SANDIA REPORT

SAND2005-5979

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Printed September 2005

Modeling Microscale Heat Transfer Using Calore

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Abstract

Modeling microscale heat transfer with the computational-heat-transfer code Calore is discussed. Microscale heat transfer problems differ from their macroscopic counterparts in that conductive heat transfer in both solid and gaseous materials may have important noncontinuum effects. In a solid material, three noncontinuum effects are considered: ballistic transport of phonons across a thin film, scattering of phonons from surface roughness at a gas-solid interface, and scattering of phonons from grain boundaries within the solid material. These processes are modeled for polycrystalline silicon, and the thermal-conductivity values predicted by these models are compared to experimental data. In a gaseous material, two noncontinuum effects are considered: ballistic transport of gas molecules across a thin gap and accommodation of gas molecules to solid conditions when reflecting from a solid surface. These processes are modeled for arbitrary gases by allowing the gas and solid temperatures across a gas-solid interface to differ: a finite heat transfer coefficient (contact conductance) is imposed at the gas-solid interface so that the temperature difference is proportional to the normal heat flux. In this approach, the behavior of gas in the bulk is not changed from behavior observed under macroscopic conditions. These models are implemented in Calore as user subroutines. The user subroutines reside within Sandia's SourceForge server, where they undergo version control and regression testing and are available to analysts needing these capabilities. A Calore simulation is presented that exercises these models for a heated microbeam separated from an ambient-temperature substrate by a thin gas-filled gap. Failure to use the noncontinuum heat transfer models for the solid and the gas causes the maximum temperature of the microbeam to be significantly underpredicted.

Acknowledgment

This project was funded by the Advanced Simulation and Computing (ASC) program at Sandia National Laboratories through the Physics and Engineering Models (PEM) project, formerly called the Materials and Physical Models (M&PM) project. The authors thank Steven N. Kempka of Sandia National Laboratories for helpful technical discussions and management guidance. The graphic-arts skills of Mitzie Bower of Sandia National Laboratories are gratefully acknowledged. The careful reviews of Michael L. Hobbs and Richard C. Givler of Sandia National Laboratories are greatly appreciated.

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Nomenclature for Solid Model

Roman Variables

a	ratio of grain radius of curvature to grain size
d	diameter or size [m]
f	phonon probability distribution function
f_o	phonon probability distribution function at thermal equilibrium
h	Planck constant, $6.6260755 \times 10^{-34}$ J · s
i	summation variable
k	phonon thermal conductivity [W/(m·K)]
k_B	Boltzmann constant. 1.380658×10^{-23} J/K
l	thickness of film [m]
n	temperature exponent in thermal conductivity (not necessarily an integer)
P	probability that a phonon reflects specularly from a film boundary
p	phonon momentum [kg·m/s]
r	phonon position [m]
T	temperature [K]
t	time [s]
v	phonon propagation velocity [m/s]
W	phonon scattering rate [1/s]
x	integration variable

Greek Variables

γ	mode of phonon polarization
ζ	external force field acting on phonons [N]
η	surface roughness of film boundary [m]
θ_D	Debye temperature [K]
λ	phonon wavelength [m]
τ	relaxation time [s]
ν	phonon frequency [1/s]
ϕ	variance for phonon scattering from rough surface
χ	radius of curvature of dominant grain size [m]
ω	phonon angular frequency [radian/s]

Superscripts

$(\dots)'$	summation variable
------------	--------------------

Subscripts

$(\dots)_{film}$	quantity associated with a film
$(\dots)_{grain}$	quantity associated with a grain
$(\dots)_{scatter}$	quantity associated with phonon scattering

$(\dots)_{transmission}$ quantity associated with phonon transmission across a grain boundary

Acronyms

B-E	Bose-Einstein
BGK	Bhatnagar-Gross-Krook
SMM	surface micromachining

Nomenclature for Gas Model

Roman Variables

C_p	specific heat at constant pressure [J/(kg·K)]
$\bar{c}$	mean molecular speed in equilibrium gas [m/s]
D	lateral extent, or “diameter”, of a body [m]
F	domain scale factor [$F > 0$]
G	thickness of gas-filled gap [m]
H	thickness of solid slab [m]
h	heat transfer coefficient [W/(m ² ·K)]
K	thermal conductivity [W/(m·K)]
k_B	Boltzmann constant, 1.380658×10^{-23} J/K
L	length of domain (out-of-page) [m]
m	molecular mass [kg]
$\hat{n}$	unit vector normal to a boundary
n	number density [#/m ³]
p	pressure [Pa]
Q	heat flow or power [W]
$\mathbf{q}$	heat flux vector [W/m ²]
q	heat flux normal to a boundary [W/m ²]
S	volumetric heat source [W/m ³]
T	temperature [K]
t	time [s]
W	width of domain [m]
$\mathbf{x}$	position vector [m]
x	Cartesian coordinate in-plane and parallel to substrate [m]
y	Cartesian coordinate in-plane and perpendicular to substrate [m]
z	Cartesian coordinate out-of-plane and parallel to substrate [m]
Z	internal energy exchange collision number [$Z \geq 1$]

Greek Variables

α	angular scattering exponent [$\alpha \geq 1$]
ζ	internal energy mode number [$\zeta \geq 0$]
γ	specific heat ratio [$1 < \gamma \leq 5/3$]
λ	molecular mean free path [m]
μ	absolute viscosity [Pa·s]
ρ	mass density [kg/m ³]
σ	accommodation coefficient [$0 \leq \sigma \leq 1$]
ω	viscosity temperature exponent [$1/2 \leq \omega \leq 1$]

Superscripts

$\overline{(\dots)}$	average value
----------------------	---------------

Subscripts

$(\dots)_A$	quantity evaluated at colder boundary
$(\dots)_B$	quantity evaluated at hotter boundary
$(\dots)_{FM}$	quantity evaluated at free-molecular conditions
$(\dots)_p$	quantity evaluated at constant pressure
$(\dots)_{\text{ref}}$	quantity evaluated at reference conditions
$(\dots)_s$	quantity associated with solid material

Acronyms

BE	Boltzmann equation
DSMC	Direct Simulation Monte Carlo
FM	free-molecular
NSSJ	Navier-Stokes Slip-Jump

1. Introduction

1.1. Overview

Microscale heat transfer issues in solids and gases are reviewed. Noncontinuum effects, not significant at the macroscale, become important at the microscale. These effects are discussed for a thin polycrystalline-silicon film and a thin gas-filled gap. The modeling approach uses the conductive-heat-transfer capabilities of Calore and is outlined. The following topics are covered.

- Chapter 1 reviews microscale heat transfer issues and application of Calore to these problems.
- Chapter 2 presents the thermal-conductivity model for thin films of polycrystalline silicon.
- Chapter 3 presents the heat-transfer-coefficient model for gas-solid interfaces.
- Chapter 4 applies these models to a heated microbeam surrounded by gas and near a substrate.
- Chapter 5 provides conclusions and discusses future work.
- Appendix A provides Calore subroutines for these models and instructions on their use.

