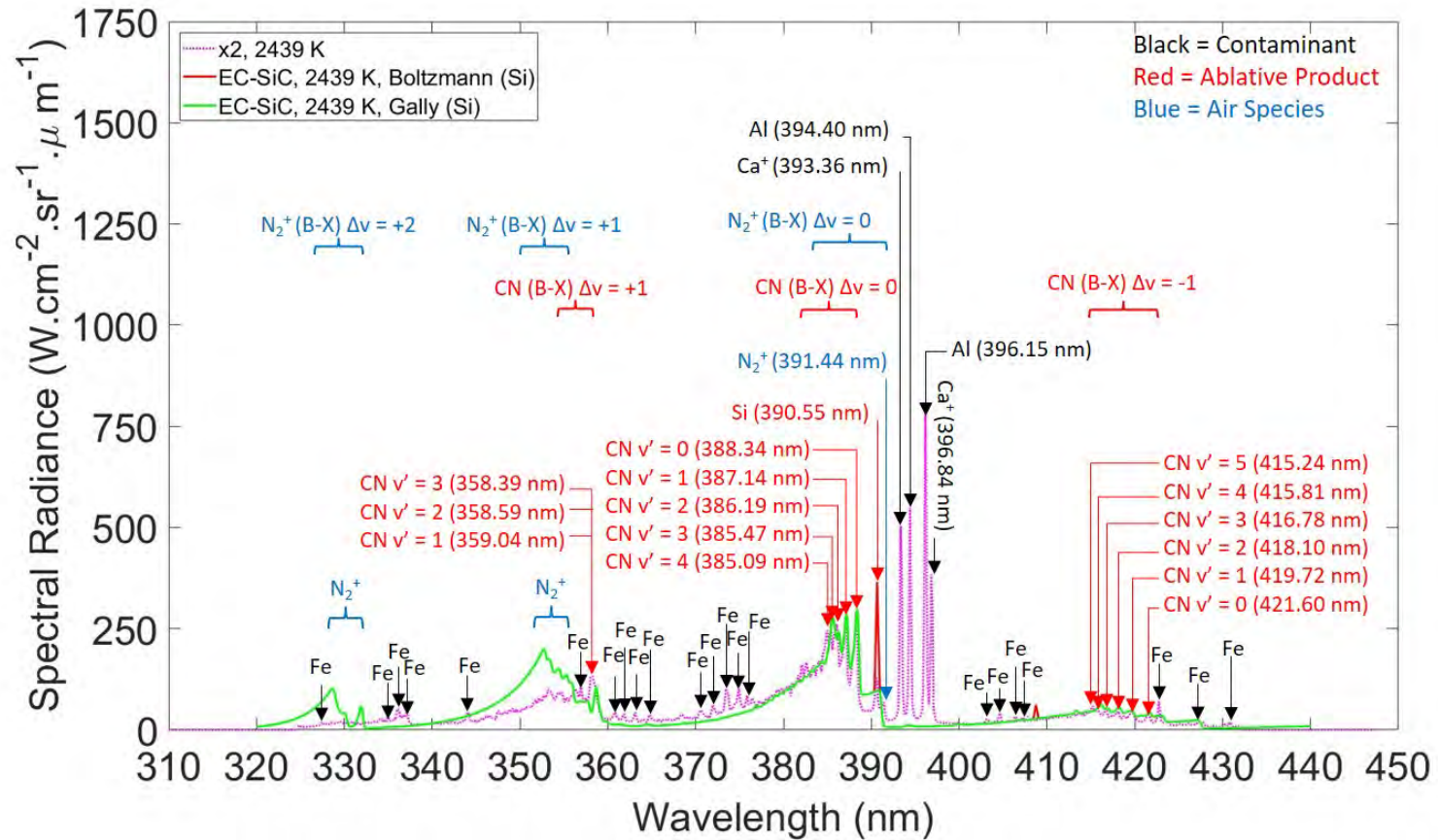


Figure 109. Experimental and simulated results for the 2439 K case for SiC-coated C-C targeting CN violet in the near-stagnation region.

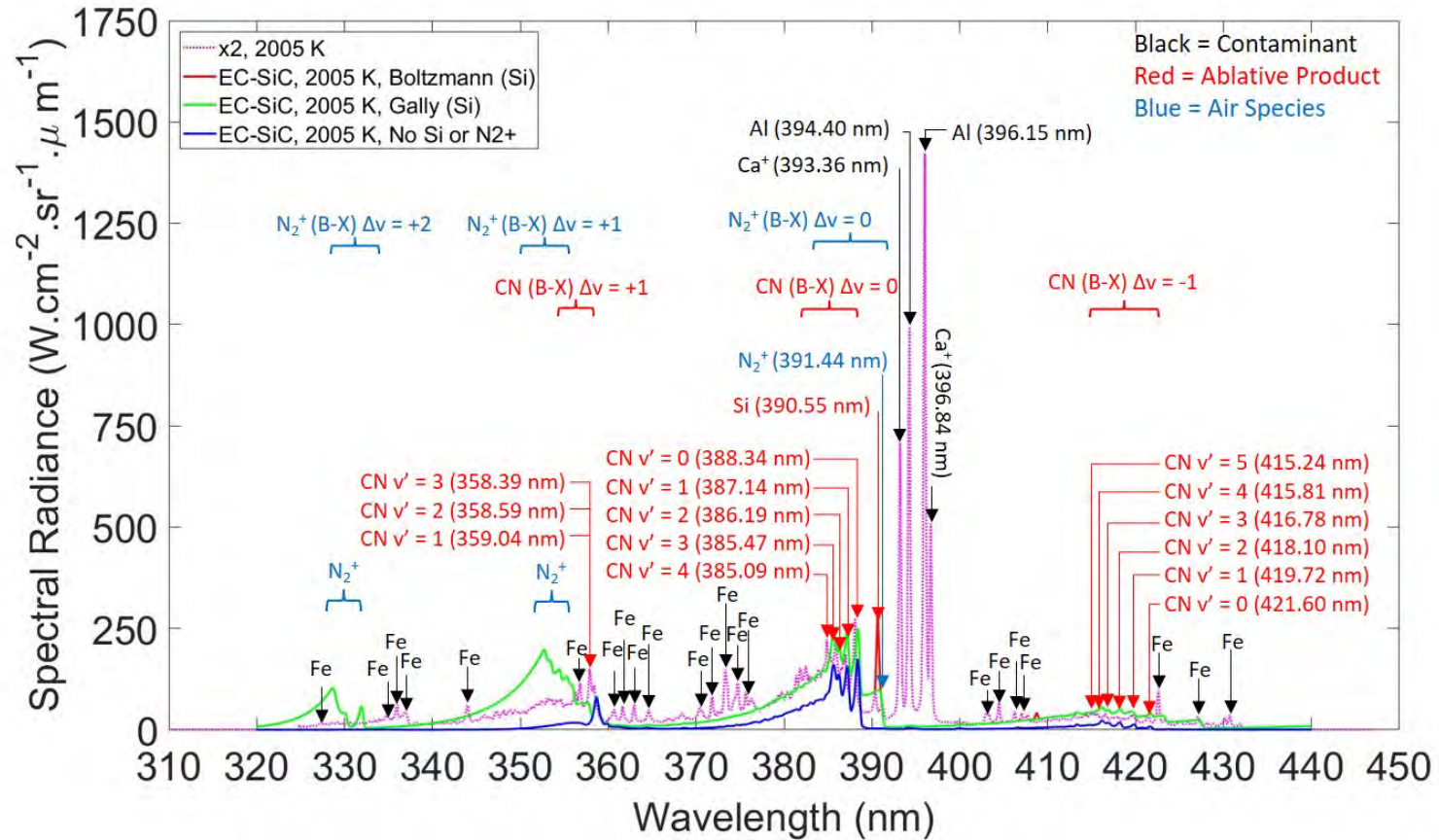


Figure 110. Experimental and simulated results for the 2005 K case for SiC-coated C-C targeting CN violet in the near-stagnation region with and without N_2^+ and atomic Si.

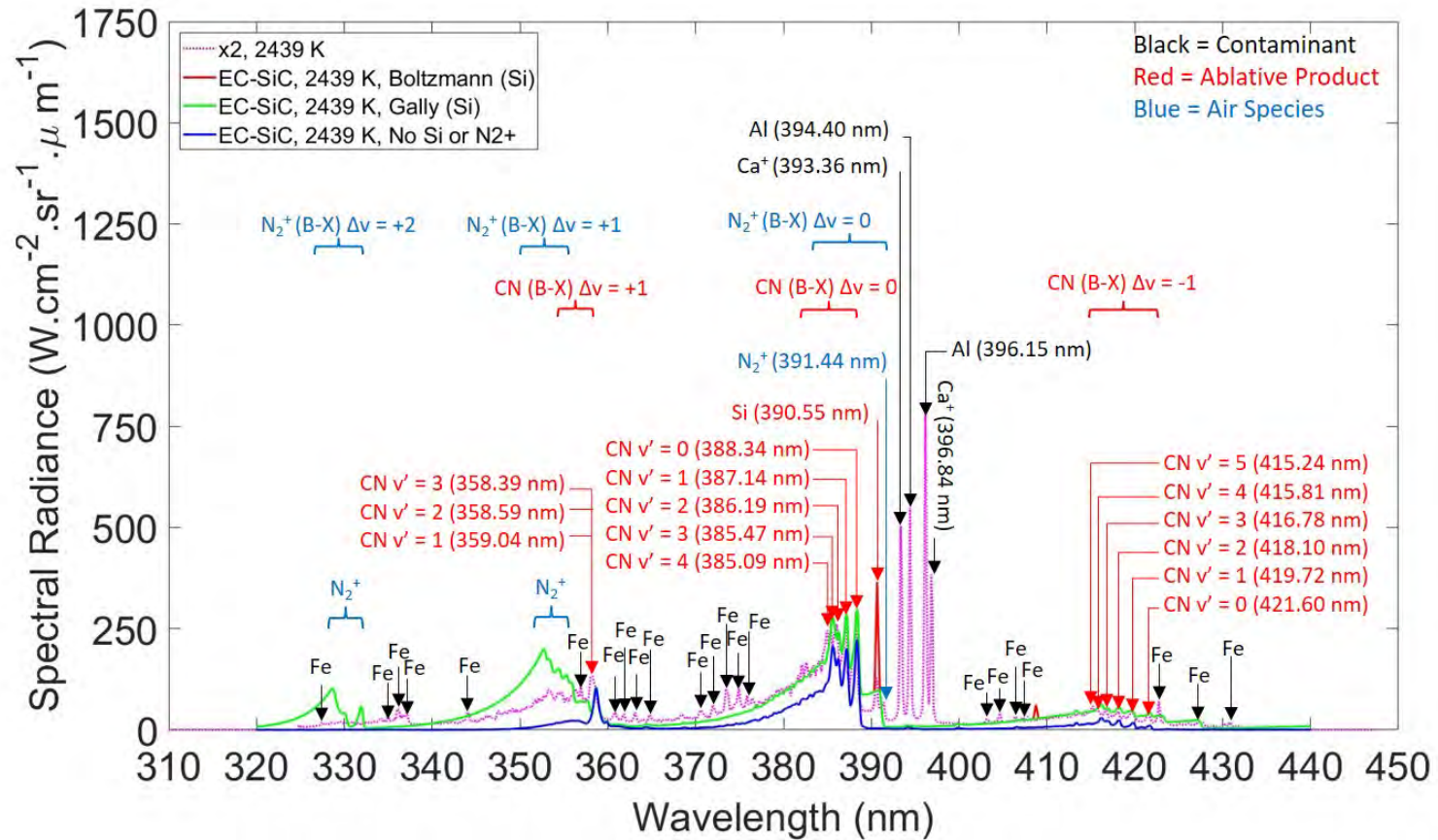


Figure 111. Experimental and simulated results for the 2439 K case for SiC-coated C-C targeting CN violet in the near-stagnation region with and without N_2^+ and atomic Si.

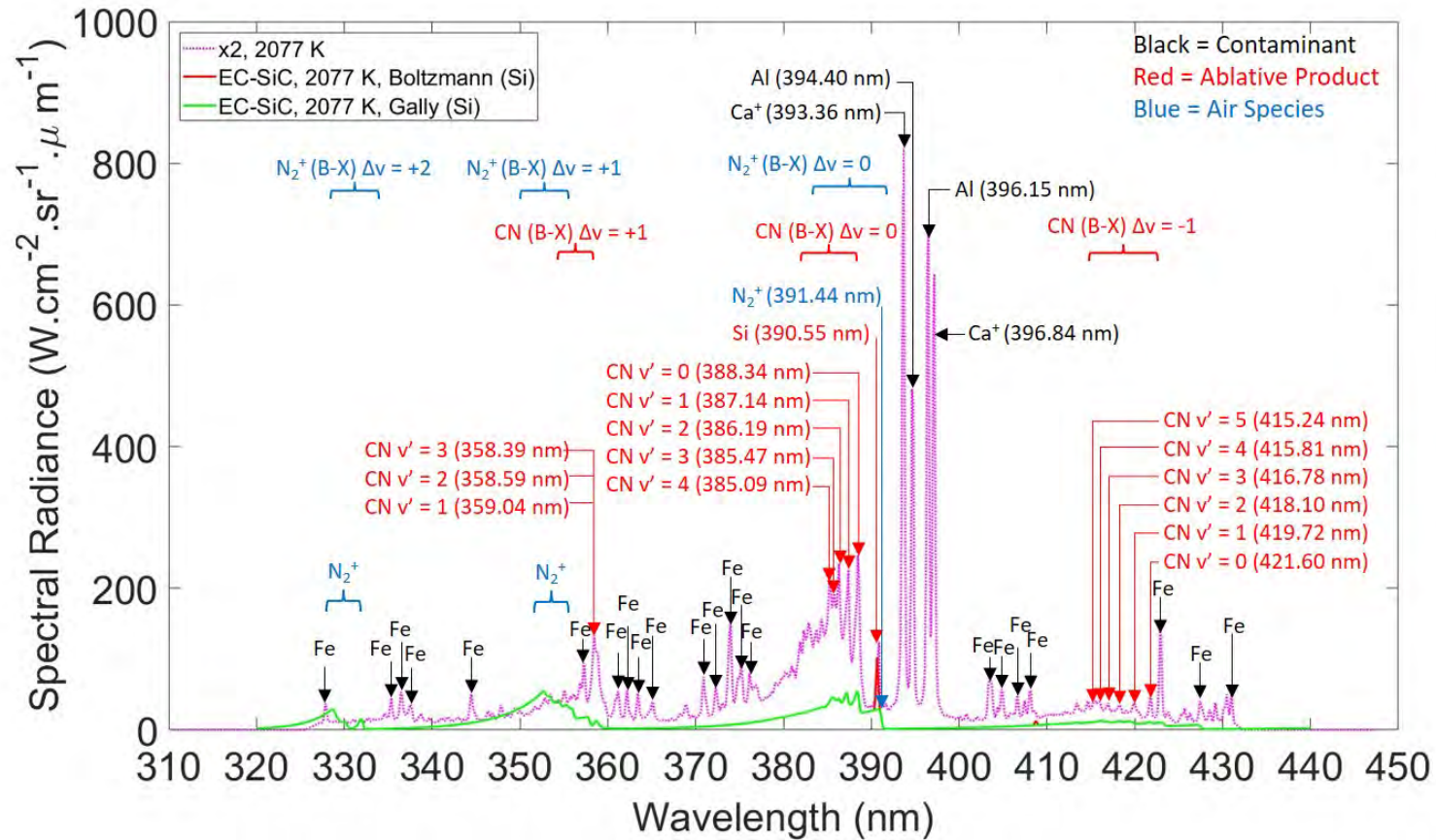


Figure 112. Experimental and simulated results for the 2077 K case for SiC-coated C-C targeting CN violet in the expansion region.

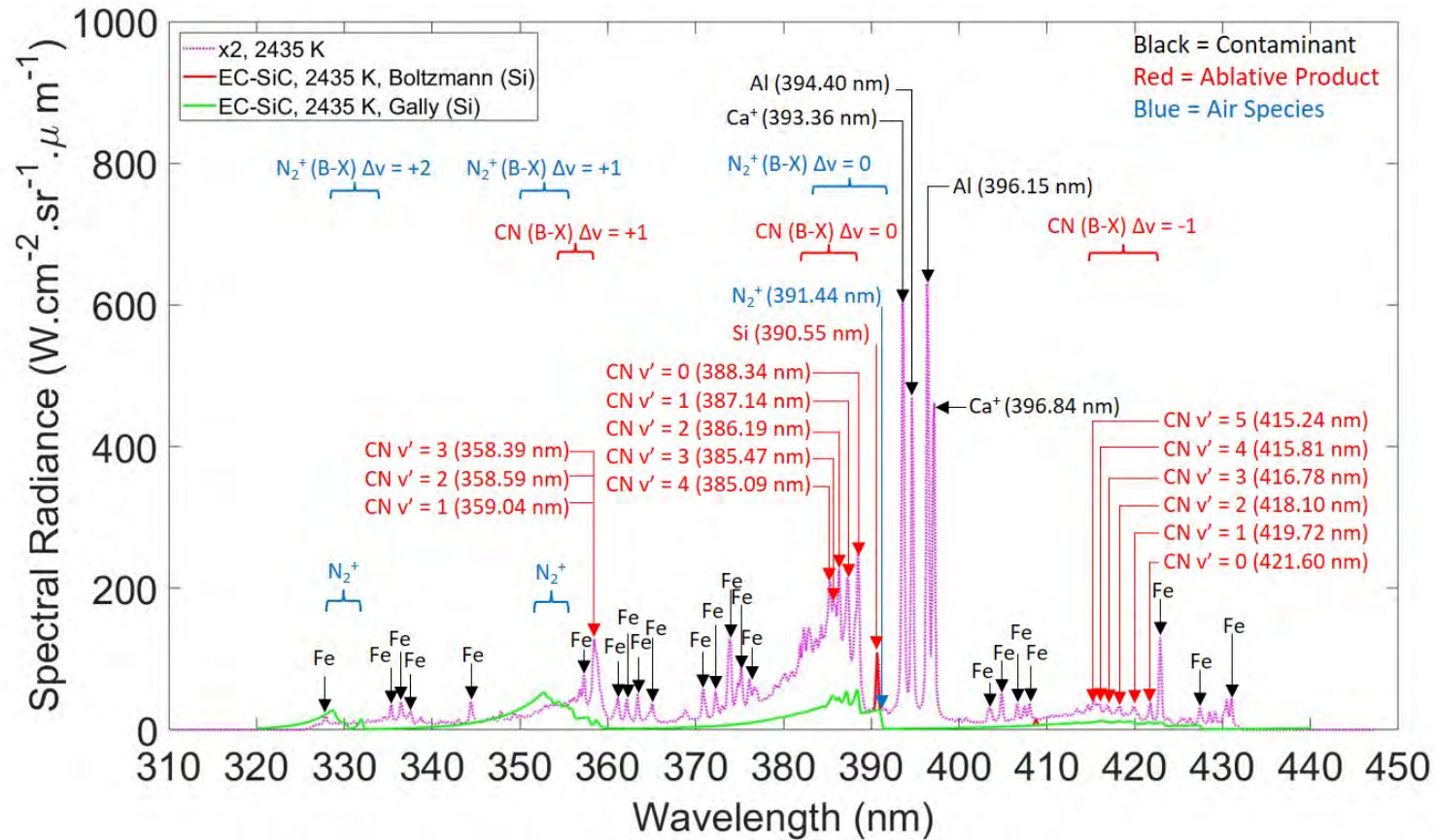


Figure 113. Experimental and simulated results for the 2435 K case for SiC-coated C-C targeting CN violet in the expansion region.