1.2. Microscale Heat Transfer Issues

Many microscale devices rely on heat transfer in the course of their operation. Figure 1.1 shows one such example: a microscale optical shutter that has laser light incident on its surface and transports this energy to the nearby substrate via conduction (Wong and Graham, 2003). The top portion of the figure shows a micrograph of one such optical shutter, and the bottom portion of the figure shows the corresponding temperature field from a Calore simulation. The temperature rise produces thermal stresses that can modify the component's shape and thereby affect its performance and, if extreme, can impact the component's mechanical integrity. Another example of a microdevice that relies on heat deposition and heat transfer for successful operation is a microscale electrothermal actuator (Plass et al., 2004). In such a device, electrical current is passed through a portion of the structure. The balance between the resultant Joule heating and the heat loss to the nearby substrate (at ambient temperature) determines the temperature rise, and the temperature rise in conjunction with the coefficient of thermal expansion determines the displacement. Thus, it is essential to be able to compute microscale heat transfer accurately.

Microscale heat transfer differs from macroscale heat transfer. The reason for this is as follows. Conductive heat transfer has a length scale associated with it that corresponds to the average distance (mean free path) traveled by the energy carriers (e.g., electrons, phonons, gas molecules) before they scatter or collide. Macroscale devices are much larger than the mean free path. In this situation, the energy carriers experience many scattering events or collisions within the bulk material before they encounter a boundary. As a result, the energy carriers achieve a nearly equilibrium distribution of their properties (e.g., a Fermi-Dirac distribution for electrons, a Bose-

Einstein distribution for phonons, a Maxwellian distribution for gas molecules), so the energy transport that results is generic to the bulk material and is therefore referred to as “continuum”. Microscale devices, however, are comparable to or smaller than the mean free path. In this situation, the energy carriers experience relatively few scattering events or collisions within the bulk material before they encounter a boundary (e.g., a material interface or a grain boundary). As a result, the energy carriers may not achieve a near-equilibrium distribution, so the energy transport that results differs from bulk behavior and is therefore referred to as “noncontinuum”.

The top diagram in Figure 1.2 illustrates three important noncontinuum processes that occur in a thin film of polycrystalline silicon. Phonons (quanta of lattice vibrational energy) are the main energy-transporting entities in this material. Possible phonon trajectories are represented by arrows. Ordinary phonon-phonon scattering in crystalline silicon is represented by blue and green trajectories that intersect and change directions. The three noncontinuum processes are represented by red arrows. The first process involves ballistic transport of phonons across the thickness of the film. When this occurs, phonons transport energy directly from one interface to another without interacting with other phonons en route. The probability of this occurring decreases exponentially with the film thickness, so this process is not important for macroscale objects but is important for microscale films. The second process involves the scattering of phonons from surface roughness at the gas-solid interface. The degree of surface roughness is highly exaggerated in the figure for illustration purposes. The nature and degree of the surface roughness affects the distribution of scattered phonons as well as the possibility of energy transfer into the adjacent gas-filled region. The third process involves the scattering of phonons from grain boundaries within a polycrystalline material. The relative importance of this effect is determined in part by the size of typical grains relative to the film thickness and to the distance that phonons travel within single-crystal bulk material before scattering. These three noncontinuum processes and their effects on heat transfer are discussed in greater detail in Chapter 2.

The bottom diagram in Figure 1.2 illustrates two important noncontinuum processes that occur for gas molecules in a thin gap bounded by two regions of solid material. Possible gas-molecule trajectories are represented by arrows. Binary collisions of gas molecules are represented by blue and green trajectories that intersect and change directions. The two noncontinuum processes are represented by red arrows and are in many ways analogous to the first two processes discussed above for phonons. The first process involves ballistic transport of gas molecules across the gap. When this occurs, gas molecules transport energy directly from one interface to another without interacting with other gas molecules en route. Again, the probability of this occurring decreases exponentially with the gap thickness, so this process is not important for macroscale gaps but is important for microscale gaps. The second process involves the reflection of gas molecules from a solid surface and the accommodation of gas molecules to the solid surface. Here, “accommodation” denotes the probability that reflecting gas molecules acquire (on average) the temperature of the solid surface. This probability is affected by the properties of the gas molecules and the solid molecules (or of the molecules resident on the surface) and by the surface roughness. Again, the degree of surface roughness is highly exaggerated in the figure for illustration purposes. It is noted in passing that there is no analogous process in the gas to the third process discussed above for phonons. These two noncontinuum processes and their effects on heat transfer are discussed in greater detail in Chapter 3.

1.3. Calore Modeling

Calore is the Sierra computational tool for performing a wide variety of heat transfer simulations (Bova et al., 2005). Calore is capable of simulating conductive and radiative heat transfer, multiple materials, a nonzero thermal resistance (inverse contact conductance) between different materials, and steady and transient behavior in two or three spatial dimensions. Calore has been developed for parallel implementation to allow the solution of large problems and for use in conjunction with other Sierra computational tools such as Adagio. The combination of Calore and Adagio makes it possible to simulate the response of a solid structure to a thermally generated stress field. This capability is important for the analysis of the microscale thermal actuator, as discussed in the previous section.

The ability of Calore to simulate conductive heat transfer is of prime importance in the simulation of microsystems for two reasons. First, conduction is the most important heat transfer mechanism in many microsystems because of their small size. Second, the equations describing conduction provide the framework for implementing models for the noncontinuum processes described in the previous section.

Within a single material, the equation of conductive heat transfer has the following form:

$$\rho C_p \left(\frac{\partial T}{\partial t} \right) = \left(\frac{\partial}{\partial \mathbf{x}} \right) \cdot \left[K \left(\frac{\partial T}{\partial \mathbf{x}} \right) \right] + S, \quad (1.1)$$

where T is the temperature, ρ is the mass density, C_p is the specific heat at constant pressure, K is the thermal conductivity, S is the volumetric heat source term, t is time, and $\mathbf{x}$ is position. In this formulation, Fourier's law is used to relate the heat flux $\mathbf{q}$ to the temperature gradient:

$$\mathbf{q} = -K \left(\frac{\partial T}{\partial \mathbf{x}} \right). \quad (1.2)$$

The quantities ρ , C_p , K , and S can be functions of temperature, position, and time. At the interface between two materials, the temperature can be discontinuous across the interface, with the temperature difference proportional to the heat flux:

$$q = h \Delta T, \quad (1.3)$$

where q is the heat flux normal to the interface, ΔT is the temperature difference across the interface, and h is the heat transfer coefficient or contact conductance. Thus, $1/h$ is the thermal or contact resistance. In the limit of an infinite heat transfer coefficient (or a vanishing thermal resistance), the temperature difference vanishes, so the temperature is continuous across the interface between the two materials.

While not considered here, the Calore versions of the above equations also incorporate convective heat transfer with a prescribed divergence-free velocity field and conductive heat transfer with a tensor thermal conductivity (Bova et al., 2005).

Perhaps somewhat paradoxically, the models for the noncontinuum processes described above are developed in the context of the continuum conductive heat transfer formulation presented above. Within this formulation, four quantities are available for model development: the mass density ρ , the specific heat at constant pressure C_p , the thermal conductivity K , and the heat transfer coefficient (contact conductance) h . The first three quantities are specific to a particular material, whereas the fourth quantity is shared by the two materials on opposite sides of an interface. Slightly different modeling strategies are employed for the solid and the gas, as outlined below.