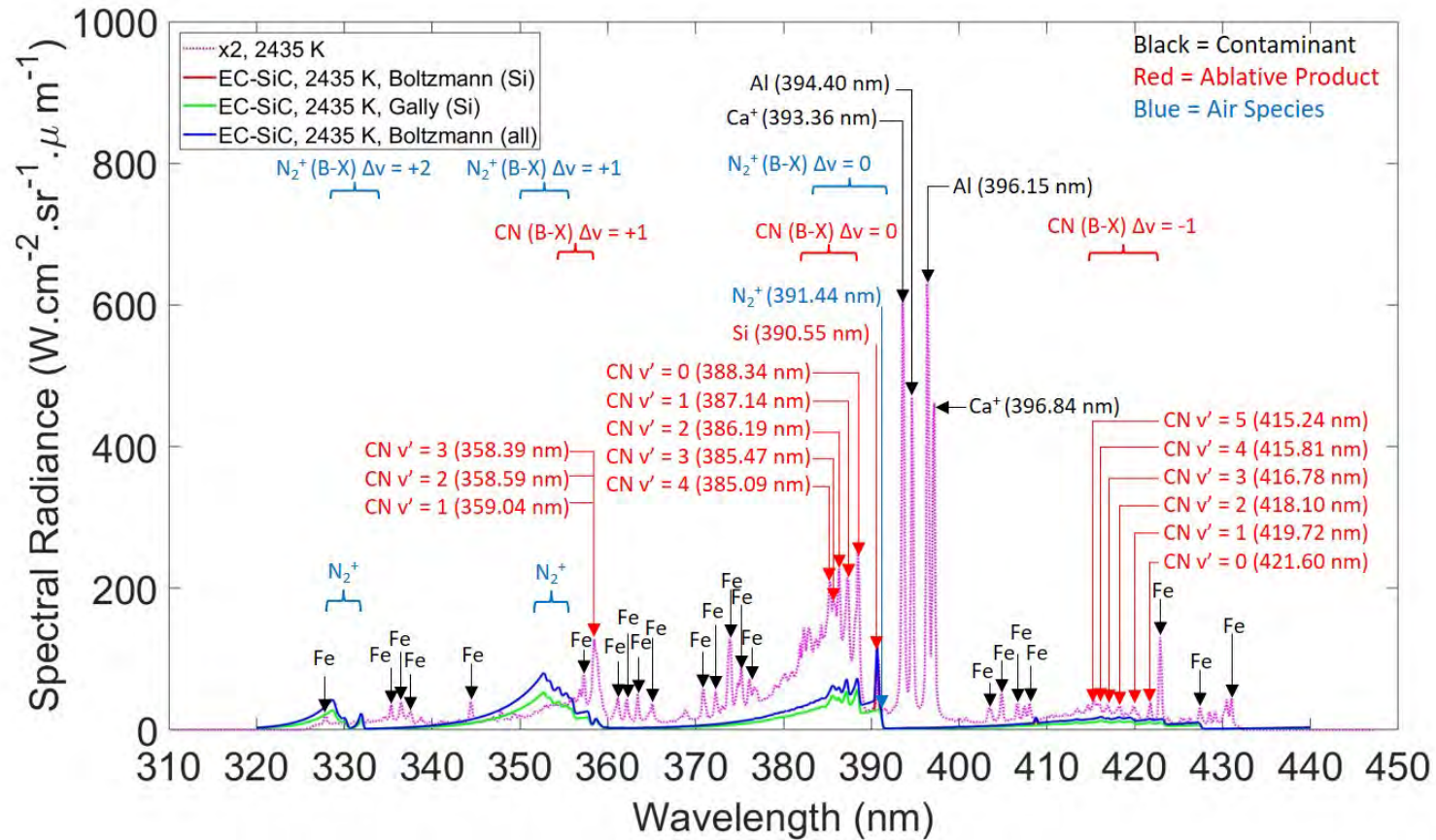


Figure 114. Experimental and simulated results for the 2435 K case for SiC-coated C-C targeting CN violet in the expansion region.

predicting experimental results by approximately 70%, the underprediction is now 60%. Note that HARA models all molecular species assuming either a Boltzmann or non-Boltzmann distribution; one cannot choose to model a particular species one way while modeling another species a different way.

Atomic Si.

Figures 115 and 116 show experimental and simulated radiations results for the 1839 K and 2352 K case, respectively, for SiC-coated C-C targeting atomic Si in the near-stagnation region using a non-Boltzmann (Gally) model to populate the electronic states. Figures 117 and 118 show the same figures using a Boltzmann model to populate the electronic states. Similarly, Figures 119 and 120 show experimental and simulated results with both atomic Si and SiO modeled assuming a Boltzmann distribution.

Simulated results for both cases calculated assuming a non-Boltzmann distribution appear to be at or near zero in value while simulated results for both cases assuming a Boltzmann distribution overpredict all potentially-identified atomic Si lines by several orders of magnitude. The only available model for SiO is a Boltzmann model, therefore the model likely overpredicts results for SiO, which were not noted during the experiments, by several orders of magnitude. To be sure that the radiation calculation is taking place for the non-Boltzmann distribution, plots of only simulated results can be viewed. These results are seen in Figures 121 and 122.

Similarly, Figures 123 and 124 show experimental and simulated radiation results for the 1968 K and 2333 K case, respectively, for SiC-coated C-C targeting atomic Si in the expansion region using the Gally model to populate the electronic states. Figures 125 and 126 show experimental and simulated results using a Boltzmann distribution. Figures 127 and 128 again show similar plots with both Si and SiO

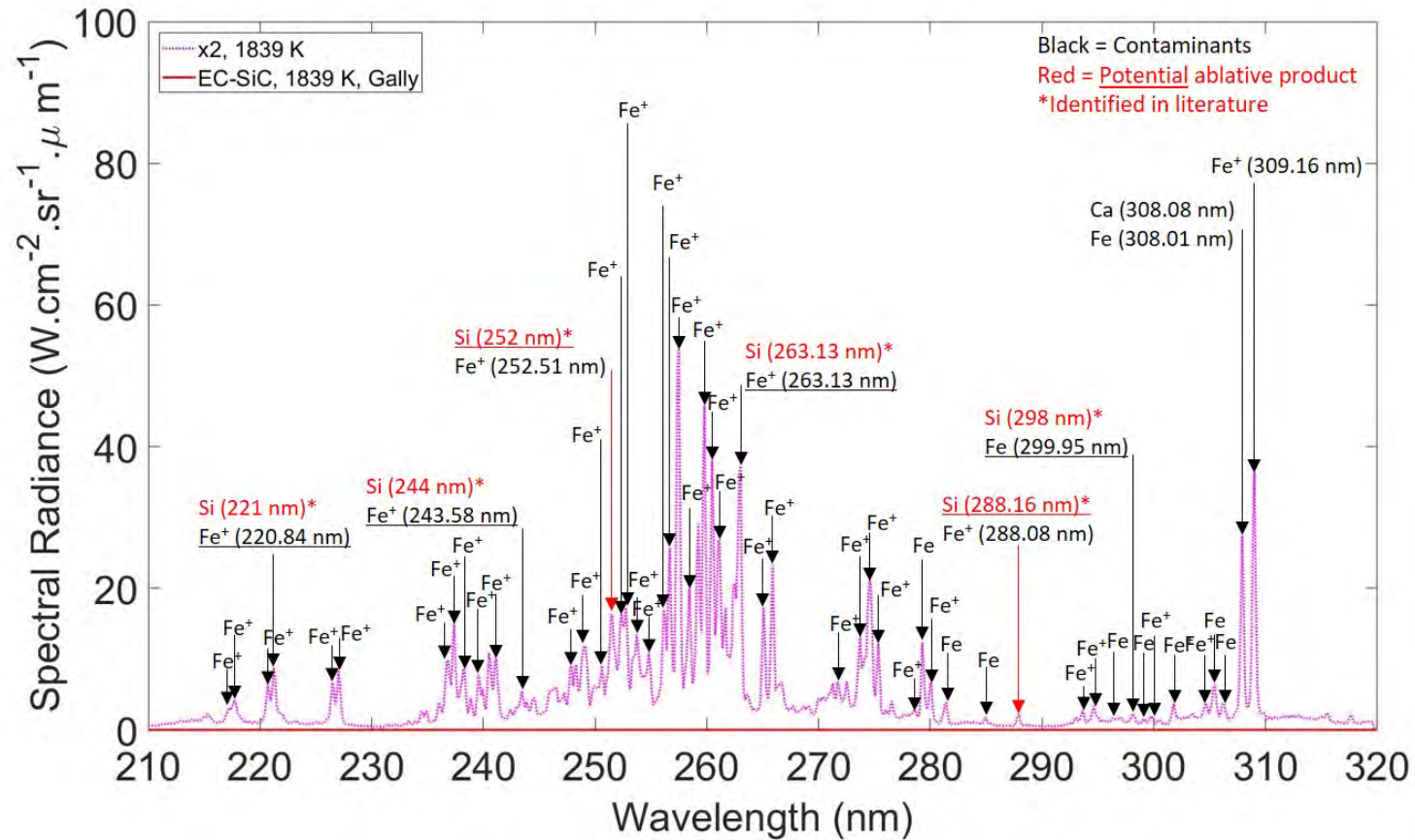


Figure 115. Experimental and simulated results for the 1839 K case for SiC-coated C-C targeting atomic Si in the near-stagnation region, assuming a non-Boltzmann (Gally) population of the electronic states.

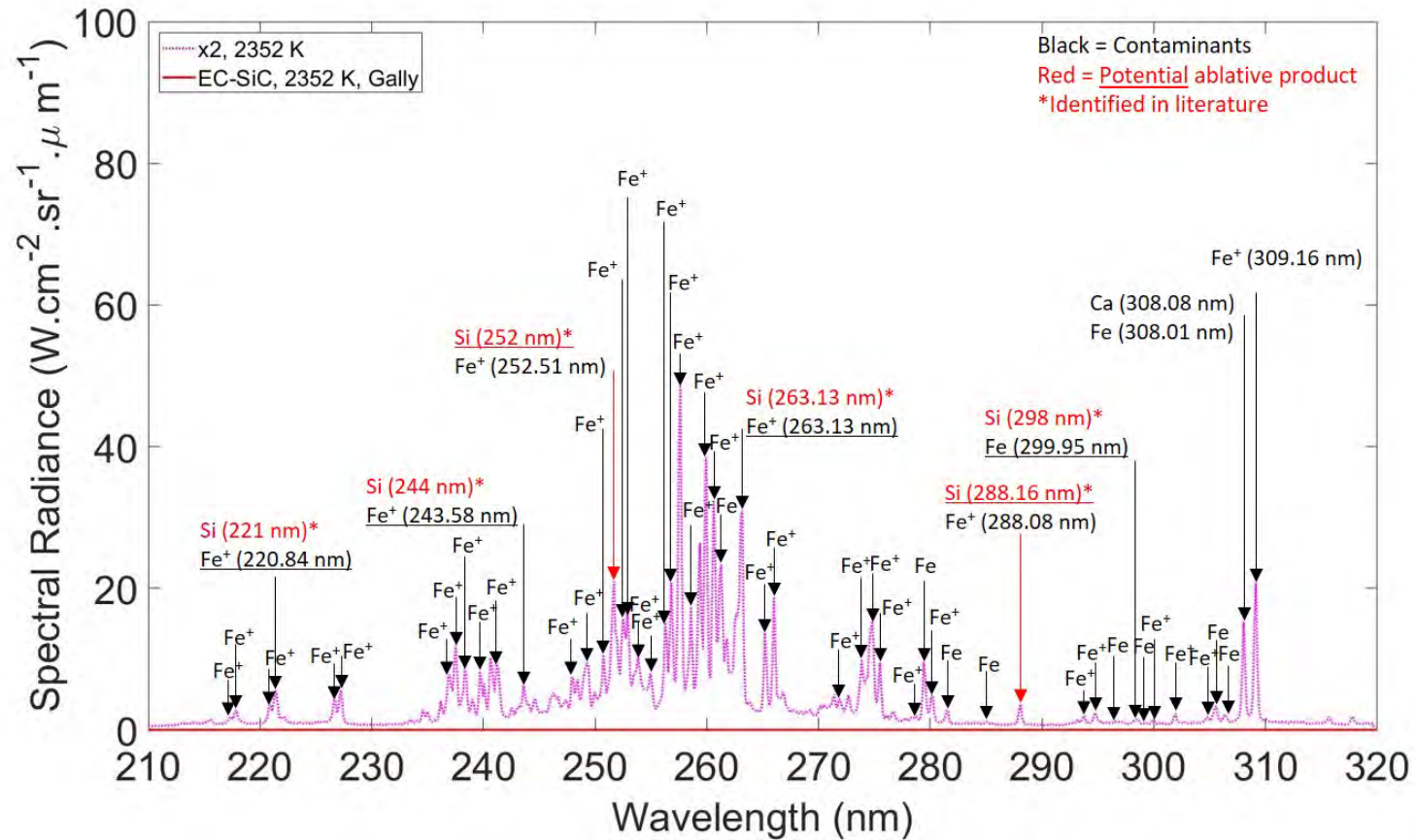


Figure 116. Experimental and simulated results for the 2352 K case for SiC-coated C-C targeting atomic Si in the near-stagnation region, assuming a non-Boltzmann (Gally) population of the electronic states.

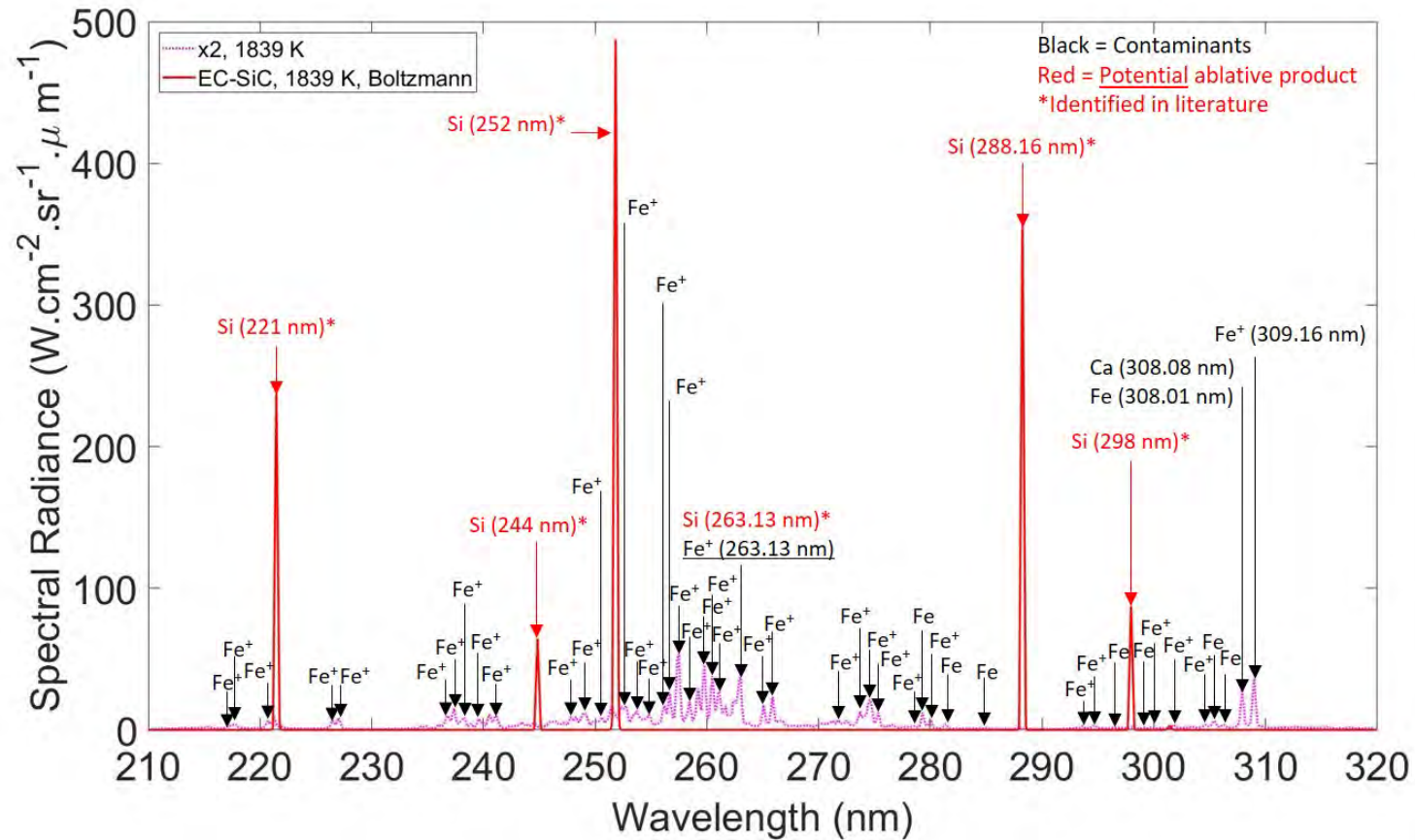


Figure 117. Experimental and simulated results for the 1839 K case for SiC-coated C-C targeting atomic Si in the near-stagnation region, assuming a Boltzmann population of the electronic states.