The following modeling strategy is employed for the solid. The mass density and the specific heat at constant pressure retain their bulk values, the thermal conductivity is modified from the bulk value, and the heat transfer coefficient is reserved for the gas. The thermal-conductivity model incorporates the effects of film thickness, surface roughness, and grain size to produce a scalar value appropriate for thermal conduction along a broad thin polycrystalline-silicon film. More specifically, the relevant metric of comparison is conduction along the film, rather than across its very small thickness. The reasons for this approach are as follows. Conduction of heat in the direction across the film is controlled by conduction of heat across the interface separating the solid film and the adjacent gas and by conduction of heat within the adjacent gas. The thermal conductivity of the gas is approximately four orders of magnitude smaller than that of the solid, and their geometric length scales are very similar (typically a few microns for each material). As a result, temperature variations across the solid film are negligibly small compared to temperature variations in the adjacent gas: the thermal conductivity of the solid is so large that the solid is locally isothermal across the film and the precise value of its thermal conductivity across the film is not important. However, the thermal conductivity along the film is of critical importance since one of the main processes for heat removal is conduction along the film to solid attachment points, through which heat is exhausted into the essentially semi-infinite substrate at ambient temperature. Therefore, the thermal conductivity along the film is the important quantity to model accurately, and the thermal conductivity across the film is set equal to this quantity since it is not important for the situations considered herein, namely broad thin solid films surrounded by a gas that is a rather good insulator. If, for other classes of applications, it were necessary to describe the thermal conductivities along and across the film accurately, a tensor thermal conductivity would be required. As discussed above, Calore has this capability. However, this additional complexity is not necessary for the present microsystems applications. Chapter 2 presents the model for the thermal conductivity of a thin film of polycrystalline silicon in full detail.

The following modeling strategy is employed for the gas. The mass density, the specific heat at constant pressure, and the thermal conductivity retain their bulk values, and the heat transfer coefficient is prescribed to represent the effects of the finite gap thickness and accommodation of gas molecules to the solid surface during reflection. The mass density is not considered to be spatially uniform or temporally constant. Instead, the gas pressure is maintained at the ambient value since most microsystems are open to the ambient environment, and the gas is allowed to move quasi-statically in response to temperature variations while remaining at constant pressure. As indicated above, the gas and solid temperatures at the interface differ by an amount

proportional to the normal heat flux crossing the interface. In contrast to the solid model discussed above, the model for the heat transfer coefficient does not incorporate the gap thickness explicitly. Instead, the heat transfer coefficient is prescribed in such a manner as to yield very nearly the correct heat transfer across a thin gas-filled gap bounded by planar solid walls for all gas pressures from rarefied to ambient or larger and for all values of the accommodation coefficient between zero and unity. For other geometries (e.g., a solid body of finite extent in an infinite or semi-infinite gas-filled region), the accuracy of this model decreases somewhat. Suggestions are presented for future improvements of the model to account for this situation. The interaction of gas molecules with the solid surface is described in terms of an accommodation coefficient. This parameter describes the combined effect of the energy exchange between the gas molecules and the solid molecules (or whatever molecules reside on the solid surface) and of the surface roughness. Here, the accommodation coefficient is considered an input parameter that is derived from experimental data for a particular combination of a gas, a solid, and their environmental history (Rader et al., 2004): the development of an accommodation-coefficient model lies far beyond the scope of this project. Chapter 3 presents the model for the gas-solid heat transfer coefficient in full detail.

The above models for microscale heat transfer in solids and gases are implemented in Calore user subroutines and are used to analyze a representative microsystem application in Chapter 4. More specifically, a heated microbeam separated from the ambient-temperature substrate by a thin gas-filled gap is considered. Similar structures are used for microscale thermal actuation induced by Joule heating. The results from this example indicate that failure to use the models discussed above can result in a significant underprediction of the microbeam temperature rise and the associated thermal stress and motion. The subroutines, the means by which they are accessed through Sandia's SourceForge server, and the details of their use are presented in Appendix A.

Figure 1.1. Optical shutter: top, micrograph; bottom, Calore heat transfer simulation.

Figure 1.2. Noncontinuum heat transfer: top, phonons in solid; bottom, gas molecules.

2. Microscale Heat Transfer in Solids

2.1. Overview

Microscale heat transfer effects in a solid need to be considered when the characteristic length of a microstructure is on the order of the mean free path of the major heat carriers, either phonons or electrons. For single-crystal silicon, the mean free path of phonons is 43 nm at room temperature, and for diamond, it is 315 nm at room temperature (Chen, 2005; Tien and Chen, 1994; Flik et al., 1992). Usually it takes several collisions for phonons to reach a state of local thermal equilibrium. Thus, for a microstructure with thickness less than a micron, the assumption that the material behaves in a continuum and equilibrium fashion may not be valid (Chen, 2005; Wong and Graham, 2003; Tien and Chen, 1994). More specifically, this implies that bulk material properties do not accurately represent the behavior of the solid. In this situation, solving the Boltzmann equation may be required in order to simulate the thermal response of a microstructure accurately.

In practice, a microstructure is packaged and integrated into a complex engineering system, which has a length scale of centimeters or larger. To model the thermal response of this integrated engineering system, all dominant heat transport mechanisms, which vary according to different characteristic length scales, must be considered. For example, the micro-switch system designed for security applications (Wong and Graham, 2003) has a feature size of 0.5 μm (its thickness). In this situation, phonon scattering from boundaries is more important than phonon scattering within the bulk material, leading to a smaller thermal conductivity than the bulk value. To address thermal problems with multiple length scales, a bridging strategy has been developed that links microscale thermal transport with continuum thermal transport. The present approach introduces the concept of an “effective thermal conductivity” and develops a phenomenological model that captures the dominant phonon-scattering mechanisms so that both large-scale and small-scale thermal effects are included in the system analysis.

2.2. Modeling Strategy

Since the focus of this work is to develop a model for use in the continuum thermal analysis code Calore (Bova et al., 2005), a subgrid physics model is developed that works well with this code. Hence, the “effective thermal conductivity” concept is employed. A more advanced approach is to build a coupled continuum/noncontinuum mechanics code, such as by coupling a Monte Carlo code (Piekos et al., 2004; Mazumder and Majumdar, 2001) with a finite-element thermal analysis code. This latter approach involves a substantial research effort. Furthermore, the resulting coupled-analysis tool is expected to require a very large CPU time to achieve a solution. Thus, this coupled-analysis approach may not be useful for design-oriented analyses.

The approach involving a subgrid physics model has the following advantages over the coupled-analysis approach: (1) it is easier to implement; (2) it is able to run faster in computer simulations; (3) it is more robust in numerical analysis. However, the subgrid physics model also has the following drawbacks. First, the local non-equilibrium state is assumed to be not too far away from the equilibrium state, so only near-equilibrium situations can be considered. Second, the thermal

conductivity is derived from Fourier's Law, which is strictly valid only for continuum situations. Third, the temperature itself must be a well-defined and globally applicable parameter.

2.3. Phonon Transport Theory

The initial focus here is to analyze the performance of surface micromachined (SMM) devices. Since these SMM devices are made of semiconductors, the dominant heat carriers in these materials are phonons, which are the quanta of lattice vibrational energy (Berman, 1976; Kittel, 1996).

The dynamics of phonon transport and scattering is governed by the Boltzmann equation:

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_r f + \zeta \cdot \nabla_p f = \left(\frac{\partial f}{\partial t} \right)_{scatter}, \quad (2.1)$$

where $f(x, p, t)$ is the probability distribution function for an ensemble of phonons, r is the position, v is the phonon propagation velocity, p is the phonon momentum, and ζ is the external force field. The scattering term has the following general form:

$$\left(\frac{\partial f}{\partial t} \right)_{scatter} = \sum_{p'} [W(p, p') \cdot f(p') - W(p', p) \cdot f(p)], \quad (2.2)$$

where $W(p, p')$ is the scattering rate from momentum p' to momentum p .

In a state of thermal equilibrium, the phonon distribution function $f_o(x, p, t)$ follows the Bose-Einstein (B-E) distribution:

$$f_o(x, p, t) = \frac{1}{\exp\left(\frac{h\nu}{k_B T}\right) - 1}, \quad (2.3)$$

where k_B is the Boltzmann constant, h is the Planck constant, ν is the phonon frequency, and T is the temperature.

In a state of thermal nonequilibrium, in which a heat flow or a temperature gradient exists, when the phonon distribution function deviates only slightly from the equilibrium condition, the scattering term can be approximated using the Bhatnagar-Gross-Krook (BGK) form:

$$\left(\frac{\partial f}{\partial t} \right)_{scatter} = \frac{f_o - f}{\tau(p)}, \quad (2.4)$$

where $\tau(p)$ is the total relaxation time. From this form, it is seen that the scattering process acts to restore the phonon distribution back to the equilibrium state.

By solving the BGK form of the Boltzmann equation (i.e., Equations (2.1) and (2.4)), the thermal conductivity k can be derived (Berman, 1976; Holland, 1963):

$$k = 4\pi \cdot k_B \cdot \left(\frac{k_B}{h}\right)^3 \cdot T^3 \cdot \sum_{\gamma} \frac{1}{v} \cdot \int_0^{\theta_{D,\gamma}/T} \tau_{\gamma}(x) \cdot \frac{x^4 e^x}{(e^x - 1)^2} \cdot dx, \quad (2.5)$$

where γ is the mode of phonon polarization, $\theta_{D,\gamma}$ is the Debye temperature, and $x = h\nu/(k_B T)$.

By assuming that each scattering process is independent from all the others, Matthiessen's rule can be used to determine the total relaxation time in terms of the relaxation times of the individual scattering processes (Berman, 1976):

$$\frac{1}{\tau_{\gamma}} = \sum_i \frac{1}{\tau_{\gamma,i}}. \quad (2.6)$$

The character of each phonon scattering process is captured through the expression of its relaxation time. This approach can calculate an effective thermal conductivity that is anisotropic and heterogeneous and that behaves nonlinearly with temperature.

2.4. Existing Models

Among the existing models, the Callaway (Callaway, 1959) and Holland (Holland, 1963) models are considered for further development. These models are selected because they have been assessed many times to predict the thermal conductivity of bulk silicon and other semiconductors (Berman, 1976). The Callaway model assumes a single dominant propagation mode for phonon transport, while the Holland model utilizes three propagation modes (one longitudinal mode and two transverse modes). Predictions from both models are compared to experimental data to evaluate the tradeoff between the “simplicity and speed of using single mode” (the Callaway model) versus the “complexity and accuracy of using multi-mode” (the Holland model).

Figure 2.1 shows the comparison of the thermal-conductivity values for single-crystal silicon from the Callaway (single-mode) and Holland (multiple-mode) models and bulk values measured by Holland and Neuringer (1962) (1.7 K to 300 K) and Glassbrenner and Slack (1964) (300 K to 1683 K). The Callaway model fails at high temperature because it has only one dominant phonon mode. This mode can capture the normal and umklapp (Kittel, 1996) scattering processes at low temperature. At high temperature, however, the normal and umklapp processes depend on temperature in different fashions. The Callaway model predicts a temperature dependence of T^{-n} , where $n < 1$. However, experimental data have a $T^{-1.2}$ temperature dependence. Based on this evaluation, the Holland model is selected as the starting point for the development of the subgrid physics model.

2.5. Scattering at a Thin-Film Boundary

In both the Callaway model and the Holland model, the relaxation time for thin-film boundary scattering is determined by dividing the thickness of a structure by the phonon propagation velocity and multiplying this value by a weighting factor. This weighting factor characterizes the effect of surface topography on phonon scattering at the thin-film boundary. In both models, a constant weighting factor of $F = 0.8$ is used. This constant value is derived from those experiments that measure the thermal conductivity of single-crystal silicon at low temperatures. At low temperatures, boundary scattering dominates since the phonon mean free path increases moderately as the temperature is decreased.

A constant weighting factor of 0.8 may produce inaccurate predictions of the thermal conductivity of a thin-film material. This approximation neglects the fact that phonons of different modes and different frequencies may interact differently at the boundary of the film. In addition, if the film is sufficiently thin (i.e., micron scales), the boundary scattering can be dominant even at room temperature. Hence, a constant weighting factor of 0.8 may be inaccurate. Figure 2.2 shows a comparison between predictions of the Holland model and experimental data for a single-crystal silicon film that is $1.5 \mu\text{m}$ thick. The Holland model significantly underpredicts the thermal conductivity of the silicon film. Hence, the thin-film boundary scattering model needs to be improved by considering the phonon spectrum and the surface topography.

The present subgrid physics model is a further development based on the work of Ziman (1960) and McConnell et al. (2001). To capture variations in the phonon-boundary interaction, the incident phonons are treated as plane waves propagating toward a wall at an angle. By comparing the reflection of two parallel waves after scattering at the film surface, the degree of coherence of the waves can be correlated, and the phase change with respect to the surface topography can be analyzed. Hence, the probability of specular reflection can be found:

$$P(\omega) = \exp(-\pi \cdot \overline{\varphi^2}) = \exp\left(-\pi \cdot \frac{16\pi^2 \eta^2}{\lambda^2}\right) = \exp\left(-4\pi \cdot \frac{\eta^2 \omega^2}{v^2}\right), \quad (2.7)$$

where η is the surface roughness, λ is the phonon wavelength, ω is the angular frequency of phonon, and φ is the variance.

For completely specular reflection, $P(\omega) = 1$. On the contrary, for completely diffuse reflection, $P(\omega) = 0$. Subsequently, the weighting factor can be related to the probability of specular reflection according to $F = (1 + P(\omega))/(1 - P(\omega))$. The relaxation time for film boundary scattering then takes the following form:

$$\frac{1}{\tau_{film}} = \frac{v}{l} \cdot \frac{1}{F} = \frac{v}{l} \cdot \left(\frac{1 - P(\omega)}{1 + P(\omega)}\right), \quad (2.8)$$

where l is the film thickness and v is the phonon propagation velocity.

2.6. Comparing Model Predictions to Experimental Data

To assess its predictive capability, the present subgrid physics model is applied to calculate the thermal conductivity of undoped single-crystal silicon films of various thicknesses as a function of temperature. Figures 2.2, 2.3, and 2.4 show model predictions and experimental data from Asheghi at Stanford (Asheghi, 1999) and Graham at Sandia, California (Graham et al., 2003).

Figure 2.2 considers a film thickness of $l = 1.5 \mu\text{m}$. The various model predictions use different parameters to describe the boundary scattering. The original Holland model uses a phonon speed of $v = 6400 \text{ m/s}$ and a constant weighting factor of $F = 0.8$. This model significantly underpredicts the thermal conductivity. The present model considers the phonon spectrum and its interaction with the surface topography. The first calculation based on this model uses a single weighted average value for the phonon propagation velocity and a relatively rough surface (rms roughness $\eta \approx 20 \text{ nm}$) to predict the relaxation time for thin-film boundary scattering. Again, the model predictions do not compare well with the experimental data. However, if the rms surface roughness is changed to $\eta = 0.1 \text{ nm}$, which is more justifiable to use for single-crystal silicon, the present model gives much better results when compared to the experimental data. In addition, if the group velocity for each mode of phonon propagation is used, the model predictions compare reasonably well with the data.