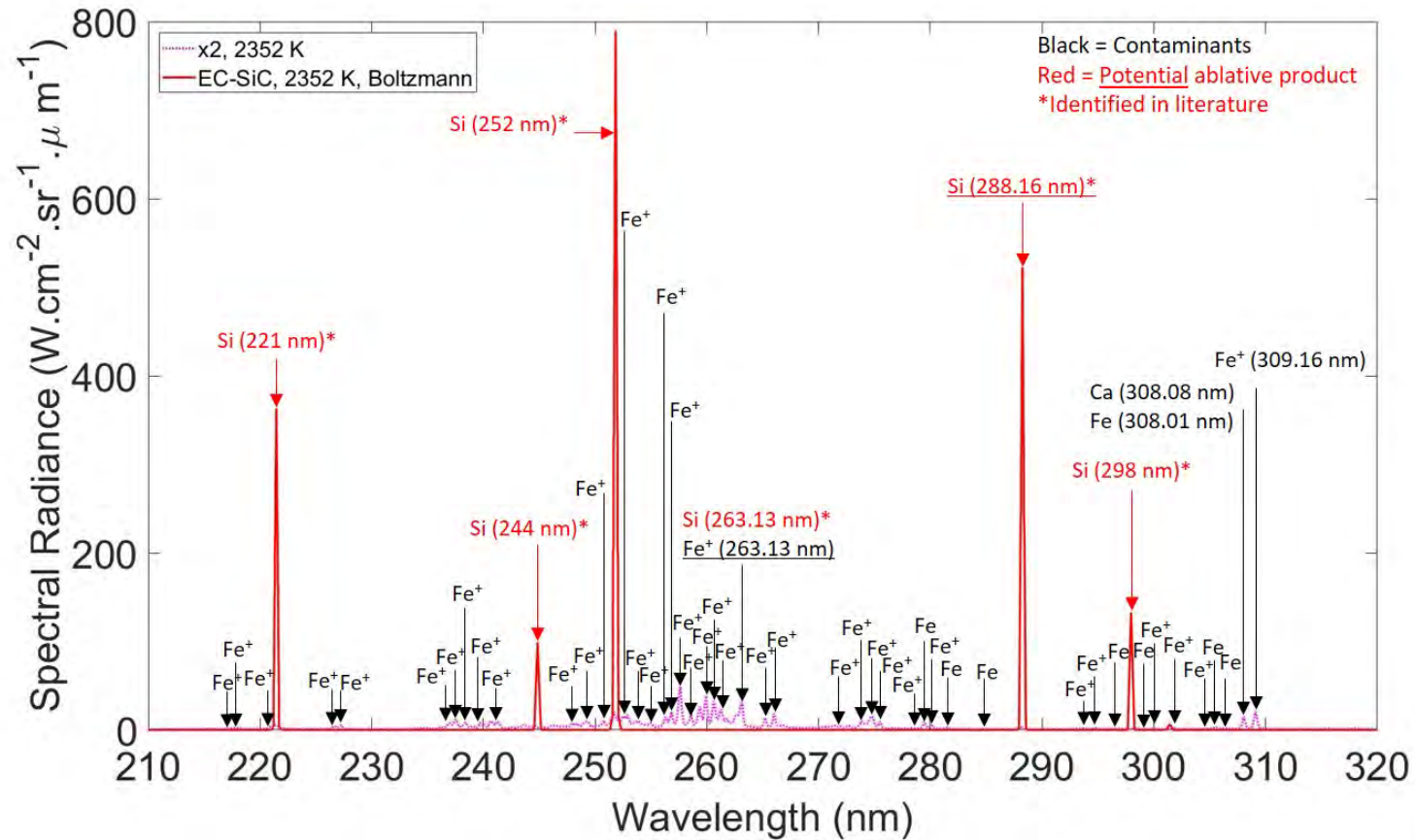


Figure 118. Experimental and simulated results for the 2352 K case for SiC-coated C-C targeting atomic Si in the near-stagnation region, assuming a Boltzmann population of the electronic states.

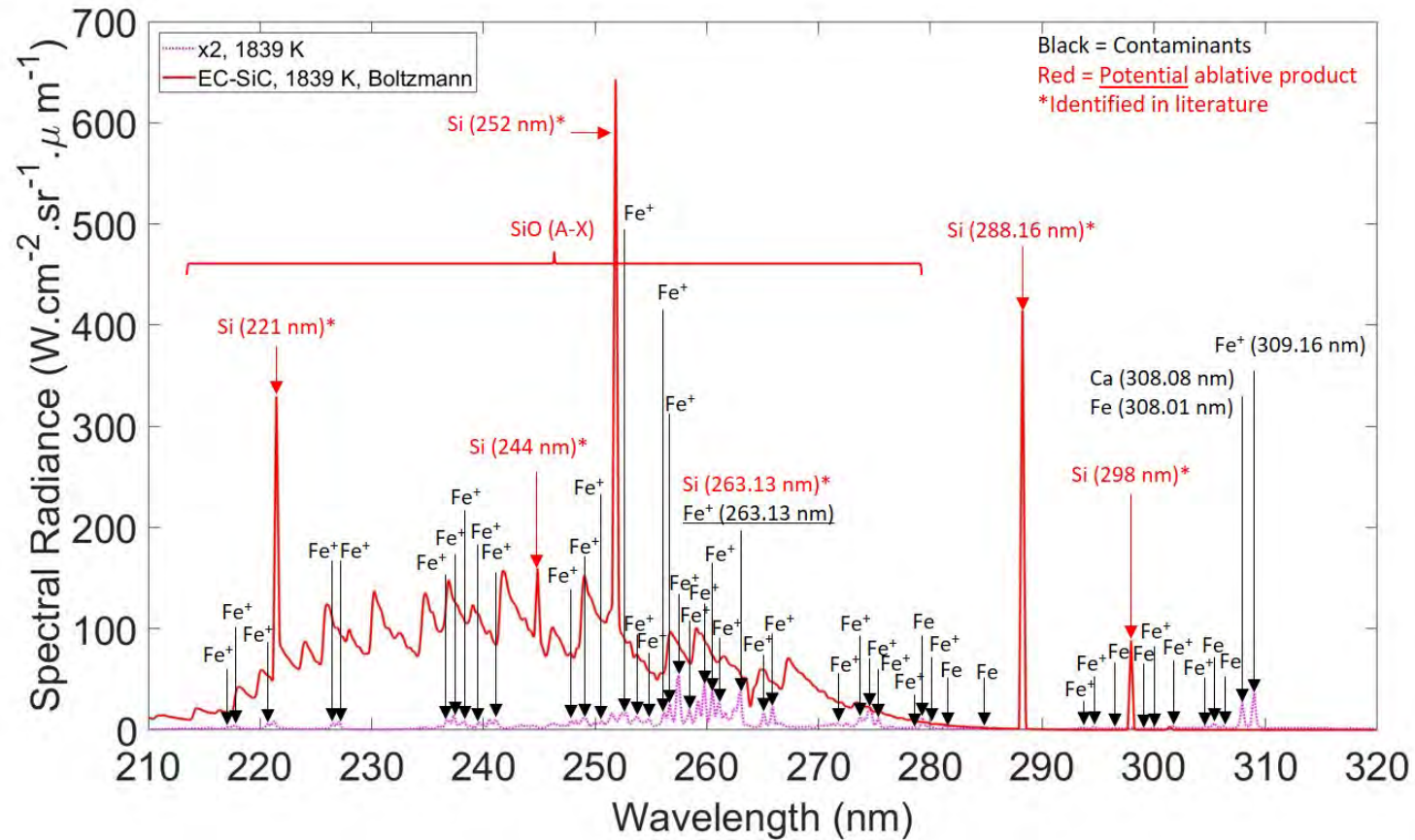


Figure 119. Experimental and simulated results for the 1839 K case for SiC-coated C-C targeting atomic Si in the near-stagnation region, assuming a Boltzmann population of the electronic states, with SiO.

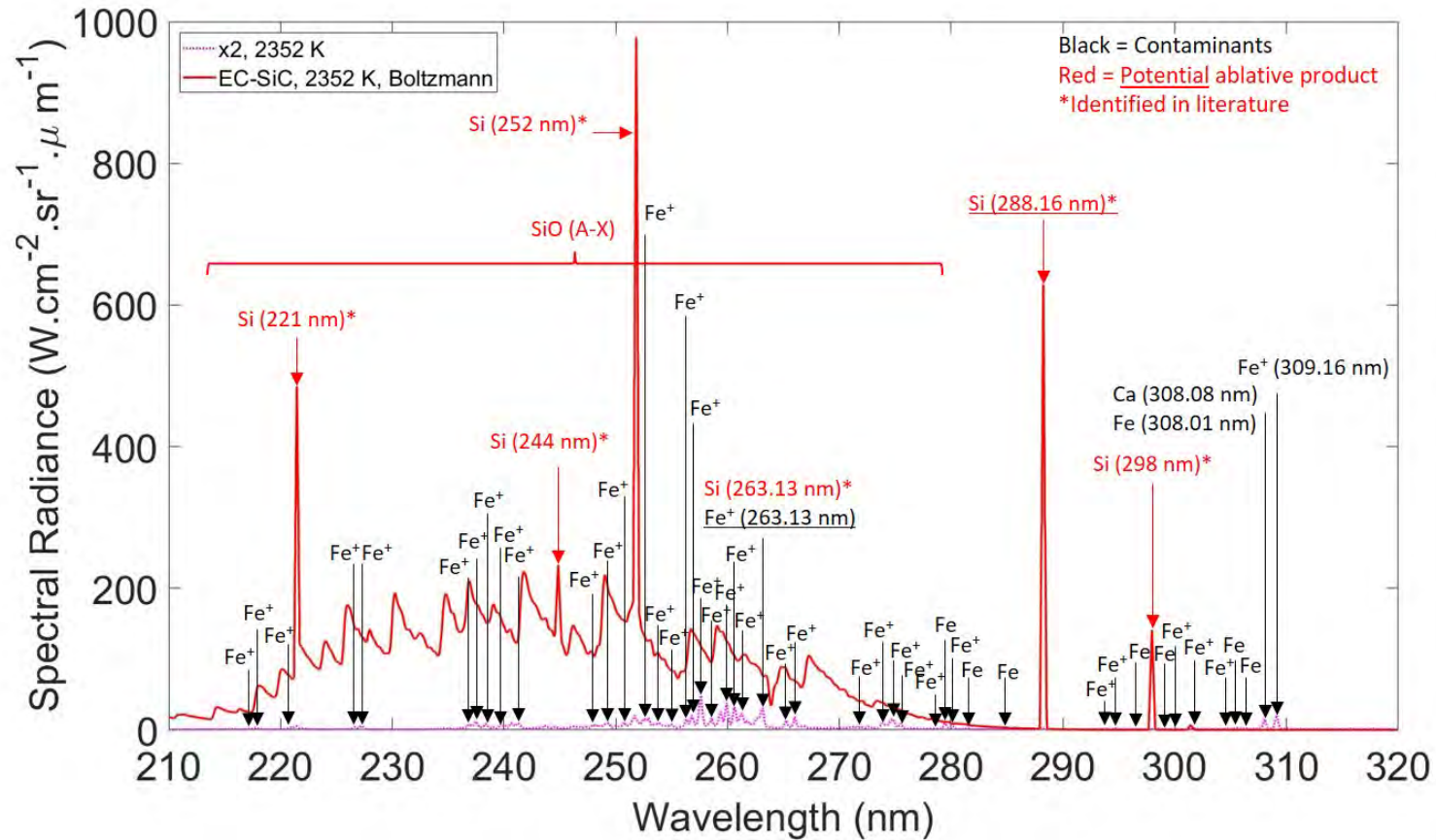


Figure 120. Experimental and simulated results for the 2352 K case for SiC-coated C-C targeting atomic Si in the near-stagnation region, assuming a Boltzmann population of the electronic states, with SiO.

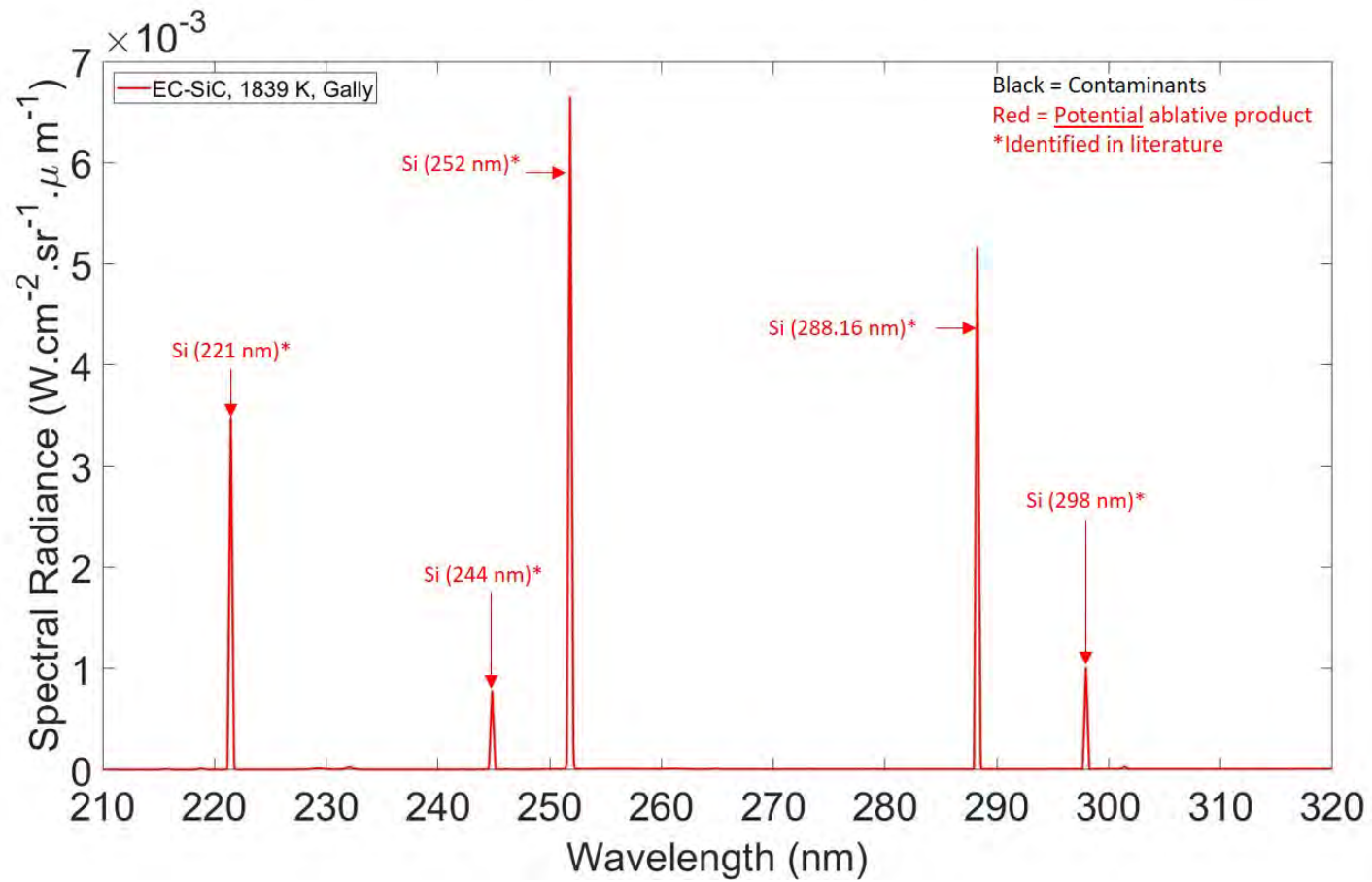


Figure 121. Simulated results for the 1839 K case for SiC-coated C-C targeting atomic Si in the near-stagnation region, assuming a non-Boltzmann (Gally) population of the electronic states.

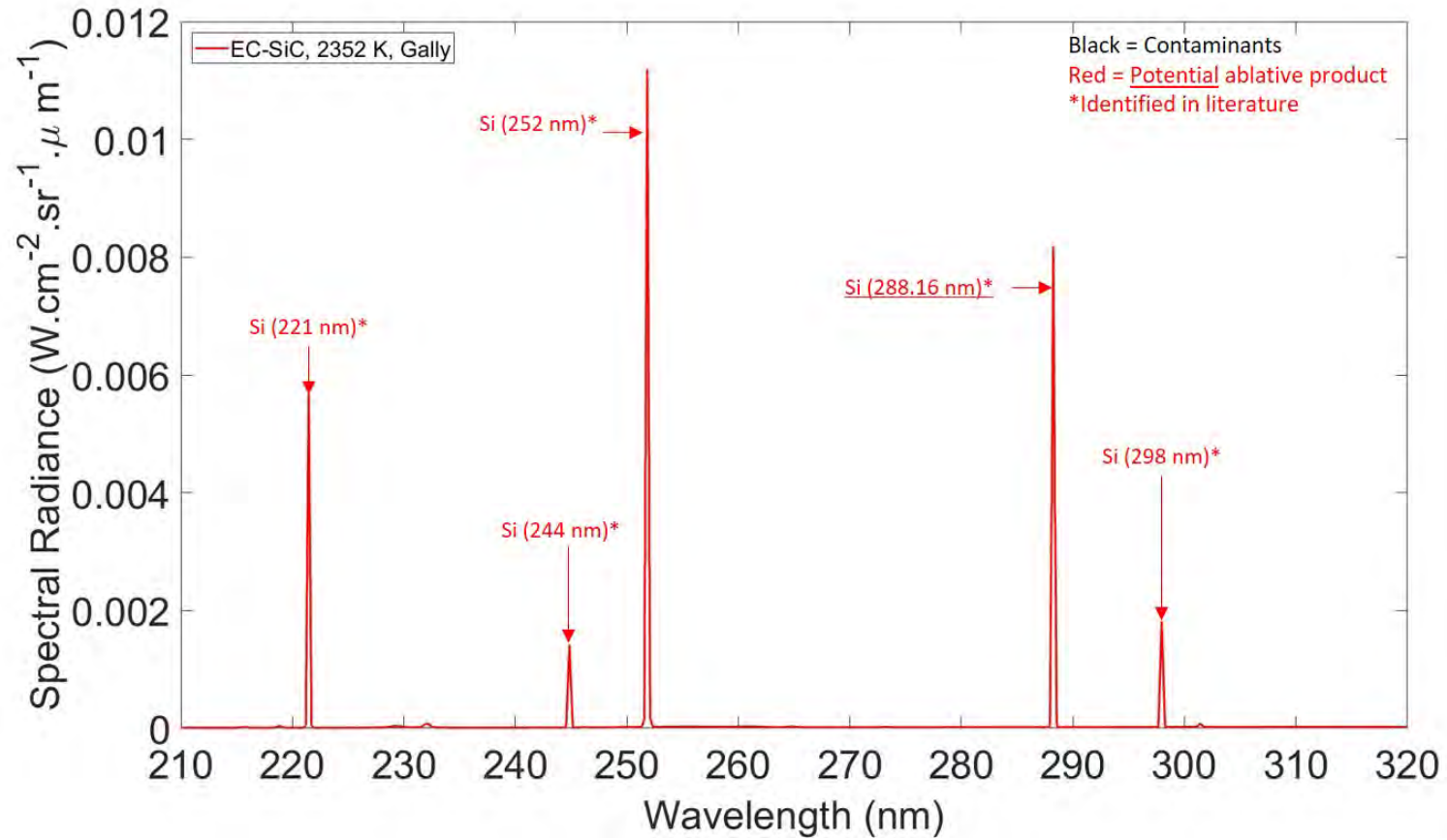


Figure 122. Simulated results for the 2352 K case for SiC-coated C-C targeting atomic Si in the near-stagnation region, assuming a non-Boltzmann (Gally) population of the electronic states.

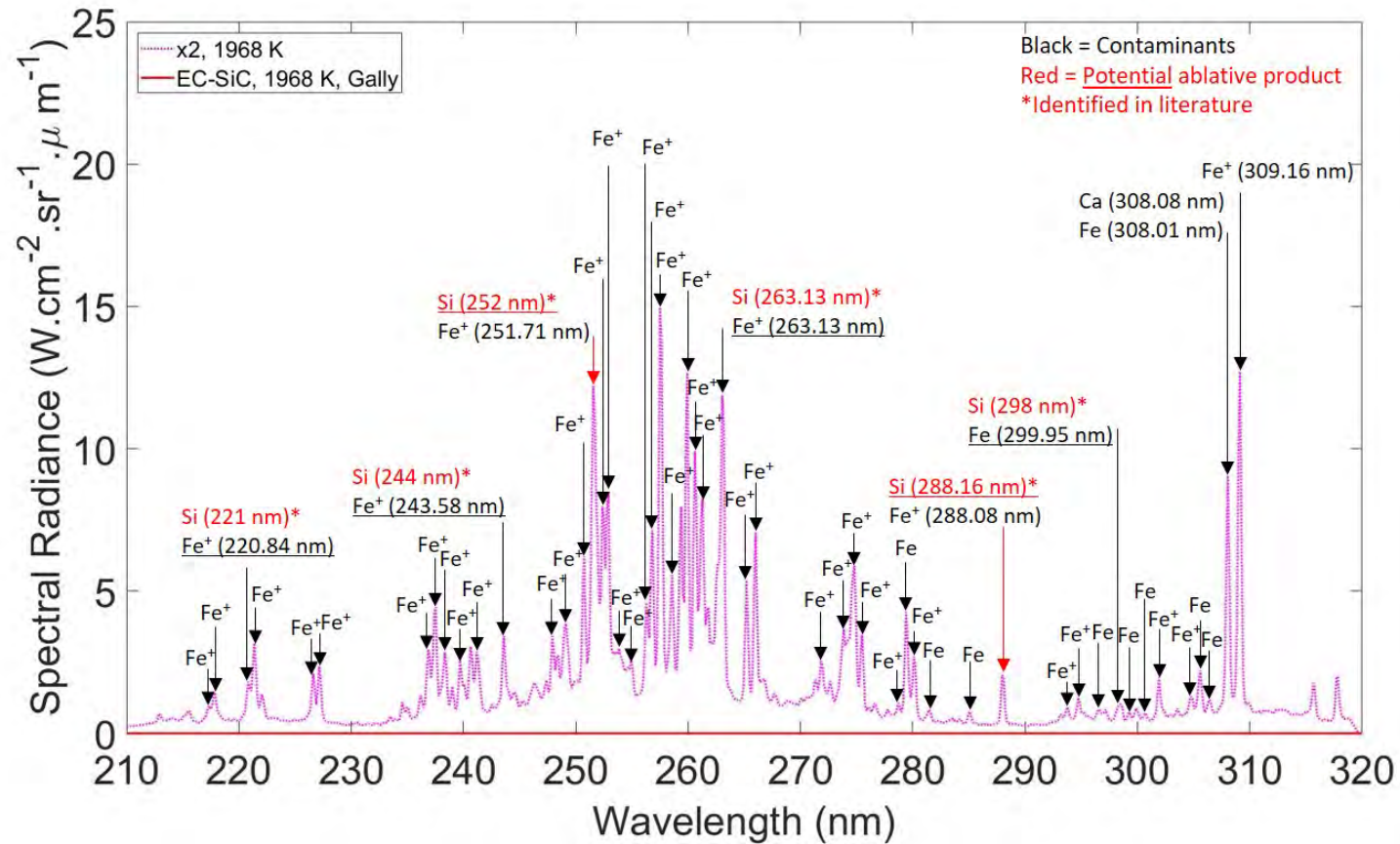


Figure 123. Experimental and simulated results for the 1968 K case for SiC-coated C-C targeting atomic Si in the expansion region, assuming a non-Boltzmann (Gally) population of the electronic states.

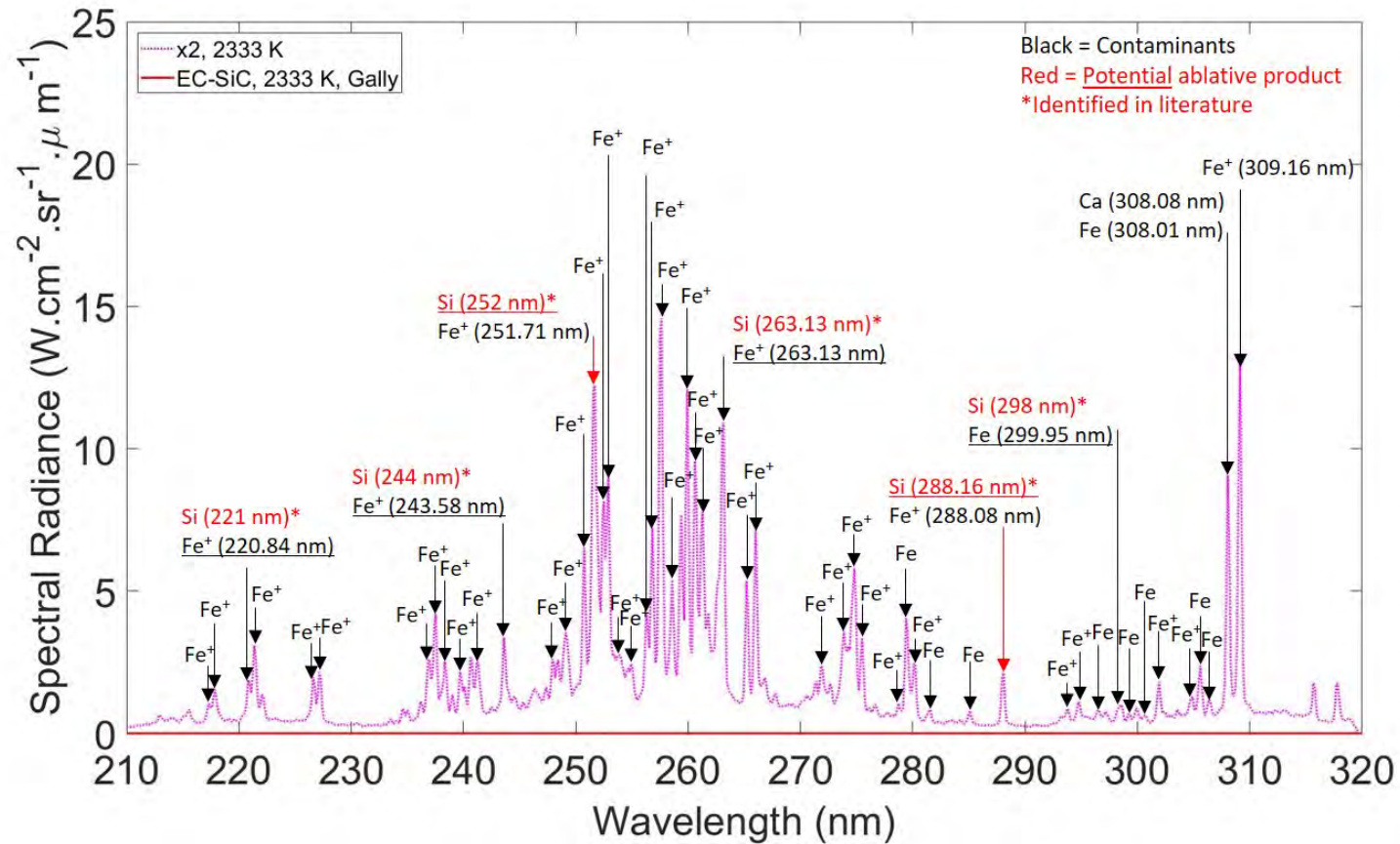


Figure 124. Experimental and simulated results for the 2333 K case for SiC-coated C-C targeting atomic Si in the expansion region, assuming a non-Boltzmann (Gally) population of the electronic states.

Figure 125. Experimental and simulated results for the 1968 K case for SiC-coated C-C targeting atomic Si in the expansion region, assuming a Boltzmann population of the electronic states.

Figure 126. Experimental and simulated results for the 2333 K case for SiC-coated C-C targeting atomic Si in the expansion region, assuming a Boltzmann population of the electronic states.

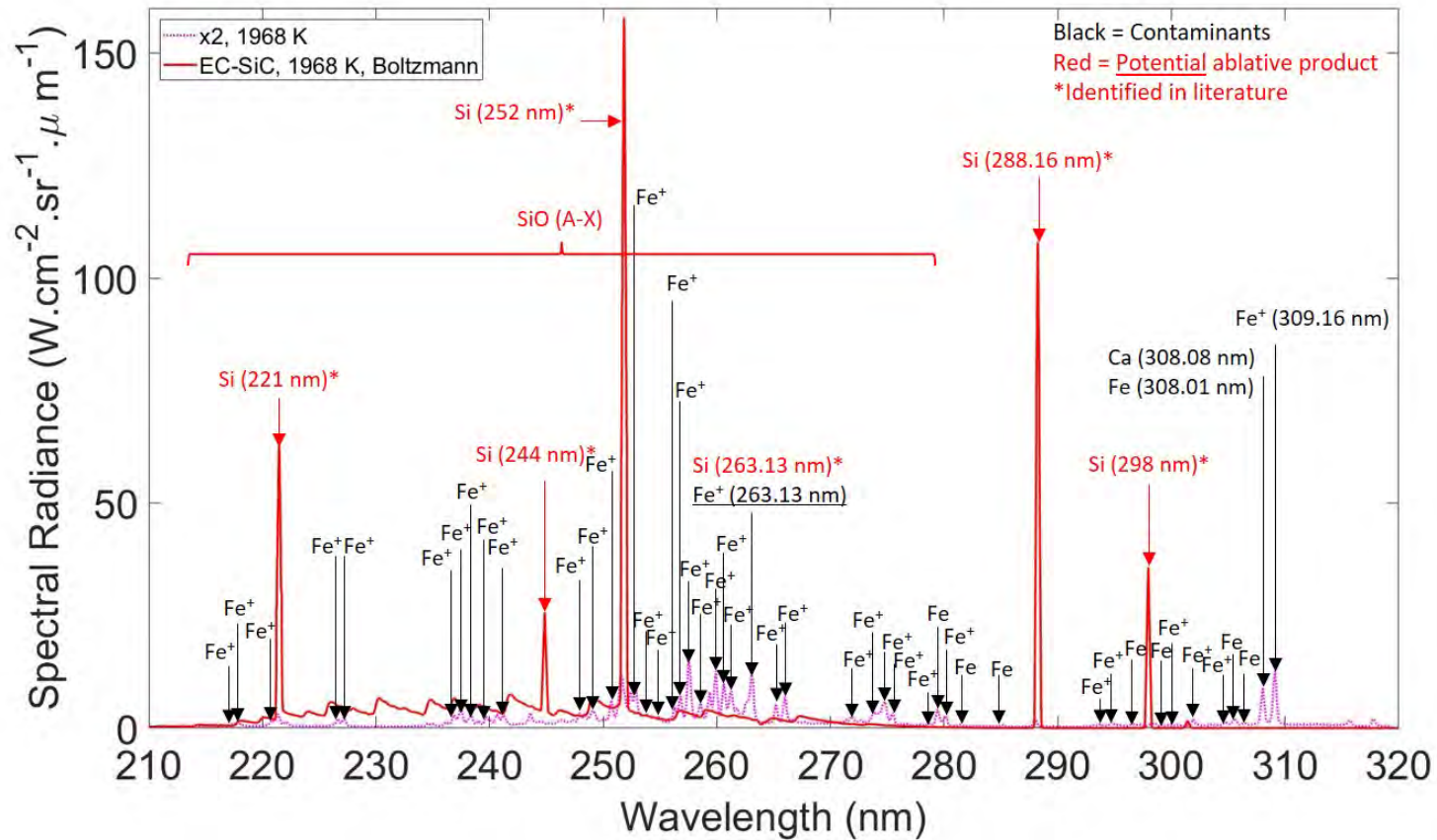


Figure 127. Experimental and simulated results for the 1968 K case for SiC-coated C-C targeting atomic Si in the expansion region, assuming a Boltzmann population of the electronic states, with SiO.

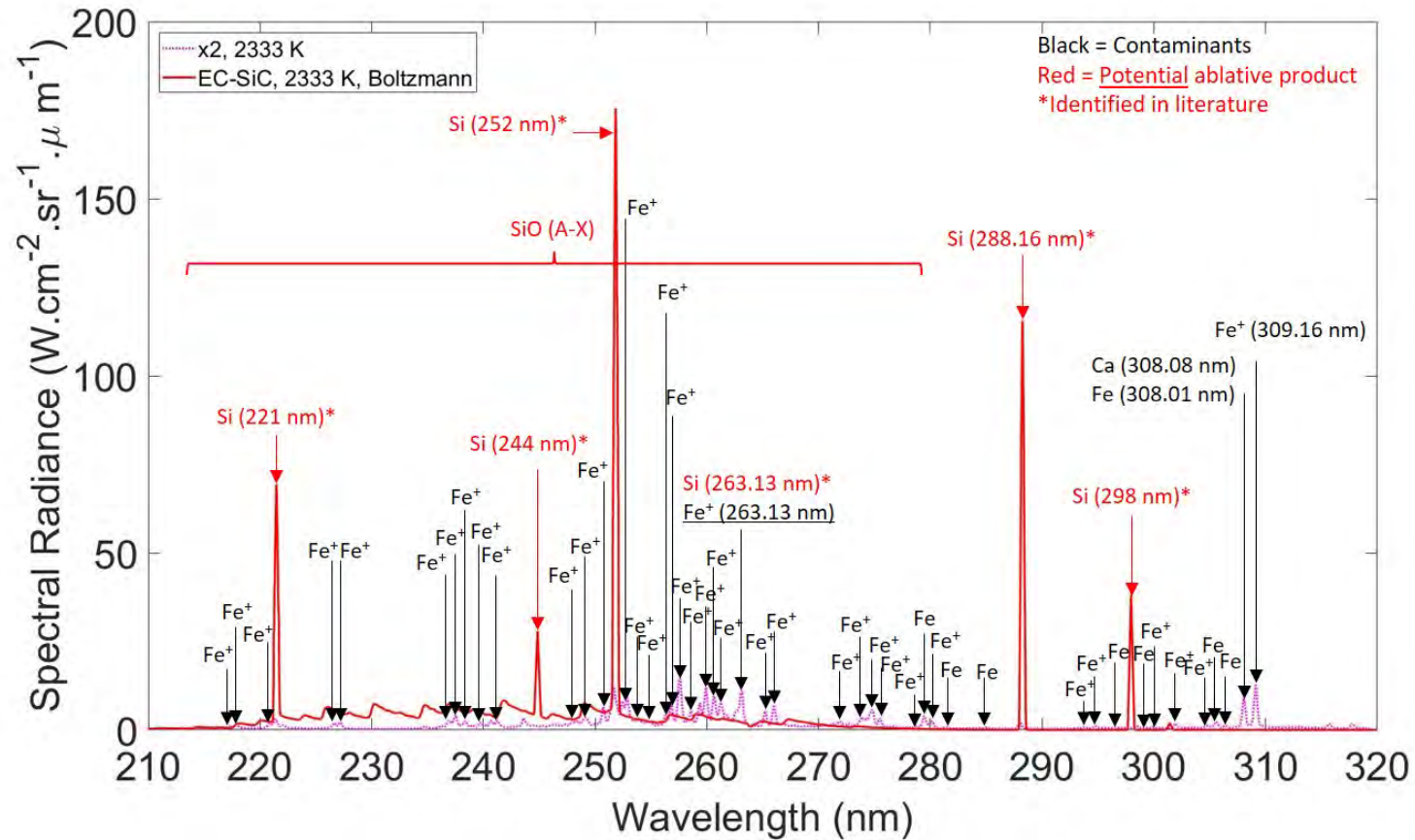


Figure 128. Experimental and simulated results for the 2333 K case for SiC-coated C-C targeting atomic Si in the expansion region, assuming a Boltzmann population of the electronic states, with SiO.