Figure 2.3 compares the model and experimental results for a film thickness of $l = 1.0 \mu\text{m}$. Additional experimental data for a film thickness of $l = 0.83 \mu\text{m}$ are also included. The present model predicts the thermal conductivity reasonably well at room temperature or above. However, at low temperature, the present model overpredicts the thermal conductivity.

Figure 2.4 shows additional results for thinner films with $l = 0.35 \mu\text{m}$ and $l = 0.42 \mu\text{m}$. The predicted thermal conductivity agrees better with the data from Graham's experiments than with the data from Asheghi's experiments. In summary, the present subgrid physics model predicts the thermal conductivity of a thin film of single-crystal silicon with reasonable accuracy.

2.7. Scattering at a Grain Boundary

Since polycrystalline silicon is commonly used instead of single-crystal silicon in many SMM devices, the next task is to predict the thermal conductivity of polycrystalline silicon. For polycrystalline silicon, the phonon scattering at grain boundaries must be included in the subgrid physics model. Similar to the boundary scattering at the film surface, the relaxation time for grain boundary scattering τ_{grain} can be derived as follows, where d_{grain} is the grain size:

$$\frac{1}{\tau_{\text{grain}}} = \frac{v}{d_{\text{grain}}} \cdot \left(\frac{1 - P_{\text{transmission}}(\omega)}{1 + P_{\text{transmission}}(\omega)} \right). \quad (2.9)$$

Then the probability of a phonon being transmitted across a grain boundary has the form below:

$$P_{transmission}(\omega) = \exp\left(-\pi \cdot \frac{\chi^2 \omega^2}{v^2}\right) = \exp\left(-\pi \cdot \frac{a^2}{d_{grain}^2} \cdot \frac{\omega^2}{v^2}\right), \quad (2.10)$$

where χ is the radius of curvature of the dominant grain size and a is a coefficient that relates the radius of curvature to the diameter of the grain.

For $P_{transmission} = 1$, the transmission of phonons across the grain boundary is perfect (100%), so there is only a minimal increase in thermal resistance. For $P_{transmission} = 0$, no phonons are transmitted across the grain boundary, so the grain boundary is a perfect insulator. In the subgrid physics model, the transmission rate is influenced by the radius of curvature, which is subsequently affected by the grain size.

The present approach assumes that there is one dominant grain size that affects phonon scattering at grain boundaries. In reality, for a polycrystalline material, this scattering process is influenced by the grain-size distribution. However, phonon scattering at the grain boundary and the associated thermal resistance may be controlled by the smallest grains in the microstructure, rather than by the larger grains. Hence, phonon scattering at grain boundaries is a very complicated phenomenon. In summary, the development of the present subgrid physics model is only an initial effort. More work is needed to extend the current model to include the boundary-scattering effect from grains with various sizes. In addition, more experiments are needed to better understand and characterize phonon transmission at grain boundaries and to validate the model.

The thermal conductivity of polycrystalline silicon is different from that of single-crystal silicon because phonon scattering at grain boundaries increases the thermal resistance. By including grain-boundary scattering in the subgrid physics model, the model does predict a smaller thermal conductivity for polycrystalline silicon than for single-crystal silicon.

Figure 2.5 plots the thermal conductivity of undoped polycrystalline silicon as a function of temperature. The calculated thermal-conductivity values for polycrystalline silicon with grain sizes of 440 nm and 580 nm, respectively, are compared to the experimental data. The effect of grain size on the thermal conductivity at room temperature is illustrated in Figure 2.6. As shown in both figures, the model predictions are reasonably accurate. However, there are some minor discrepancies between the model predictions and the experimental measurements. More thermal conductivity experiments are planned to resolve these differences.

2.8. Calore Implementation

Currently, the “effective thermal conductivity” subgrid physics model discussed above is written in FORTRAN as a specialized user subroutine for Calore. This subroutine is contained in the file `kpolysi.f`, which is described in Appendix A. This subroutine has been used in Calore to analyze the thermal and mechanical responses of micro-electro-thermal-mechanical actuators. Results of these simulations are presented in Chapter 4.

Figure 2.1. Model predictions using single-mode and multiple-mode phonon transport. Callaway and Holland models are compared to bulk-silicon experimental data. Boundary scattering effect becomes important only at low temperature.

Figure 2.2. Calculated and measured thermal conductivity of a 1.5-μm silicon film. Film is undoped single-crystal silicon.

Figure 2.3. Calculated and measured thermal conductivity of a 1.0-μm silicon film. Film is undoped single-crystal silicon.

Figure 2.4. Calculated and measured thermal conductivity of a 0.35- μm silicon film.
Film is undoped single-crystal silicon. Measured values are at different thicknesses.

Figure 2.5. Effect of temperature on thermal conductivity for two grain sizes.
Film is undoped polycrystalline silicon.

Figure 2.6. Effect of grain size on thermal conductivity at room temperature.
Film is undoped polycrystalline silicon.

3. Microscale Heat Transfer in Gases

3.1. Overview

The noncontinuum gas-phase heat transfer model implemented in Calore is reviewed. In this Navier-Stokes Slip-Jump (NSSJ) model, Fourier's law of continuum heat conduction is retained, and continuum values for all gas properties are used, but a temperature discontinuity proportional to the normal heat flux is imposed at gas-solid interfaces. Implementation of this model in Calore is discussed. The model is applied to two microscale geometries, the microgap and the microbeam. The Calore results are in excellent agreement with results from other codes in which the same model is implemented and are generally in good agreement with results from Direct Simulation Monte Carlo (DSMC) simulations, in which noncontinuum gas behavior is treated rigorously. Causes for modest but systematic differences between the Calore and DSMC results are discussed, and future efforts will focus on extending the model to account for these effects.

3.2. Model Development

The goal of this portion of the effort is to develop a model to represent microscale gas-phase heat transfer that can be implemented within the Calore framework (Bova et al., 2005). By necessity, the model is required to represent noncontinuum heat transfer effects that are nonnegligible and can be dominant at microscale conditions (Karniadakis and Beskok, 2002). At atmospheric conditions, the mean free path λ , the distance that molecules travel on average between pairwise collisions, is extremely small. For example, the mean free path of nitrogen at STP is $0.0583 \mu\text{m}$ (Gallis et al., 2005). When the mean free path is much smaller than a representative geometric length scale, noncontinuum effects on heat transfer in the gas are small and can be neglected. Conversely, when the mean free path is comparable to or larger than the geometric length scale, noncontinuum effects become important. At atmospheric conditions, the former situation is obtained for macroscopic systems, whereas the latter situation is obtained for microscale systems.

The mean free path depends on the composition, the temperature, and the pressure of the gas. For example, the mean free path of helium is approximately three times that of argon at the same temperature and pressure. For a given composition, the mean free path increases at least linearly with temperature and is inversely proportional to the pressure. The temperature dependence is of some importance since temperature differences in microsystems can vary by up to a factor of three (Wong and Graham, 2003; Gallis et al., 2005), but the pressure dependence is particularly significant since microsystems can be packaged at pressures that are one to several orders of magnitude smaller than atmospheric pressure.