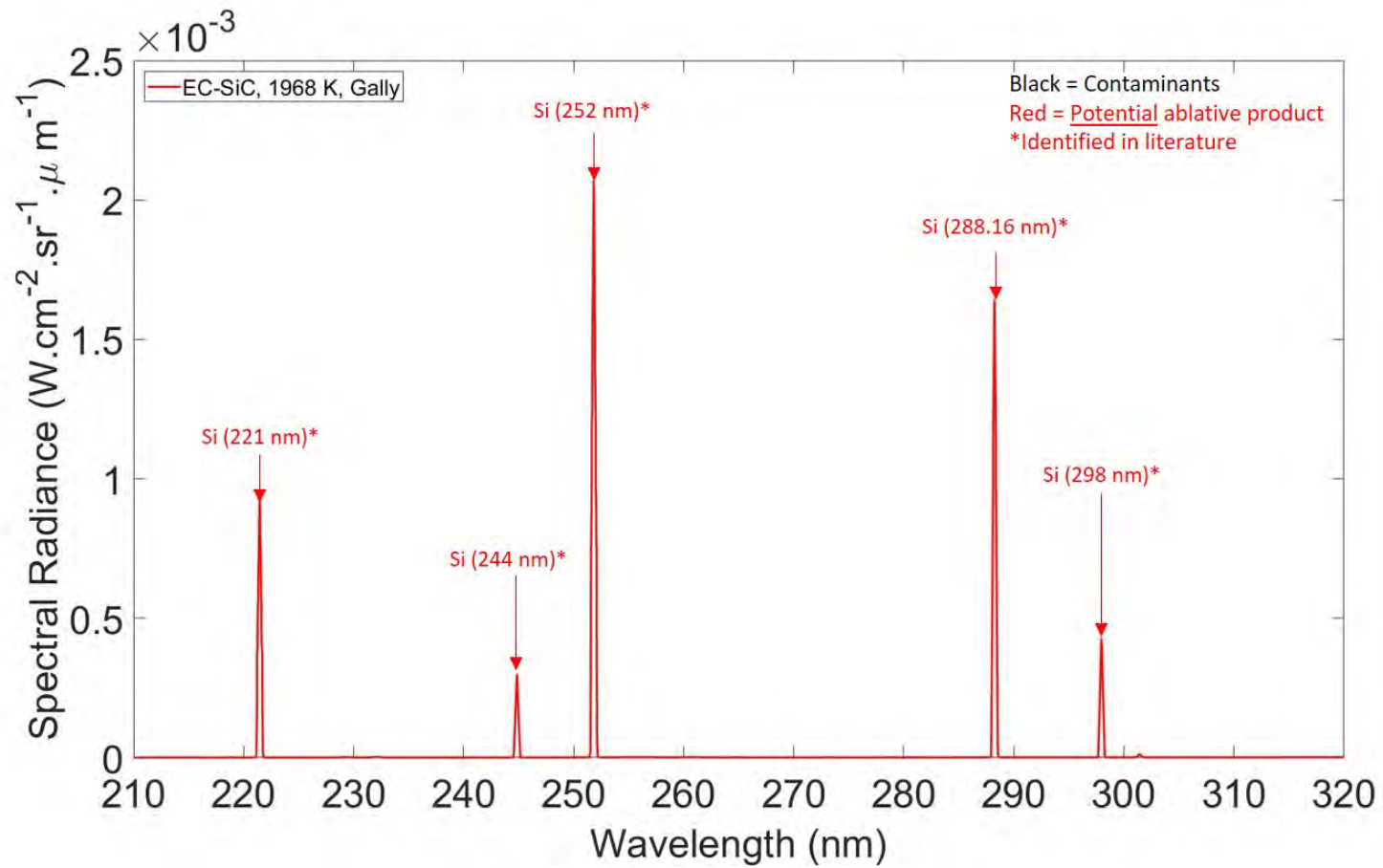


Figure 129. Simulated results for the 1968 K case for SiC-coated C-C targeting atomic Si in the expansion region, assuming a non-Boltzmann (Gally) population of the electronic states.

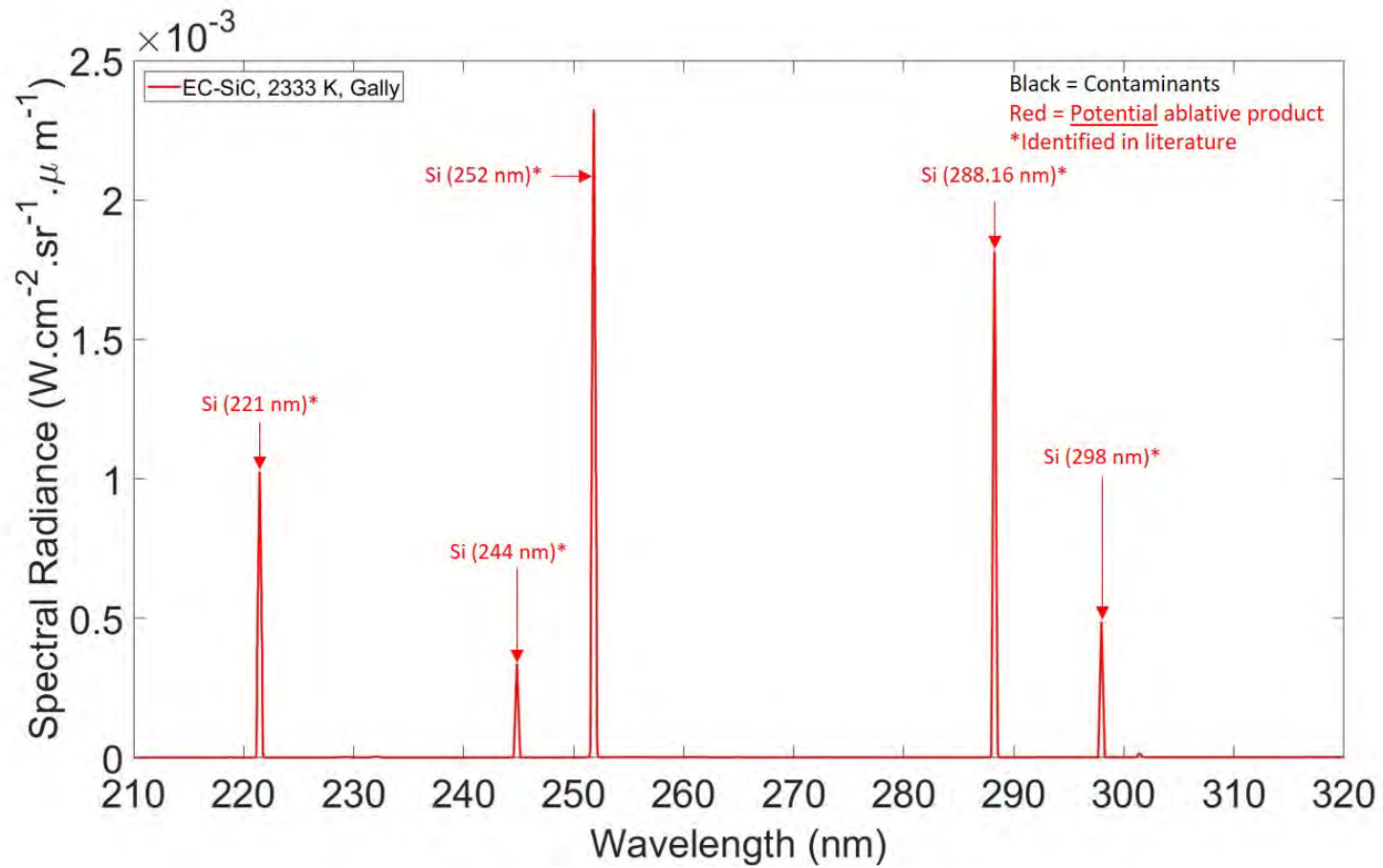


Figure 130. Simulated results for the 2333 K case for SiC-coated C-C targeting atomic Si in the expansion region, assuming a non-Boltzmann (Gally) population of the electronic states.

modeled assuming a Boltzmann distribution.

The same trends of simulated results obtained using a non-Boltzmann distribution underpredicting experimental results and simulated results obtained using a Boltzmann distribution overpredicting experimental results are again observed. Simulated results for SiO are significantly lower in the expansion region compared to the near-stagnation region, but still overpredict experimental results, which were again not observed during the experiments. Similarly, plots of only simulated results obtained assuming a non-Boltzmann distribution are shown in Figures 129 and 130 to once again confirm that the expected radiation calculation is taking place.

The overprediction of simulated results assuming a Boltzmann distribution can be expected based on the overpopulation of the excited electronic states. The underprediction of simulated results assuming a non-Boltzmann distribution can likely be attributed to several factors. One factor is the potential underprediction of the ablation rate of the equilibrium-char ablation model, which was previously shown to predict 50% less CN than the finite-rate ablation model for C-C; therefore, it is possible that the ablation model is resulting in approximately 50% less atomic Si entering the flowfield than is actually entering the flowfield. Another contributing factor may be the chemical reaction that results in ionization of the Si atom. This reaction, shown in Table 3, is included in the LAURA code but does not contain a reference as many of the other chemical reactions do and is purely an estimate provided by the code developers. The number density of Si ions is used directly by the non-Boltzmann model so any errors in this calculation would lead to errors in simulated radiation. Therefore, this reaction rate very well may be wrong and overpredicting or underpredicting the ionization of the Si atom and should be investigated further.

C₂ Swan.

Figure 131 shows experimental and simulated results for SiC-coated C-C targeting C₂ Swan in the near-stagnation region. Simulated results obtained assuming both a Boltzmann and non-Boltzmann distribution are included. Compared to the experimental results, both simulated results appear to be at or near zero. To be sure that the simulations are taking place, Figure 132 shows only simulated results for this case. This figure confirms that simulated radiation results are being computed, however their magnitude is significantly lower than experimental results, indicating that the belief that C₂ Swan radiation was not observed during the experiments is correct. It should also be noted that there is barely a distinguishable difference between simulated results obtained assuming a Boltzmann and non-Boltzmann distribution. This observation may be the result of C₂ being a trace species in the flowfield; if its presence was greater, perhaps there would be a more significant difference between the two radiation models.

Atomic N and O.

Figure 133 shows experimental and simulated radiation results for SiC-coated C-C targeting atomic N and O in the near-stagnation region. The simulated results computed using a Boltzmann distribution to populate the electronic states drastically overpredict the intensity by several orders of magnitude while the CR model also significantly overpredicts simulated results. Compared to the other two models, the Gally model, which uses the Saha-Boltzmann equation to populate the excited electronic states, is in excellent agreement with the experimental results. This finding suggests that using the Saha-Boltzmann equation to populate the electronic states most accurately replicates the X2 experiments, since the population of the electronic states is the only difference between the three models, as shown in Figure 4.

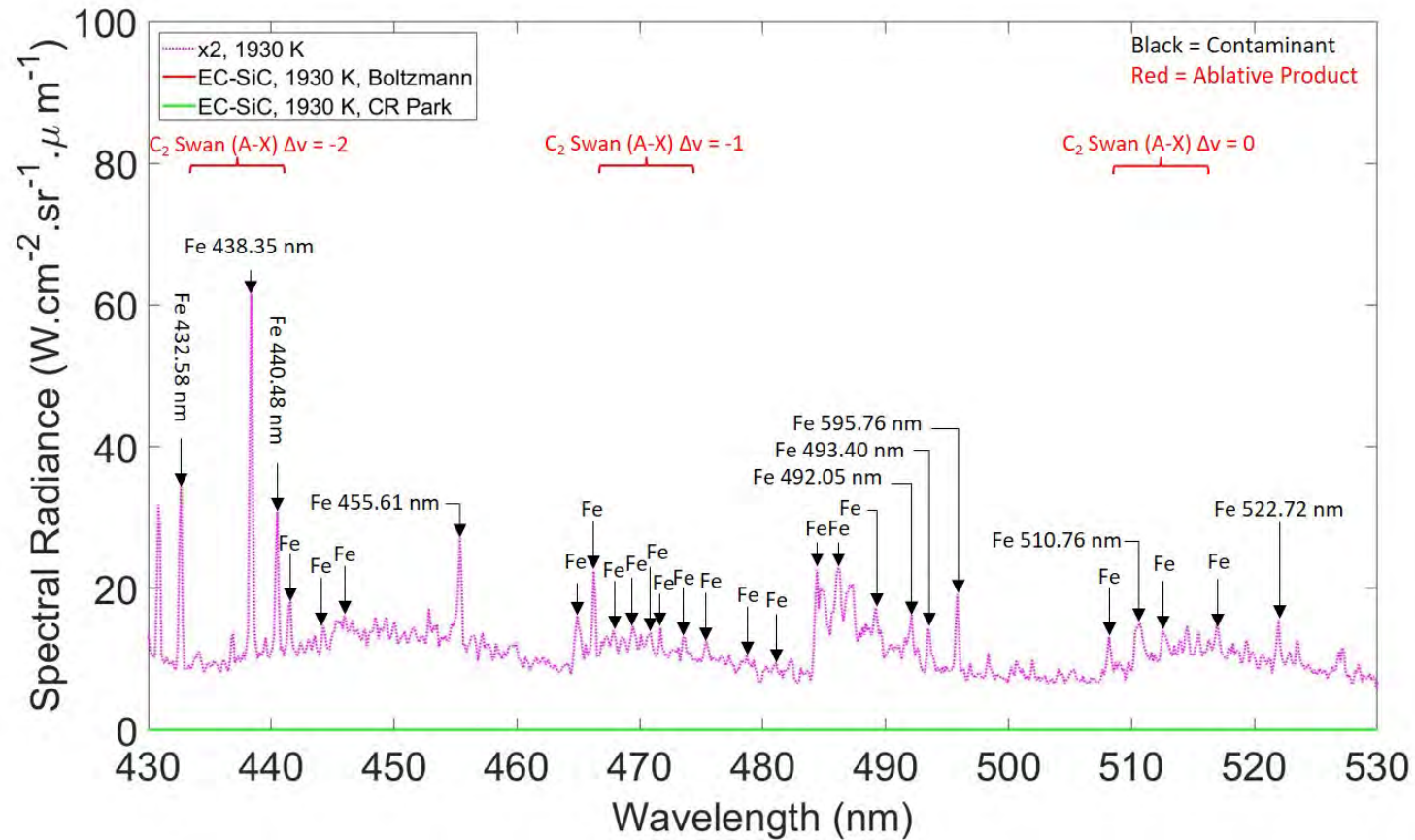


Figure 131. Experimental and simulated results for the 1930 K case for SiC-coated C-C targeting C₂ Swan in the near-stagnation region, for both Boltzmann and non-Boltzmann (CR Park) population of the electronic states.

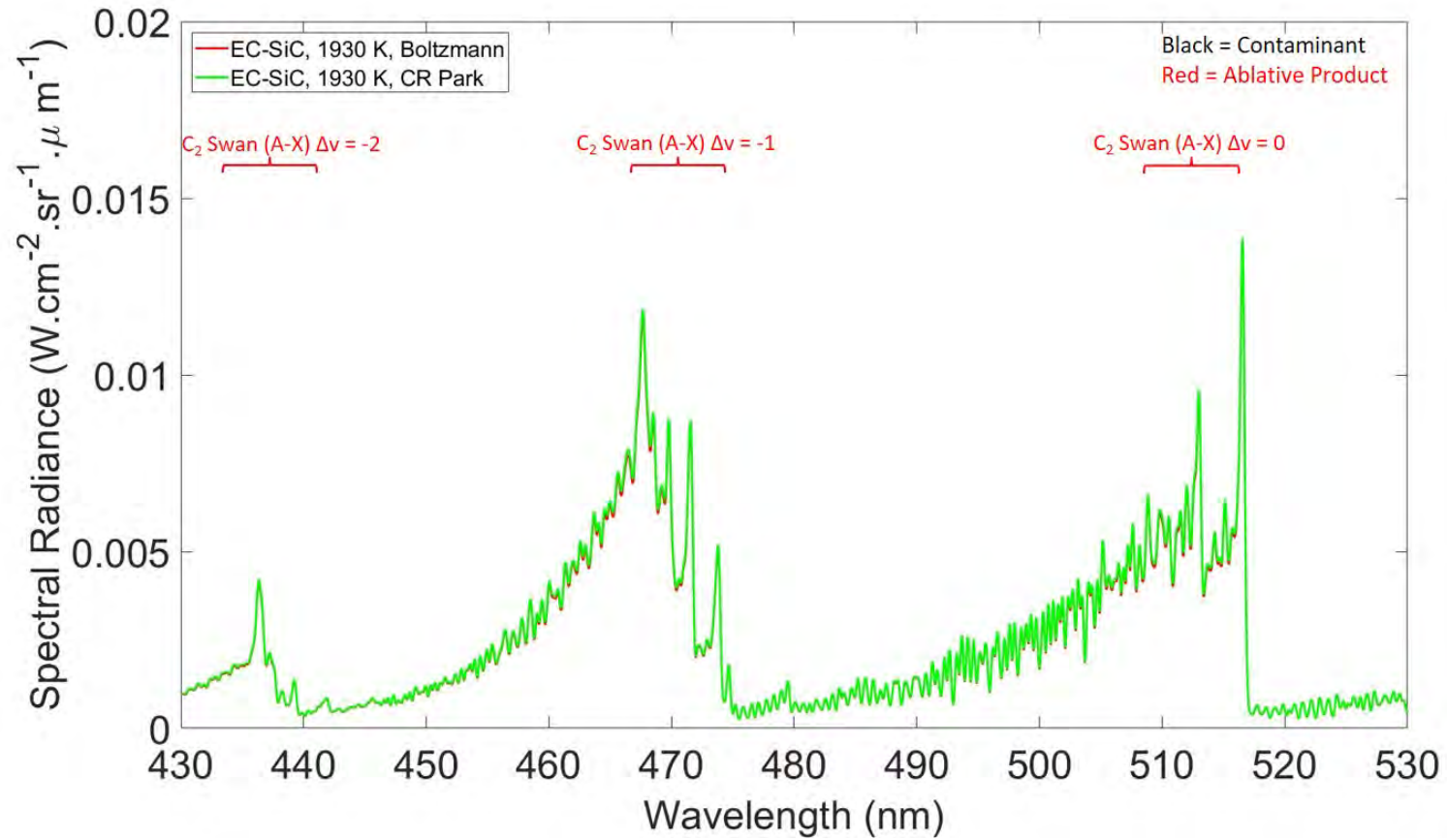


Figure 132. Simulated results for the 1930 K case for SiC-coated C-C targeting C₂ Swan in the near-stagnation region, for both Boltzmann and non-Boltzmann (CR Park) population of the electronic states.