The noncontinuum gas-phase heat transfer model discussed below is developed according to several basic principles. First, the model must match the general framework of Calore. In this context, the above statement implies that the model must use one of the modes of heat transfer currently implemented in Calore. Conductive heat transfer (i.e., Fourier's law) is chosen because it is the correct formulation in the continuum limit and because, as extended below, it can treat certain generic situations with good accuracy even for nearly free-molecular gas conditions.

Second, the model must predict the gas-phase heat transfer from one solid object to another with good accuracy. In this viewpoint, the temperature field in the gas-filled region is of lesser intrinsic importance, being of interest only so far as it contributes to determining the gas-phase heat flux accurately. Third, the model must be generic. It cannot depend upon the use of a particular geometry or coordinate system (or time frame). Fourth, the model must be local. It should not require global information about the geometry or the temperature field. The precise definition of “local” is admittedly vague in this context. For example, whether the distance from a point on a gas-solid interface to the “closest” adjacent gas-solid interface is a “local” quantity is an open question. Fourth, the model must recover continuum behavior and should reproduce known noncontinuum results wherever possible. As indicated above, the use of conductive heat transfer ensures the former and enables the latter in certain circumstances.

As indicated above, the noncontinuum model for gas-phase heat transfer is developed within the context of continuum conductive heat transfer. More specifically, within a single material (here, a gas), the following equation is applied:

$$\rho C_p \left(\frac{\partial T}{\partial t} \right) = \left(\frac{\partial}{\partial \mathbf{x}} \right) \cdot \left[K \left(\frac{\partial T}{\partial \mathbf{x}} \right) \right] + S, \quad (3.1)$$

where T is the temperature, ρ is the mass density, C_p is the specific heat at constant pressure, K is the thermal conductivity, S is the volumetric heat source term, t is time, and $\mathbf{x}$ is position. In this formulation, Fourier’s law is used to relate the heat flux $\mathbf{q}$ to the temperature gradient:

$$\mathbf{q} = -K \left(\frac{\partial T}{\partial \mathbf{x}} \right). \quad (3.2)$$

The quantities ρ , C_p , K , and S can be functions of temperature, position, and time.

When two materials (here, a gas and a solid) are in contact, the temperature is allowed to be discontinuous across the interface separating these materials. In this situation, the temperature difference (“jump”) ΔT is taken to be proportional to the normal heat flux q , with the proportionality expressed in the following form:

$$q = h \Delta T. \quad (3.3)$$

Here, the heat transfer coefficient h can in principle be a function of the temperatures and other properties of the two materials, of interface-specific quantities such as accommodation coefficients (Karniadakis and Beskok, 2002), and of position and time. This model belongs to the general class of models known as Navier-Stokes Slip-Jump (NSSJ) models (Gallis et al. 2005).

In the formulation outlined above, four gas-phase quantities are available for modeling: the mass density ρ , the specific heat at constant pressure C_p , the thermal conductivity K , and the heat transfer coefficient h (which can also depend on solid-phase and interface properties). These are specified below so as to reproduce continuum conductive heat transfer in the continuum limit by definition and to reproduce many aspects of noncontinuum gas-phase heat transfer by design.

The mass density is taken to obey the ideal gas law:

$$\rho = \frac{mp}{k_B T}. \quad (3.4)$$

Here, p is the pressure, m is the molecular mass, and k_B is the Boltzmann constant. When the temperature in the above equation equals the translational temperature, this equation is exact even under noncontinuum conditions (Bird, 1994). Although the above is always true for a monatomic gas, the above may not be true for a polyatomic gas under noncontinuum conditions because its translational and internal temperatures may differ (Bird, 1994). Here, the gas pressure is assumed to be uniform in space and constant in time (it is typically taken to be the ambient value). While appropriate for the open geometries found in microsystems, this assumption is not applicable for certain situations (e.g., a closed heated gas-filled volume) and can be relaxed if necessary. When the gas temperature varies in time and the pressure is fixed, the above equation implies quasi-static gas motion. The associated convective heat transfer is small and is ignored here.

The specific heat at constant pressure is taken to have the following form:

$$C_p = \left(\frac{\gamma}{\gamma - 1} \right) \left(\frac{k_B}{m} \right). \quad (3.5)$$

Here, the specific heat ratio γ is related to the number of available internal energy modes ζ :

$$\gamma = \frac{5 + \zeta}{3 + \zeta}. \quad (3.6)$$

This equation indicates that γ lies in the range $1 < \gamma \leq 5/3$ and reproduces the well-known values of $\gamma = 5/3$ for $\zeta = 0$ (a monatomic gas) and $\gamma = 7/5$ for $\zeta = 2$ (a rigid-rotor diatomic gas). The specific heat relation is exact for a monatomic gas but is approximate for a polyatomic gas whenever the translational and internal temperatures are not equal.

The thermal conductivity is taken to have the continuum value even for noncontinuum conditions. Because of its convenience, accuracy, and use in noncontinuum simulations (Bird, 1994), the following form is used to represent the temperature dependence of the thermal conductivity:

$$K = K_{\text{ref}} \left(\frac{T}{T_{\text{ref}}} \right)^{\omega}. \quad (3.7)$$

Here, ω is the temperature exponent, which generally lies in the range $1/2 \leq \omega \leq 1$, and “ref” denotes reference values. If desired, another functional form such as the well-known Sutherland formula can be implemented (Karniadakis and Beskok, 2002). The accuracy of using the continuum thermal conductivity has been demonstrated under two types of conditions known to produce noncontinuum behavior in a gas: large mean free paths (Gallis et al., 2005) and large heat fluxes (Gallis et al., 2004). Both of these situations are illustrated in subsequent sections.

The heat transfer coefficient at the gas-solid interface is the main method for incorporating noncontinuum effects and is taken to have the following form:

$$h = \left(1 + \frac{\zeta}{4}\right) \left(\frac{\sigma}{2 - \sigma}\right) \left(\frac{p\bar{c}}{T}\right). \quad (3.8)$$

Here, σ is the accommodation coefficient at the gas-solid interface, which lies in the range $0 \leq \sigma \leq 1$ and can be thought of as the probability that a gas molecule exchanges energy with the solid during reflection. More precisely, σ is the ratio of the difference between the incident and reflected gas-phase energy fluxes to the difference that would be obtained if all gas molecules reflected diffusely from the solid at the solid temperature on average (Bird, 1994). In the above expression, maximum heat transfer is achieved when $\sigma = 1$, whereas zero heat transfer (insulating behavior) is obtained when $\sigma = 0$. The quantity $\bar{c}$ is the mean molecular speed of an equilibrium distribution of gas molecules at temperature T :

$$\bar{c} = \sqrt{\frac{8k_B T}{\pi m}}. \quad (3.9)$$

Only gas-phase properties (p , T , $\bar{c}$, and ζ) and interface properties (σ) enter into the above expression for h : no solid-phase properties appear explicitly. In principle, σ can depend on solid-phase, gas-phase, and interface properties, including roughness, as well as on position and time. In the examples that follow, σ is uniform in space, constant in time, and the same for all gas-solid surfaces. These restrictions can be relaxed as necessary. It is noted that, when the gas pressure is uniform in space and constant in time, the heat transfer coefficient is inversely proportional to the square root of the gas temperature at the gas-solid interface. In this model, the continuum limit is obtained when $h \rightarrow \infty$, whereas the free-molecular limit is obtained when $h \rightarrow 0$.

Although it nowhere appears in any of the relations above, the mean free path is often a convenient quantity to calculate. Two forms are particularly convenient (Gallis et al., 2005):

$$\lambda = \frac{2\mu}{\rho\bar{c}} = \frac{\pi\mu\bar{c}}{4p}. \quad (3.10)$$

Here, μ is the absolute viscosity, which has a temperature dependence identical to that of the thermal conductivity, where again “ref” denotes reference values:

$$\mu = \mu_{\text{ref}} \left(\frac{T}{T_{\text{ref}}}\right)^\omega. \quad (3.11)$$

The above two equations indicate that the mean free path is proportional to $T^{\omega + 1/2}$ and inversely proportional to p . These relations make precise the general comments earlier in this section. After some algebra, the interface condition $q = h\Delta T$ is seen to be equivalent to $\Delta T \propto \lambda(\hat{\mathbf{n}} \cdot \nabla T)$, a more common form (Karniadakis and Beskok, 2002).

3.3. Calore Implementation

The noncontinuum model for gas-phase heat transfer is incorporated into the Calore framework in the following manner. The mass density and the thermal conductivity are temperature-dependent and are determined by linear interpolation from look-up tables covering a broad temperature range that contains the expected temperature values. Subroutines that incorporate this information can be developed as needed. The specific heat at constant pressure is simply a constant.

The heat transfer coefficient applied at a gas-solid interface is best implemented as a subroutine. Appendix A presents FORTRAN source code for the subroutines used in the simulations presented in the following section. These subroutines are contained in the file `gasnoncon.f`. Appendix A also presents instructions for accessing this file from Sandia’s SourceForge server.

The subroutines require five input parameters, which are taken to be global constants independent of position and time and which are not changed by the subroutine: the gas pressure p , the accommodation coefficient σ , the Boltzmann constant k_B , the molecular mass m , and the specific heat ratio γ . The subroutines do not require a particular set of units to be used; however, the units of the above quantities, together with the unit for the temperature T , must be consistent. The consistent units used below are p in Pa, σ a pure number, k_B in J/K, m in kg, γ a pure number, and T in K. In the future, any combination of the following dependencies could be considered: $p = p(t)$, $\gamma = \gamma(T)$, $\sigma = \sigma(\mathbf{x}, t, p, T, T_s)$, where T_s is the solid temperature. There is no plan to implement any of these dependencies, but they are physically allowable. The five required inputs are made available to the subroutine as “real data” in the Calore input file. The below example is for nitrogen at 10^6 Pa.

```
real data 1.e6, 1.0, 1.380658e-23, 46.5e-27, 1.4
```

Calore also makes available to the subroutine certain “region data” (information pertaining to the physical region being examined), which includes the temperatures on both sides of the gas-solid interface at the element Gauss points (Bova et al., 2005). However, Calore does not identify the materials to which the temperatures correspond. One way to circumvent this limitation is for the user to pass to the subroutine some (problem-dependent) information that enables the subroutine to correctly identify the material corresponding to each temperature. For the two situations considered herein, maximum and minimum tests can be used to make this correspondence because the temperature decreases monotonically from the heated silicon part through the gas to the ambient-temperature substrate. Thus, the user passes a flag selecting the maximum test at the upper gas-solid interface for one instance of the boundary condition but selecting the minimum test at the lower gas-solid interface for the other instance of the boundary condition.

The contact boundary condition in Calore, which is used to apply the heat transfer coefficient at the interface, does not support instance data (Bova et al., 2005). A request to enable instance data as part of the contact boundary condition has been submitted to the Calore development team. At present, an individual subroutine must be provided for each gas-solid interface, within which the user provides a means of identifying the solid temperature. Future Calore developments may include the ability to associate a temperature at an interface with its corresponding material.

3.4. Microgap and Microbeam Results

Two Calore test problems that apply the noncontinuum gas-phase heat transfer model of the previous section are presented below: the “microgap” and the “microbeam”. In each situation, a gas-filled region separates two solid silicon regions, one hot and the other cold. Different gases (argon and nitrogen) and different temperature differences (small and large compared to ambient) are examined. Only steady situations are considered. In all cases, the quantity of interest is the heat flux or heat flux per unit length from the hot solid to the cold solid. The correctness of the Calore implementation of the model is verified by comparison of Calore results with analytical solutions where known and with FIDAP results (Fluent, 1998) obtained using the same model (but not the same implementation). The accuracy of the model is assessed by comparison of these results with corresponding results from the Direct Simulation Monte Carlo (DSMC) method. The DSMC method uses computational molecules to simulate the behavior of real molecules and by doing so is able to accurately represent gas behavior under both continuum and noncontinuum conditions (Bird, 1976; Bird, 1978; Wagner, 1992; Bird, 1994; Bartel et al., 2001; Gallis et al. 2004; Gallis et al., 2005).

The gas-phase and solid-phase material properties used in all simulations are presented in Tables 3.1-3.2 (Bird, 1994; White, 1984; Emsley, 1989). In this section and in this section alone, the previously described sophisticated models that incorporate the grain-size dependence and the temperature dependence of the thermal conductivity of polycrystalline silicon are not used. Instead, the properties of single-crystal silicon at 300 K in Table 3.2 are used (Emsley, 1989). In the particular problems considered in this section, the heat transfer is controlled entirely by the gas (radiative heat transfer is ignored here). The gas and solid regions are of similar sizes, all of the heat has to flow through the gas to get from the hot solid region to the cold solid region, and the thermal conductivity of the gas is four orders of magnitude smaller than that of the solid. Thus, the solid regions are nearly isothermal. Therefore, to enable a more quantitative assessment of the noncontinuum gas-phase heat transfer model, the solid properties are simplified. In the following chapter, the noncontinuum effects from both the gas and the solid are coupled.

The microgap geometry is shown schematically in Figure 3.1. In the Calore simulations, the geometry has three 1- μm -thick parallel layers: two solid slabs bounding a gas layer. All lateral boundaries are insulating, the bottom and top boundaries are at fixed temperatures T_A and T_B , respectively, and the gas-solid interfaces use the heat transfer coefficient described in the previous section to relate the heat flux to the temperature jump. In the FIDAP and DSMC simulations, only the gas layer is treated. As discussed above, neglecting the solid regions makes almost no discernible difference in the results because the solid thermal conductivity is four orders of magnitude larger than that of the gas (see Table 1) so the solid regions are almost isothermal.

A Calore mesh is shown in Figure 3.2. Each of the three slabs is $2 \times 2 \times 1 \mu\text{m}$ in extent. The 8-node brick elements have dimensions of $0.2 \times 0.2 \times 0.1 \mu\text{m}$, so each slab has 10^3 elements. The Calore simulations are thus three-dimensional although the situation is mathematically one-dimensional. Simulations with a more refined mesh created by halving the elements in all three directions produce almost identical results. The two-dimensional computational mesh used in the FIDAP simulations is more refined and uses more accurate 9-node quadrilateral elements. The Calore and FIDAP heat-flux values typically agree to four significant figures.

The DSMC simulations use a one-dimensional mesh with uniform cells and a constant time step. For 10^6 Pa, a 1000-cell mesh and a 0.5-ps time step are used. For lower pressures, a 100-cell mesh and a 5.0-ps time step are used. In all cases, 30 computational molecules per cell are used. For these values, numerical errors are below 1%, based on extensive simulations using a wide variety of meshes, time steps, and computational molecules per cell (Rader et al., 2005). Stochastic errors are also kept below 1% by acquiring $O(10^9)$ molecular samples per cell (Rader et al., 2005).