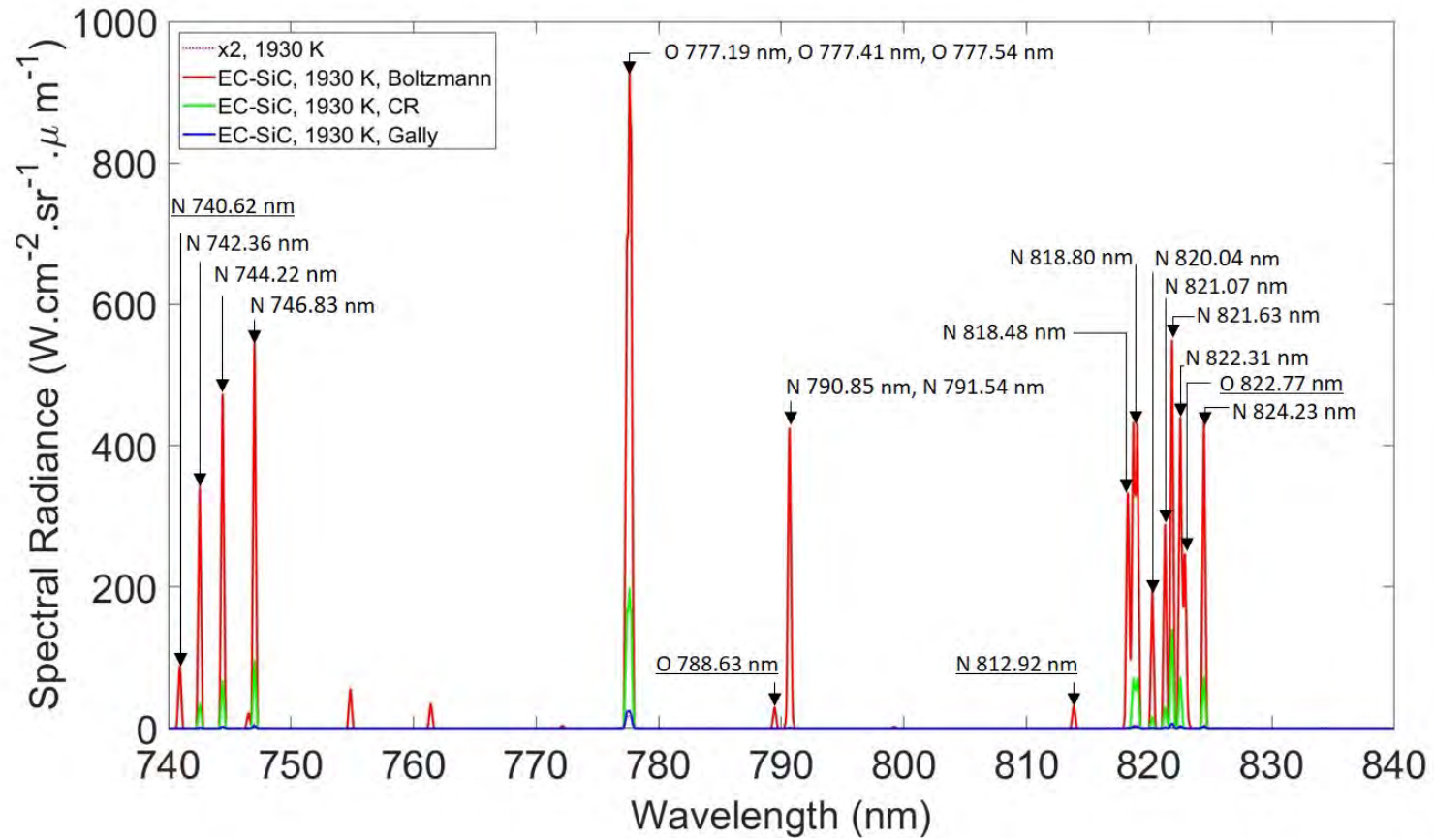


Figure 133. Experimental and simulated results for the 1930 K case for SiC-coated C-C targeting atomic N and O in the near-stagnation region, for both Boltzmann and non-Boltzmann (CR, Gally) population of the electronic states.

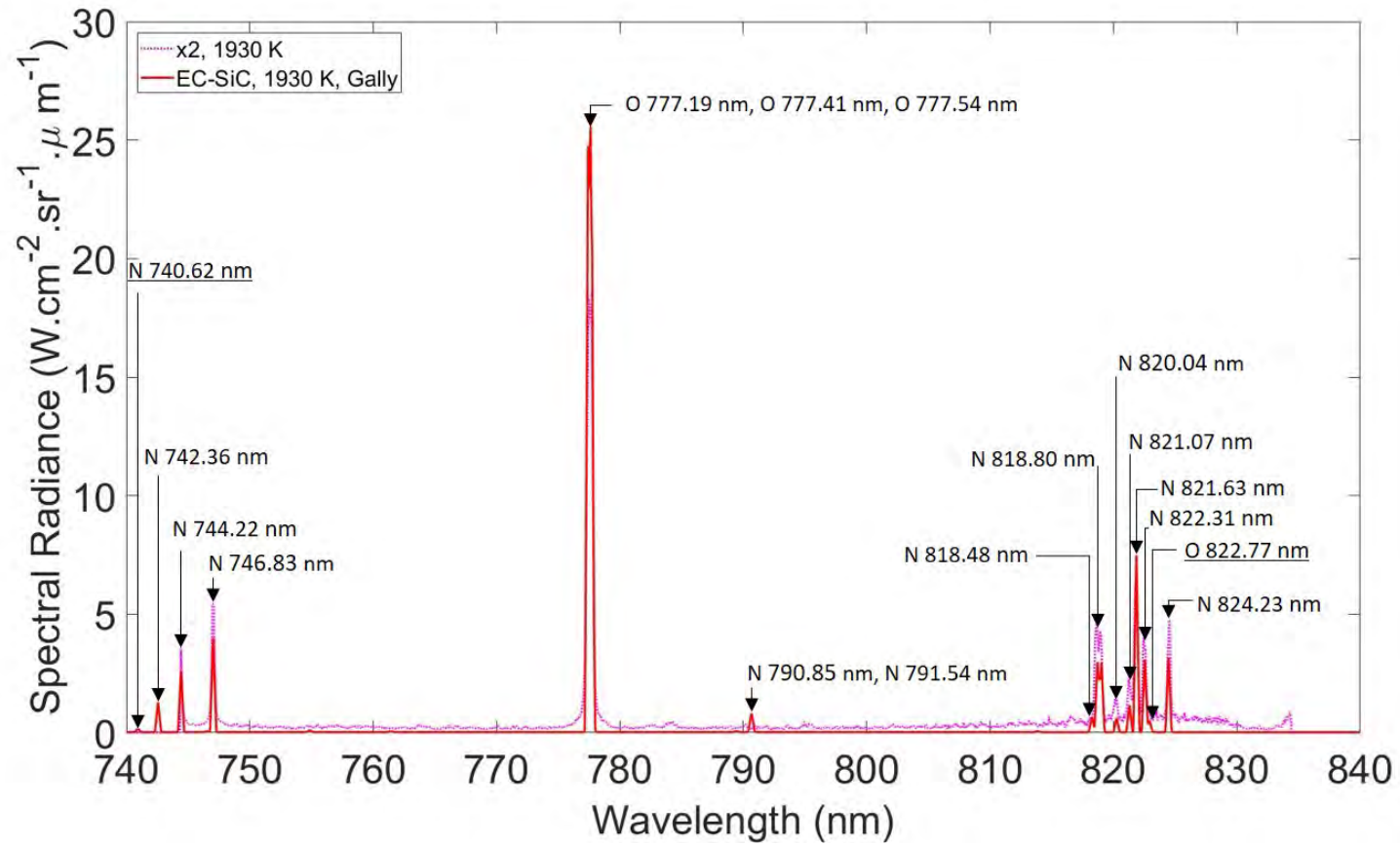


Figure 134. Experimental and simulated results for the 1930 K case for SiC-coated C-C targeting atomic N and O in the near-stagnation region, using only the Gally model to populate the electronic states.

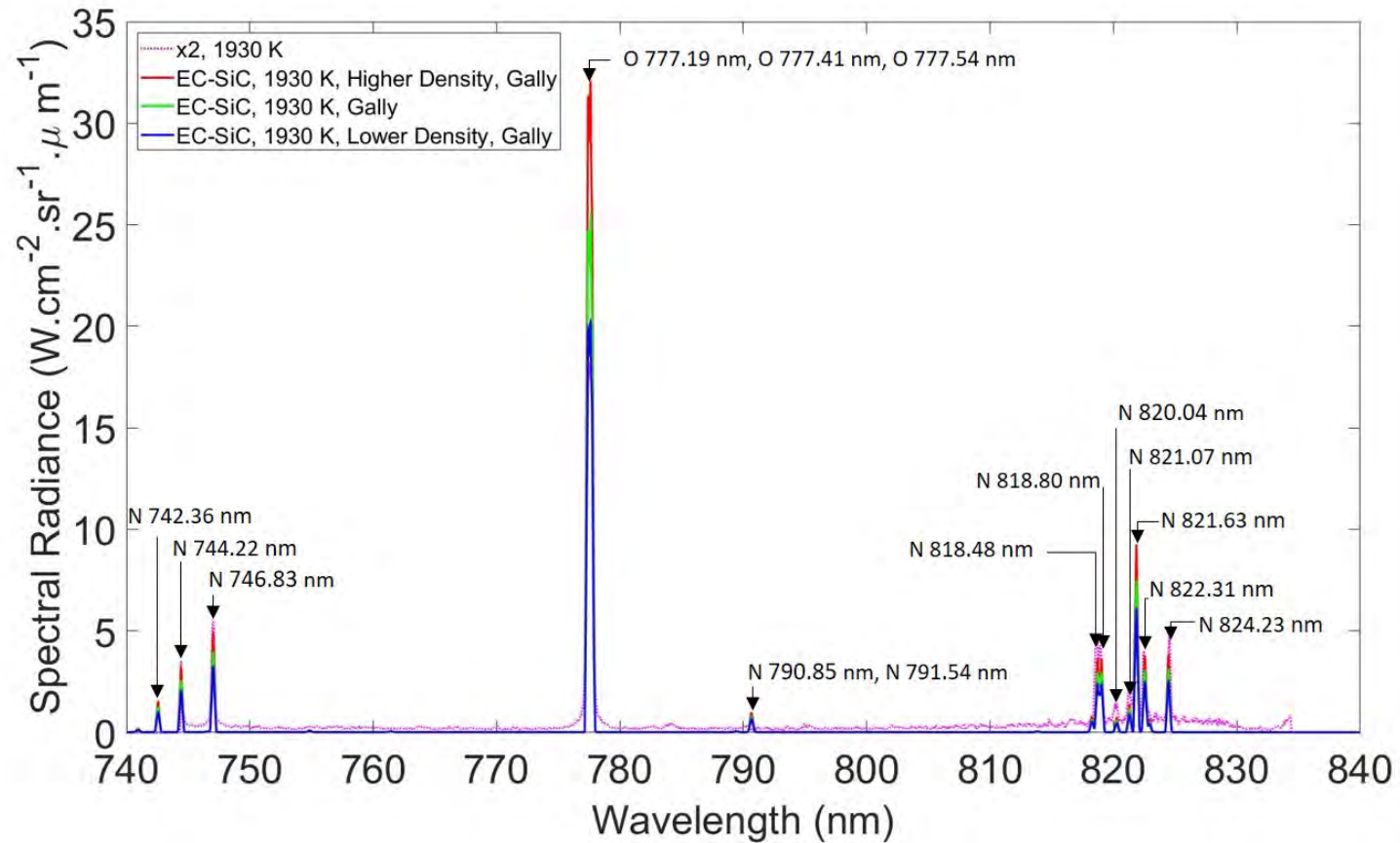


Figure 135. Experimental and simulated results for the 1930 K case for SiC-coated C-C targeting atomic N and O in the near-stagnation region with high and low density, using only the Gally model to populate the electronic states.

Figure 134 shows a similar plot of experimental and simulated results using only the Gally model. In general, the simulated results overpredict radiation of atomic O by about 35% while they underpredict atomic N by approximately 30%. Finally, Figure 135 shows experimental and simulated results with high and low values for density, as shown in Table 6. Density was selected as the flowfield parameter to vary to determine the impact of varying flowfield parameters since it has the largest uncertainty at approximately $\pm 8\%$. As shown in Figure 135, this implementation leads to approximately a variation in the radiation of $\pm 25\%$, which explains the difference between simulated results obtained using the Gally model and experimental results.

6.4 Summary

Simulations were run using the LAURA and HARA simulation codes following the process detailed in this chapter to replicate shock tube experiments. This technique involves a four-step process for computing the flowfield solution with ablation as well as a post-processing step to compute radiation using a stand-alone version of the HARA radiation code. This process required several files and inputs that normally are not needed. The main advantage of using the stand-alone version of the HARA code is that it allowed the user-defined points of the line-of-sight replicating that of the spectrometer to be hard-coded into the code.

Simulated radiation results for C-C in the near-stagnation region were in excellent agreement with experimental results. Simulated results obtained using the finite-rate ablation model were within 5% of the experimental results while simulated results obtained using the equilibrium-char ablation model underpredicted the experimental results by 40%. It was shown that the equilibrium-char ablation model predicts up to 50% less CN than the finite-rate ablation model, leading to this underprediction in

radiation. Simulated results for C-C in the expansion fared slightly worse, with the finite-rate model underpredicting experimental results by 25% while the equilibrium-char model again underpredicted by 40%.

Simulated results for SiC-coated C-C in the near-stagnation region matched experimental results surprisingly well; the 2005 K case was overpredicted by 15% while the 2439 case was overpredicted by 5%. It is believed that there may be an underprediction of CN radiation, which is the result of the equilibrium-char ablation model potentially underpredicting production of CN, that is being offset by an overprediction of N_2^+ radiation. The potential overprediction of N_2^+ radiation results from overpopulation of the excited electronic states for this transition. The significance of N_2^+ radiation is far lower in the expansion region, which may contribute to the order-of-magnitude underprediction in CN radiation for SiC-coated C-C in the expansion region. Assuming a Boltzmann distribution for the electronic state population of molecular species (i.e. CN and N_2^+) improves simulated results slightly, however improvements to the ablation model could potentially be much more impactful.

Using a Boltzmann distribution to compute radiation of atomic Si overpredicted by orders of magnitude compared to experimental data; a similar observation was made when including SiO in the simulated results, since the only model available for SiO assumes a Boltzmann distribution. Conversely, the Gally model underpredicted significantly. A main reason for this observation may again be the underprediction of the ablation rate, which could suggest that approximately 50% less Si is being introduced into the flowfield than is actually occurring. Again, improving the ablation model for SiC may greatly improve this shortcoming. The chemical reaction governing ionization of Si may also be a contributing factor. This reaction does not have a reference source as many of the other reactions do and should be investigated further.

The Gally model, which is one of two available non-Boltzmann models for atomic

N and O (the other being the CR model), provided the best comparison to experimental results. This result suggests that the Gally model is populating the electronic states for these species most in line with the experimental setup. Although there was approximately a 30% difference between simulated and experimental results, these results are in line with the experimental error. Results were obtained using high and low values for density, which is the flowfield parameter with the highest uncertainty at $\pm 8\%$, resulted in a $\pm 25\%$ variation in simulated radiation.

VII. Conclusions

High-temperature materials have long been a critical technology area for hypersonic vehicles, highlighted by a 2014 SAB study. Many researchers continue to investigate candidate materials, however the ability to model ablation and heating rates remains a significant challenge, particularly in wake flows. These efforts are further hampered by the lack of data in realistic hypersonic flight environments. C-C and SiC are two candidate materials, but both have issues with oxidation; C-C oxidizes at temperatures as low as 700 K and while SiC forms a protective oxide layer under certain conditions, it experiences significant mass loss and strength degradation at temperatures of approximately 1800 K. Characterization of the latter focuses heavily on the transition from passive to active oxidation.

Multiple experimental campaigns were conducted at the X2 superorbital expansion facility at the University of Queensland in order to build a comprehensive dataset to be used to evaluate state-of-the-art flowfield, ablation, and radiation models, in completion of Research Objective 2. The combination of the two experimental campaigns constitute one of the most comprehensive assessments of C-C and SiC-coated C-C, with calibrated spectral emission measurements obtained in the UV, vis/nIR, and MWIR regions. In the first experimental campaign, SiC-coated C-C was investigated for the first time at the X2 facility, satisfying Research Objective 1, along with uncoated C-C, expanding a relatively new preheating concept and enabling testing of additional materials. Different thicknesses, coating thicknesses, and fiber orientations were investigated in the near-stagnation and expansion regions at various locations above the model. It was found that fiber direction did not affect heating of the samples, with minor differences being attributed to slightly different thicknesses. Further, samples that were 6 mm thick did not break while those that were 3 mm thick did; the breaking likely occurred during the driver gas rather than the test gas,

but samples repeatedly breaking could affect the integrity of the model. A 1 mm thick coating survived the shot completely intact while the substrate was exposed on samples with a 300 μm thick coating, which was likely the result of the heavier helium/argon driver gas but was easily remedied by allowing for additional coating cycles. CN violet emissions were observed with increasing intensity with surface temperature while oxidation products (i.e. CO and CO₂) were not detected; a number of potential atomic Si lines were also identified.

The second experimental campaign built on the lessons learned from the first experimental campaign; all samples were made with a 6 mm thick substrate and all SiC-coated samples had a 1 mm thick coating. This design choice allowed test articles to be reused for multiple shots, which had never been done at the X2 facility, allowing quicker turnaround between shots and limiting the number of parts that need to be made. Flight-representative test articles can be quite expensive and manufacturing of complex composites can also take quite a long time; reuse of test articles can help ease this burden. CN violet emissions were again the dominant feature, while atomic N and atomic O were also observed at significantly lower intensity levels. A number of atomic Si lines were also identified, although not all of the lines observed by Panerai [26] could be distinguished from the facility contaminants.

The experiments showed higher intensity levels for SiC-coated C-C compared to C-C in the expansion region for CN violet, which suggests that the SiC coating is ablating at a higher rate than uncoated C-C and the ablation products are entering the flowfield at a higher rate; intensity for C-C was higher than SiC-coated C-C in the near-stagnation region. Spatial profiles of spectral radiance for SiC-coated C-C averaged between 384 and 389 nm, corresponding to CN violet, showed a distinct rise in intensity approximately 5 mm downstream of the shock, which is approximately where the expansion corner is located. This same trend was observed when averaging

spectral radiance from 250 to 253 nm, which is where atomic Si lines are suspected; a line at 288.16 nm, also believed to be atomic Si, showed this trend as did the previously-identified atomic Si line at 390.55 nm. This same observation could not be conclusively made when averaging between 467 and 474 nm, corresponding to C₂ Swan bands, due to the constant non-zero continuum.

Simulations were conducted using the process developed for this research, which was detailed in Chapter 6 in fulfillment of Research Objective 3, for comparison to experimental results. This process requires various aspects of the simulation, including grid adaptation, ablation, and radiation, to be added gradually over multiple steps. One of the most critical aspects of this process is to hold surface temperature as constant. Failure to do so results in the same converged solution regardless of the initial temperature. Surface temperature is updated as part of the solution process, so care must be taken to ensure that it is kept constant. Keeping surface temperature constant greatly increases the time required to achieve a converged solution; utilizing additional computing resources will not work as LAURA is unable to enforce the constant surface temperature boundary condition, likely due to the way tasks are assigned. The culmination of this computational study completes Research Objective 4.

Simulated radiation results for C-C were found to be in excellent agreement with experimental results, particularly when using the finite-rate ablation model. Results obtained with the equilibrium-char ablation model were shown to underpredict experimental results by 40%, which speaks to the benefit of using a high-fidelity model. The creation of a similar surface kinetics model for SiC would greatly enhance the ability to model ablation of this material and should be pursued.

The comparison between experimental and simulated results for atomic Si showed that neither a Boltzmann nor the present non-Boltzmann (Gally) model adequately

replicate the experimental results. The results obtained using a Boltzmann model overpredict by several orders of magnitude, while results using the Gally model underpredict significantly. The Gally model may yield more accurate results if a finite-rate ablation model were to be applied. Additionally, implementation of more accurate chemical reaction rates for the reaction governing the ionization of Si may improve this model. Regardless, developing a new non-Boltzmann model, similar to the CR model available for atomic N and O, may yield better simulated results and should be explored. Additionally, the development of a non-Boltzmann model for SiO would be beneficial. Although SiO radiation was not observed during the experimental campaigns, it may be significant for different flight regimes or if larger quantities of SiC are used.

It was observed that the simulations overpredicted radiation of N_2^+ . This overprediction is likely due to the overpopulation of the excited electronic states for this transition. Other sources of electron-impact excitation rates should be considered, particularly for their relevancy to the conditions being modeled for this work, for implementation into the HARA code. Choosing a source with lower excitation rates may result in lower population of the excited electronic states and thus, simulated radiation results that better match experimental results.

One of the significant challenges with interpreting experimental data of this nature is the identification of the spectral lines. The X2 facility has a number of known contaminants that make interpreting the experimental data even more challenging. Incorporating known contaminants into existing radiation codes, including HARA, could make identification of experimental spectra drastically easier. A main challenge in implementing this feature would be determining how much of a particular species to add to the flowfield. This parameter could be tuned to match experimental data. Alternatively, it may be easier to identify experimental spectral lines if materials

other than steel and aluminum are used for the primary and secondary diaphragm; additional materials should be considered, if they have not already.

The research undertaken in this dissertation focused on expanding hypersonic flows. Adding a turning corner to a two-dimensional compression wedge, such as the one used at the University of Queensland, would allow the recompression shock of wake flows to be simulated. The simulated results obtained throughout this research showed that shock temperatures are significantly higher than surface temperatures investigated. If similar temperatures are present in a wake recompression shock, spectral emissions could be significant despite much lower species concentrations; this significance may be especially true for atomic Si given its relative abundance compared to other species.

Conducting hypersonic experiments with a full three-dimensional wake will remain a significantly challenging task, especially if complex carbon composites are to be used. Efforts to machine C-C into three-dimensional conical shapes were undertaken early in this research with very poor results; only one cone was semi-successfully produced as the tooling used by the AFIT model shop repeatedly broke due to the extremely abrasive nature of C-C. This cone, shown in Figure 136 experienced problems with delamination. Before continuing with efforts to machine parts in such a way, a full model must be designed. For heated experiments, it would be best to start with graphite samples as they can be made much more cheaply as a proof-of-concept.

The experimental campaigns undertaken during this research represent one of the most comprehensive assessments of interaction of ablative materials with hypersonic flowfields. The abundance of data collected during the two experimental will be made available to both code developers and TPS designers to help improve existing models and designs, satisfying Research Objective 5. Further, the process developed and detailed in this dissertation to use the LAURA and HARA simulation codes can now

be applied to any geometry, including actual hypersonic vehicles. This research may one day lead to increased survivability and lethality of hypersonic weapon systems by improving the ability to model ablation and radiation, thereby reducing safety factors on thermal protection thickness and thus increasing payload.



Figure 136. Attempt at machining a 3D cone out of C-C.

Appendix A. AFRL Heating Experiment

Background.

An experiment was conducted 18-22 December 2017 with the support of personnel from AFRL. This experiment took place in building 65 on Wright-Patterson AFB utilizing AFRL/RQ's black body furnace. An optical pyrometer was set up by AFRL/RX personnel, who also assisted in post-test data processing. This experiment was conducted as a result of difficulties with temperature estimation during the first experimental campaign at the University of Queensland (UQ). The goal was to build heating profiles (i.e. temperature vs. power) for uncoated C-C and both types of SiC-coated C-C samples used during the experiments at UQ. From these heating profiles, it was hoped to obtain better temperature estimates for the second experimental campaign at UQ. Further, measurement of the time required to reach steady temperature at each power setting would aid in determining how long to heat test specimens during the second experimental campaign at UQ. It should be noted that the AFRL heating experiments utilized water cooling, which nearly eliminated any concern of melting or otherwise destroying any part of the test setup, while UQ currently does not have the ability to cool any part of the heating mechanism.

Test Setup.

The setup for this experiment is shown in Figure 137. The black body furnace proved capable of providing over 20,000 W of power while set to 45% of its maximum power setting. The spot size of the optical pyrometer, which was roughly the size of a dime, is shown in Figure 138. Power setting was controlled remotely by specifying a percentage of maximum power. The terminology used by AFRL for this power control was "drive voltage". For example, a drive voltage value of 1.0 corresponds to 10% maximum power while a drive voltage of 4.5 corresponds to 45% maximum

power. Diagnostic runs with scrap samples of approximately the same dimensions as actual test articles were conducted to determine what power setting to use to obtain a range of powers similar to those of the first experimental campaign at UQ.

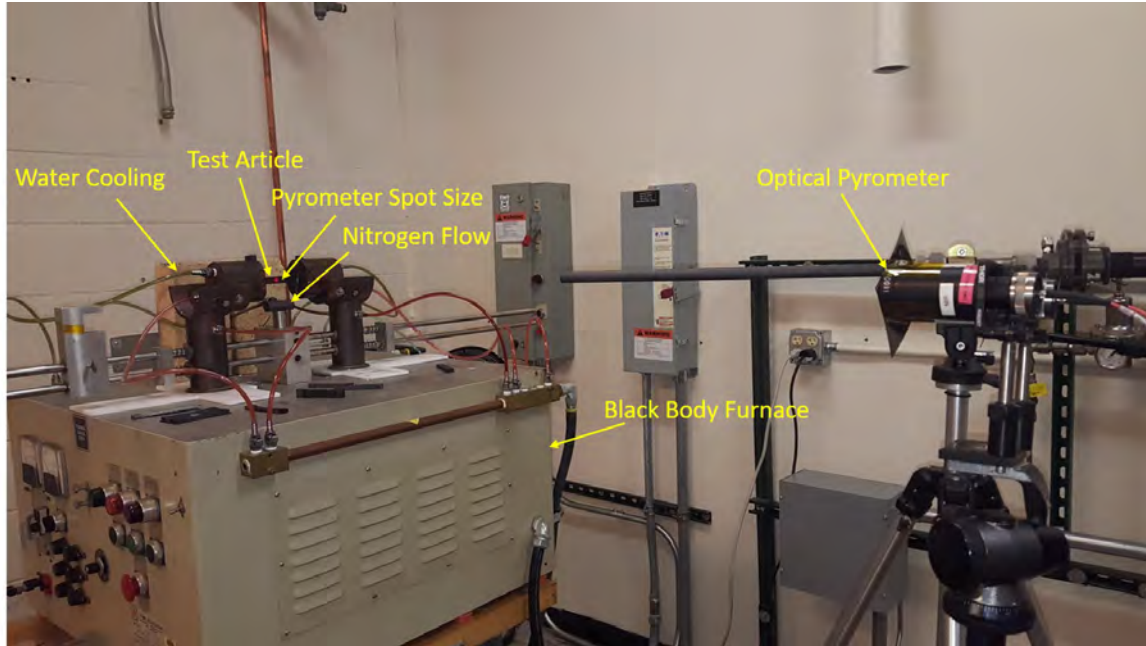


Figure 137. Setup for AFRL Heating Experiment.

A limited number of test articles were produced since it was unknown prior to diagnostic runs how much power this black body furnace was capable of producing or if scheduling would permit this experiment. Therefore, test articles were reused as long as their condition would allow it, up to five or six times. Nitrogen was flowing over the test articles as they were heated in an effort to prevent or delay oxidation, thus limiting mass loss. This approach was undertaken in an effort to preserve the test articles and also to replicate the vacuum conditions that test articles are heated under at UQ immediately before the shot.

Results.

During the experiments, three C-C samples and two of each type of SiC-coated samples were examined. The following subsections will present results for each ma-

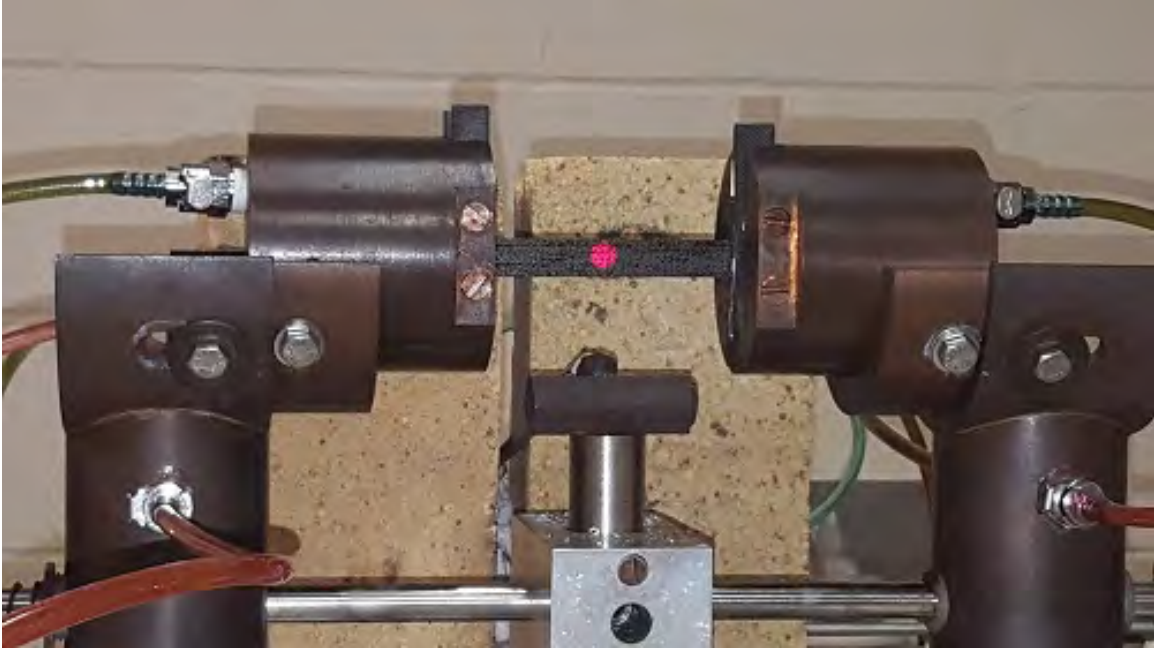


Figure 138. Spot Size of AFRL Optical Pyrometer.

terial.

C-C.

Tables 18, 19, and 20 show the heating condition for each C-C sample, as well as measured temperature and time to reach steady temperature while Figure 139 shows temperature vs. power for all three samples. Tables 21, 22, and 23 show temperature vs. time for each condition. In these tables, as well as others throughout this appendix, entries with an asterisk (*) indicate that no signal was detected by the pyrometer. In general, there was good consistency between the samples with a significant increase in time to reach a steady temperature at lower power settings. For the temperatures corresponding to the those measured during the experiments at UQ, it took between 15 and 35 seconds to reach a steady temperature. It should be noted that when the third sample was heated with a drive voltage of 4.5, the sample failed 8.4 seconds into the test and would likely have achieved a slightly higher temperature. This temperature of approximately 3600 K is believed to be the highest temperature

ever measured in this facility.

Table 18. Heating profile for first C-C sample.

Drive Voltage	Voltage, V	Current, A	Power, W	Temperature, K	Time To Steady Temperature, s
3.0	14	870	12180	2990	15
2.7	12.8	720	9216	2920	15
2.3	11.1	630	6993	2600	15
1.9	9.3	455	4231.5	2320	20
1.7	8.3	380	3154	2210	30
1.5	7.3	305	2226.5	2050	35
1.15	5.5	190	1045	1600	60
1.0	4.4	130	572	1330	90

Table 19. Heating profile for second C-C sample.

Drive Voltage	Voltage, V	Current, A	Power, W	Temperature, K	Time To Steady Temperature, s
3.0	13.9	850	11815	2980	15
2.7	12.7	729	9258.3	2950	15
2.3	11.0	625	6875	2550	15
1.9	9.2	460	4232	2310	20
1.7	8.2	380	3116	2350	30
1.15	5.3	200	1060	1510	60
1.0	4.5	150	675	1170	90

Table 20. Heating profile for third C-C sample.

Drive Voltage	Voltage, V	Current, A	Power, W	Temperature, K	Time To Steady Temperature, s
4.5	18.2	1150	20930	3590	8.4
3.5	15.7	895	14051.5	3280	20
1.7	8.2	350	2870	2050	30
1.5	7.1	270	1917	1900	35
1.15	5.2	160	832	1500	60
1.0	4.5	125	562.5	1190	90

Original SiC Coating.

Tables 24 and 25 show the heating condition for the two SiC-coated C-C samples with the original SiC coating while Figure 140 shows temperature vs. power for both samples. Tables 26 and 27 show temperature vs. time for each condition. There was again good consistency between the two samples. Compared to C-C, the SiC-coated C-C samples took much longer to reach steady temperature and required a higher

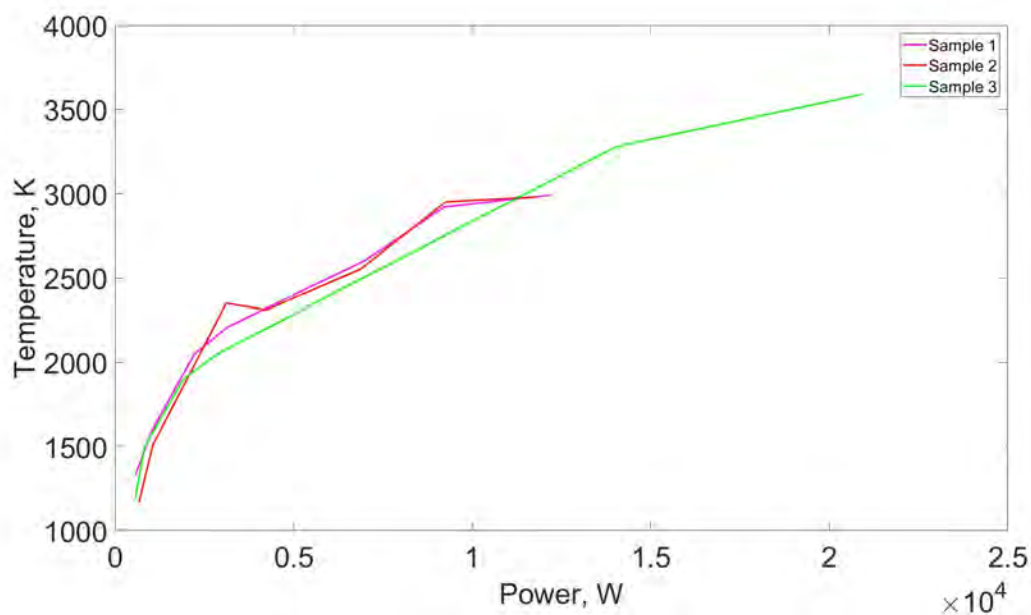


Figure 139. Temperature vs. Power for C-C.

Table 21. Temperature vs. time for first C-C sample.

		Time, s												
		5	10	15	20	25	30	35	40	50	60	70	80	90
Drive Voltage	3.0	1640 K	2670 K	2990 K										
	2.7	1610 K	2690 K	2920 K										
	2.3	1460 K	2310 K	2600 K										
	1.9	1200 K	1840 K	2200 K	2320 K									
	1.7	*	1440 K	1890 K	2100 K	2180 K	2210 K							
	1.5	*	1340 K	1690 K	1890 K	1985 K	2025 K	2050 K						
	1.15	*	*	660 K	1270 K	1390 K	1460 K	1500 K	1550 K	1590 K	1600 K			
	1.0	*	*	*	*	1080 K	1110 K	1130 K	1150 K	1180 K	1220 K	1240 K	1310 K	1330K

Table 22. Temperature vs. time for second C-C sample.

		Time, s												
		5	10	15	20	25	30	35	40	50	60	70	80	90
Drive Voltage	3.0	1620 K	2670 K	2980 K										
	2.7	1900 K	2760 K	2950 K										
	2.3	1440 K	2280 K	2550 K										
	1.9	1230 K	1850 K	2190 K	2310 K									
	1.7	*	1520 K	2000 K	2210 K	2310 K	2350 K							
	1.15	*	*	1110 K	1230 K	1330 K	1390 K	1410 K	1450 K	1500 K	1510 K			
	1.0	*	*	*	*	*	860 K	1110 K	1140 K	1160 K	1150 K	1140 K	1150 K	1170K

Table 23. Temperature vs. time for third C-C sample.

		Time, s												
		5	10	15	20	25	30	35	40	50	60	70	80	90
Drive Voltage	4.5	3360 K												
	3.5	2000 K	3000 K	3160 K	3280 K									
	1.7	*	1170 K	1520 K	1810 K	1960 K	2050 K							
	1.5	*	*	1330 K	1570 K	1720 K	1830 K	1900 K						
	1.15	*	*	*	1080 K	1150 K	1210 K	1330 K	1430 K	1500 K				
	1.0	*	*	*	*	*	*	*	*	640 K	1130 K	1150 K	1170 K	1190 K

power setting for a signal to be detected by the pyrometer. For the temperatures corresponding to the those measured during the experiments at UQ, it took between 35 and 70 seconds to reach a steady temperature. For both samples, the testing halted when a noticeable outgassing was observed, which is believed to be the transition from passive to active oxidation. This transition occurred at a higher temperature than was reported in the literature so it is likely that the nitrogen flowing over the samples was effective in delaying this transition, though it could not prevent it.

Table 24. Heating profile for first SiC-coated C-C sample, original coating.

Drive Voltage	Voltage, V	Current, A	Power, W	Temperature, K	Time To Steady Temperature, s
2.3	10.9	490	5341	2555	35
1.9	9.1	370	3367	2185	60
1.7	8.1	320	2592	1980	65
1.5	7.1	265	1881.5	1680	65
1.15	5.0	160	800	1195	80
1.0	*	*	*	*	*

Table 25. Heating profile for second SiC-coated C-C sample, original coating.

Drive Voltage	Voltage, V	Current, A	Power, W	Temperature, K	Time To Steady Temperature, s
2.3	10.9	445	4850.5	2655	35
1.9	9.0	335	3015	2285	60
1.7	8.1	290	2349	1890	70
1.5	6.9	210	1449	1510	65
1.15	*	*	*	*	*
1.0	*	*	*	*	*

Table 26. Temperature vs. time for first SiC-coated C-C sample, original coating.

		Time, s												
		5	10	15	20	25	30	35	40	50	60	70	80	90
Drive Voltage	2.3	1130 K	1690 K	2100 K	2330 K	2500 K	2445 K	2555 K						
	1.9	*	1180 K	1520 K	1780 K	1940 K	2040 K	2090 K	2130 K	2170 K	2185 K			
	1.7	*	1090 K	1340 K	1530 K	1670 K	1770 K	1840 K	1890 K	1920 K	1945 K	1980 K		
	1.5	*	*	860 K	1210 K	1310 K	1400 K	1475 K	1540 K	1620 K	1670 K			
	1.15	*	*	*	*	*	855 K	650 K	410 K	*	*	1135 K	1195 K	
	1.0	*	*	*	*	*	*	*	*	*	*	*	*	*

New SiC Coating.

Figures 28 and 29 show the heating condition for the two SiC-coated C-C samples with the new SiC coating while Figure 141 shows temperature vs. power for both

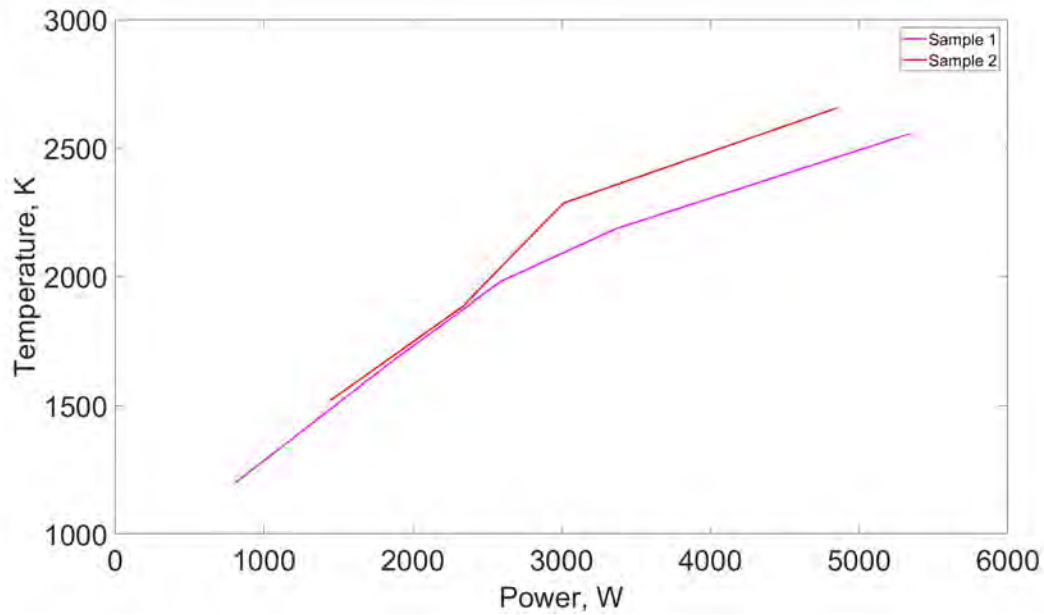


Figure 140. Temperature vs. Power for SiC-coated C-C, original SiC coating.

Table 27. Temperature vs. time for second SiC-coated C-C sample, original coating.

		Time, s												
		5	10	15	20	25	30	35	40	50	60	70	80	90
Drive Voltage	2.3	*	1625 K	2090 K	2370 K	2550 K	2590 K	2655 K						
	1.9	*	*	1325 K	1575 K	1795 K	1925 K	2080 K	2145 K	2190 K	2285 K			
	1.7	*	*	*	1240 K	1390 K	1520 K	1590 K	1640 K	1795 K	1845 K	1890 K		
	1.5	*	*	*	1140 K	1230 K	1280 K	1340 K	1390 K	1480 K	1510 K			
	1.15	*	*	*	*	*	*	*	*	*	*	*	*	*
	1.0	*	*	*	*	*	*	*	*	*	*	*	*	*

samples. Tables 30 and 31 show temperature vs. time for each condition. Like with the original SiC coating, samples with the new SiC coating took longer to reach a steady temperature than the uncoated samples. The time required was generally similar for the original and new SiC coating. The big exception to this trend was that for both samples with the new SiC coating, it took an extremely long time to reach a steady temperature at a drive voltage of 1.5. For one of the samples, it took nearly three minutes while it took nearly two for the other. As with the original SiC coating, testing was halted when both samples exhibited an outgassing. This phenomena was again believed to be the transition from passive to active oxidation, which again occurred at a higher temperature than what others have reported due to the nitrogen flowing over the samples

Table 28. Heating profile for first SiC-coated C-C sample, new coating.

Drive Voltage	Voltage, V	Current, A	Power, W	Temperature, K	Time To Steady Temperature, s
2.1	10.0	345	3450	2450	33
1.9	9.0	315	2835	2220	30
1.7	8.0	270	2160	2035	35
1.5	7.0	240	1680	1890	170
1.15	5.1	155	790.5	1340	60
1.0	*	*	*	*	*

Table 29. Heating profile for second SiC-coated C-C sample, new coating.

Drive Voltage	Voltage, V	Current, A	Power, W	Temperature, K	Time To Steady Temperature, s
2.1	9.9	360	3564	2475	40
1.9	9.0	330	2970	2285	45
1.7	8.0	290	2320	2100	70
1.5	7.0	260	1820	1870	100
1.15	5.0	155	775	1195	60
1.0	*	*	*	*	*

Heating profiles for uncoated C-C and SiC-coated C-C are shown in Figures 142, 143, and 144. Curve fits were generated using Matlab[®], which are shown in these figures. For the uncoated C-C and the new SiC-coated C-C, a two-term power model provided the best fit while a second-order polynomial was the best fit for the original

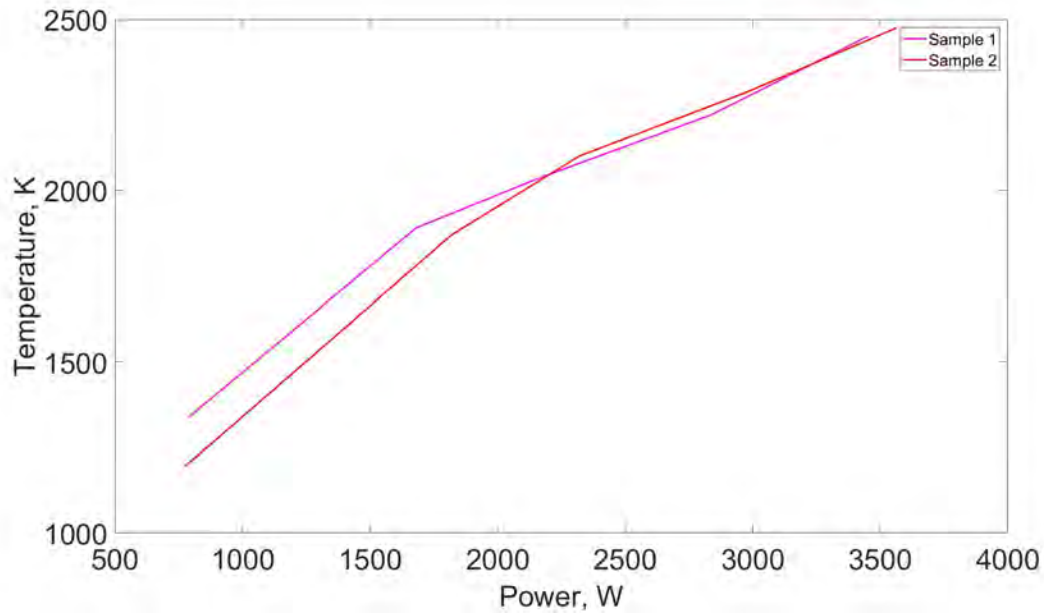


Figure 141. Temperature vs. Power for SiC-coated C-C, new SiC coating.

Table 30. Temperature vs. time for first SiC-coated C-C sample, new coating.

		Time, s												
		5	10	15	20	25	30	35	40	50	60	70	80	90
Drive Voltage	2.1	*	1450 K	1915 K	2155 K	2330 K	2410 K							
	1.9	*	1435 K	1665 K	1915 K	2075 K	2190 K	2200 K	2225 K	2245 K	2250 K	2260 K		
	1.7	*	1280 K	1430 K	1600 K	1785 K	1935 K	2035 K						
	1.5	*	*	1290 K	1370 K	1480 K	1555 K	1550 K	1595 K	1645 K	1685 K	1710 K	1720 K	1725 K
	1.15	*	*	*	*	*	*	1250 K	1250 K	1300 K	1340 K			
	1.0	*	*	*	*	*	*	*	*	*	*	*	*	

Table 31. Temperature vs. time for second SiC-coated C-C sample, new coating.

		Time, s												
		5	10	15	20	25	30	35	40	50	60	70	80	90
Drive Voltage	2.1	*	1525 K	1995 K	2255 K	2375 K	2425 K	2465 K	2475 K					
	1.9	*	1275 K	1680 K	1960 K	2130 K	2220 K	2260 K	2275 K	2285 K				
	1.7	*	*	1320 K	1590 K	1815 K	1925 K	1995 K	2040 K	2070 K	2090 K	2100 K		
	1.5	*	*	1140 K	1290 K	1415 K	1525 K	1590 K	1645 K	1725 K	1800 K	1820 K	1840 K	1850 K
	1.15	*	*	*	*	*	*	*	*	1145 K	1195 K	1190 K	*	
	1.0	*	*	*	*	*	*	*	*	*	*	*	*	

SiC coating. In all cases, the R^2 values, which provide a statistical measure of how close the data are to the fit, were close to 0.98 or greater, indicating a very good fit. These heating profiles were used during the second X2 experimental campaign to help estimate surface temperatures and to select heating conditions to achieve surface temperatures corresponding to the first X2 experimental campaign.

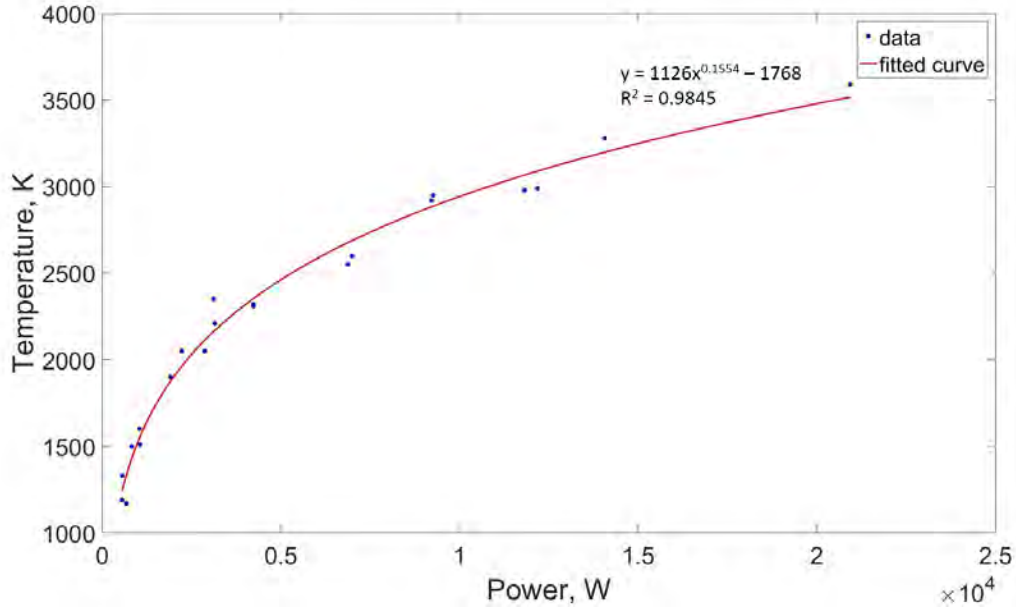


Figure 142. Temperature vs. Power for C-C.

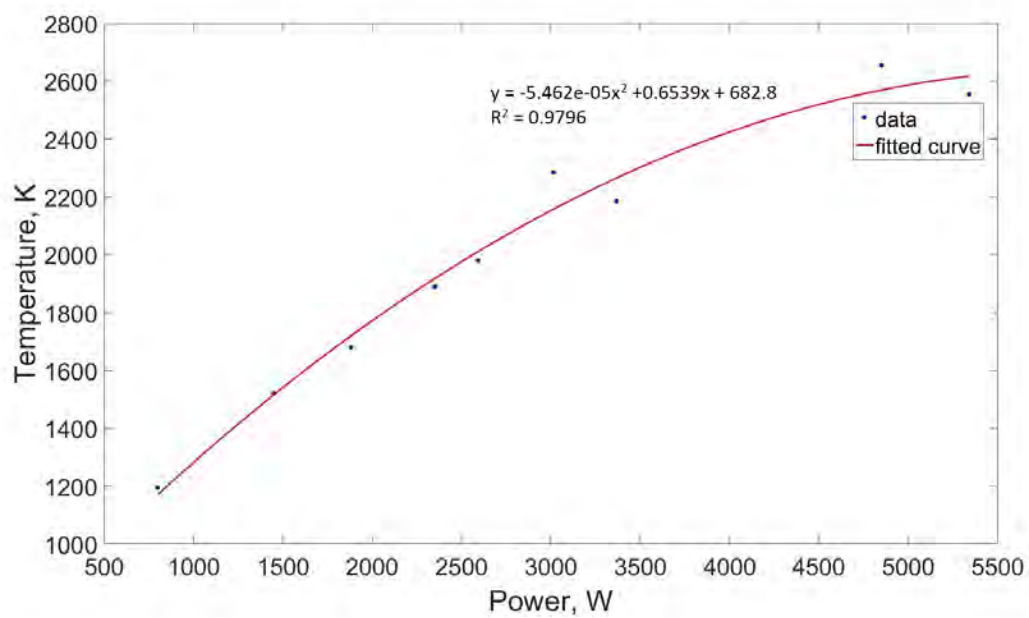


Figure 143. Temperature vs. Power for SiC-coated C-C, original SiC coating.

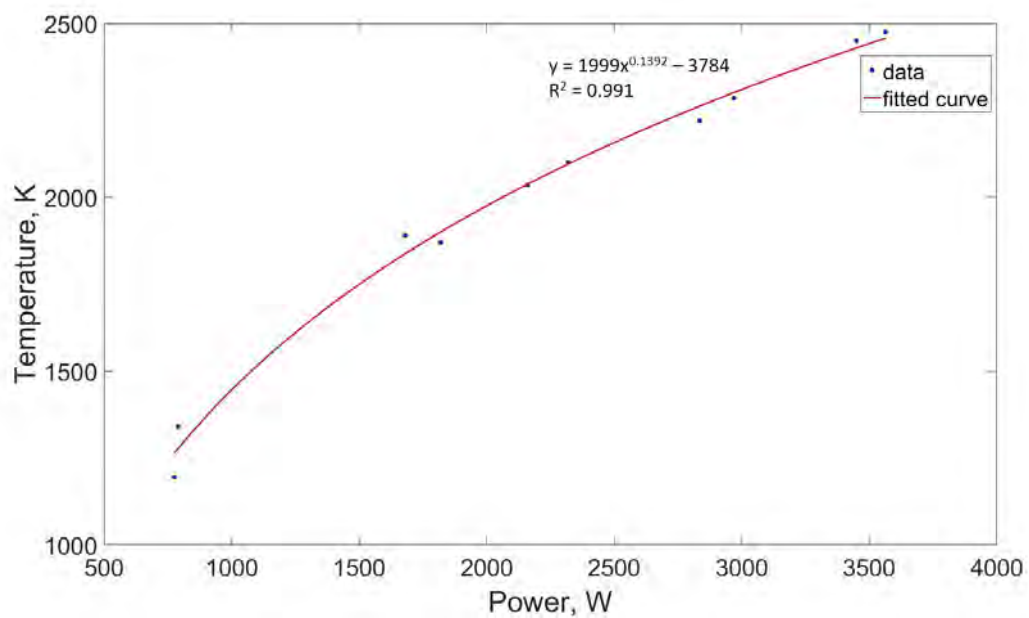


Figure 144. Temperature vs. Power for SiC-coated C-C, new SiC coating.

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Vita

Major Brian Donegan was born in Framingham, Massachusetts. After graduating from Milford High School in 2003, he studied Aeronautical Engineering at Rensselaer Polytechnic Institute. he graduated with a Bachelor of Science degree in May 2007. At the same time, he commissioned into the United States Air Force through the Reserve Officer Training Corps, Detachment 550, at Rensselaer Polytechnic Institute.

Major Donegan's first active duty assignment was to Headquarters Air Combat Command at Langley Air Force Base, Virginia. During this assignment, he earned a Master of Engineering degree in Aerospace Engineering from Old Dominion University in 2010. In 2011, Major Donegan was reassigned to Space and Missile Systems Center at Los Angeles Air Force Base, California. During this assignment, he worked on hypersonic technology development and as a test director for the Global Positioning Systems Directorate. In 2015, he entered the Aeronautical Engineering PhD program at the School of Engineering and Management, Air Force Institute of Technology.

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Thermal protection is required for vehicles entering planetary atmospheres to protect against the severe heating loads experienced. Modeling ablation and heating rates, particularly in the wake region, remains a significant challenge. To better understand this complex phenomenon, experiments were conducted at the X2 expansion tunnel at the University of Queensland. Preheated strips of C-C and SiC-coated C-C were mounted in a two-dimensional compression wedge and tested in Earth entry flow. Calibrated spectral measurements were obtained for surface temperatures from approximately 1900 K to 2700 K. Emissions for C-C and SiC appeared similar in the near-stagnation region, while emissions for SiC-coated C-C displayed a distinct rise downstream of the shock, which suggests a higher concentration of ablative species. There was generally good agreement for CN emissions, which were most dominant, while the agreement was not as good for the other radiative phenomena investigated. It is believed that the underprediction of the ablation rate of the equilibrium-char model is a key factor.						
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					(937) 255-3636 x4567; robert.greendyke@afit.edu	