Two gases are considered: argon and nitrogen (see Table 3.1). Gas pressures from 10^2 to 10^6 Pa, accommodation coefficients of 1.0, 0.9, 0.5, and 0.1, and boundary temperatures T_A and T_B of 285 and 315 K and 150 and 450 K are examined, which yield nominal gas-temperature gradients of 30 and 300 K/ μm , respectively. As stated above, the solid properties are taken to be those of pure silicon at 300 K (see Table 3.2).

The steady temperature fields from the Calore simulations for both gases and for all pressures at an accommodation coefficient of unity with boundary temperatures of 285 and 315 K are shown in Figure 3.3. In all cases, the argon and nitrogen temperature fields are qualitatively similar: the solid regions are nearly isothermal, as expected. At low pressures, the gas region is nearly isothermal, as expected for free-molecular flow (Bird, 1976). The free-molecular limit is discussed in greater detail below. At high pressures, the temperature variation becomes almost linear across the gas layer (this is exact in the limit of a small temperature difference, which yields a uniform thermal conductivity), and the temperature jumps at the gas-solid interfaces become small, as expected for continuum flow.

Figures 3.4, 3.5, 3.6, and 3.7 show the heat flux as a function of gas pressure and accommodation coefficient for both gases with both sets of boundary temperatures. The nitrogen heat flux is always larger than the argon heat flux for corresponding conditions (note the log-log nature of these plots) because of the two internal energy modes that the diatomic nitrogen molecule has but that the monatomic argon molecule lacks. The Calore values are in excellent agreement with the FIDAP values for all conditions (typically to four significant figures) and are in good agreement with the DSMC values for most conditions. In particular, the model correctly predicts not only continuum gas-phase heat transfer (the right sides of the plots) but also free-molecular gas-phase heat transfer (the left sides of the plots). The heat flux is independent of pressure at high pressures, as expected for continuum conditions, and is linear in pressure at low pressures, as expected for free-molecular conditions. However, small differences are observed between the Calore and DSMC values for order-unity accommodation coefficients and pressures of 10^4 - 10^5 Pa, for which values the mean free path is comparable to the 1- μm gap thickness. More specifically, the Calore values are typically a few percent higher than the DSMC values. The cause of this discrepancy is discussed in the following section.

The good agreement between the Calore and DSMC microgap heat-flux values for all conditions indicates that Calore can be used with confidence to predict the gas-phase heat transfer across microscale gaps between solids for monatomic and polyatomic gases, for small to large temperature differences, for low to high pressures (from free-molecular to continuum conditions), and for poor to good accommodation. The microgap geometry considered here is a typical feature of many microsystems fabricated using the SUMMIT V process (Sniegowski and de Boer, 2000). As shown below, however, this good agreement depends on the simple geometry of the microgap.

The microbeam simulation geometry is shown in Figure 3.8. The microbeam itself has an I-beam cross section with three layers. The top layer is $3.8\text{ }\mu\text{m}$ wide and $2.25\text{ }\mu\text{m}$ thick, the middle layer is $0.65\text{ }\mu\text{m}$ wide and $2.0\text{ }\mu\text{m}$ thick, and the bottom layer is $3.8\text{ }\mu\text{m}$ wide and $2.5\text{ }\mu\text{m}$ thick. A gap of $2.0\text{ }\mu\text{m}$ separates the lower surface of the microbeam from the upper surface of the adjacent substrate. The substrate is $0.1\text{ }\mu\text{m}$ thick and extends across the entire lower surface of the computational domain. Insulating boundary conditions are applied on the top, the side, the front, the back, and the symmetry plane of the domain. The lower substrate surface is held at a temperature of $T_A = 298\text{ K}$, and the symmetry surface of the microbeam cross section is held at a temperature of $T_B = 873\text{ K}$. This latter boundary condition replaces the volumetric heat source from Joule heating within the microbeam, which would otherwise be prescribed so as to produce this temperature. As for the microgap, the large solid thermal conductivity renders the solid regions nearly isothermal, so replacing the volumetric heat source with the temperature boundary condition hardly affects the temperature field.

One three-dimensional Calore computational mesh is shown in Figure 3.8. Within this mesh, the gas-microbeam portion occupies a region of $12 \times 16 \times 1\text{ }\mu\text{m}$, and the substrate portion occupies a region of $12 \times 0.1 \times 1\text{ }\mu\text{m}$. Both portions are meshed with 8-node brick elements of dimensions $0.1 \times 0.1 \times 0.5\text{ }\mu\text{m}$, which together yield 38,640 elements. The FIDAP mesh (not shown) uses graded refinement and 9-node quadrilateral elements for high accuracy. The Calore and FIDAP heat-flux values typically agree to three significant figures.

In the DSMC simulations, only the gas region is treated. The DSMC simulations use a two-dimensional mesh with uniform $0.05\text{-}\mu\text{m}$ square cells and a constant time step of 50 ps , with an average of 60 computational molecules per cell. Thus, each simulation uses almost 5 million molecules. Because of the large temperature variations, the hottest cells end up with only 20-30 computational molecules per cell when steady conditions are achieved. Since the cell size is required to be smaller than the mean free path, only pressures below 10^5 Pa are simulated with DSMC. Under the above conditions, the numerical error is around 1%, and the stochastic uncertainty is kept to a comparable value by acquiring large numbers of molecular samples.

Only one gas is considered in these simulations: nitrogen, with properties as in Table 3.1. Except in the continuum case of Figure 3.9, boundary temperatures T_A and T_B of 298 and 873 K are used with gas pressures in the range of $10^2\text{-}10^6\text{ Pa}$ and accommodation-coefficient values of 1.0, 0.8, 0.5, and 0.2. To investigate the effect of domain size on heat flux, Calore simulations are performed not only with the $12 \times 16\text{-}\mu\text{m}$ gas-microbeam portion of the domain but also with additional domains for which these two dimensions are multiplied by a scale factor F in the range $0.8 \leq F \leq 16$. In these cases, the substrate height ($0.1\text{ }\mu\text{m}$) and the domain extent in the third dimension ($L = 1\text{ }\mu\text{m}$) remain unchanged.

Two steady temperature fields from Calore simulations are shown in Figure 3.9. Here, the gas pressure is $p = 10^5\text{ Pa}$, the accommodation coefficient is $\sigma = 0.5$, and the domain scale factor is $F = 4$. The right temperature field is produced using the heat transfer coefficient in Equation (3.8) at the gas-solid interface. The left temperature field is produced by replacing the heat-transfer-coefficient condition at the gas-solid interface with a zero-temperature-jump condition. Also, the temperature T_B is modified to produce the same power from the microbeam to the substrate, as would be the case with Joule heating. Thus, the right temperature field

represents noncontinuum gas behavior, whereas the left temperature field represents continuum gas behavior. The neglect of noncontinuum effects in the gas causes the microbeam temperature to be significantly underpredicted (here, by about 150 K). Thus, it is important to include noncontinuum effects when computing the gas-phase heat transfer.

Figures 3.10 and 3.11 show the effect of gas pressure, accommodation coefficient, and domain size on the temperature field. Calore temperature fields are shown for gas pressures from 10^2 Pa, which is nearly free-molecular, to 10^6 Pa, which is nearly continuum, for all four accommodation coefficients (0.2, 0.5, 0.8, and 1.0), and for two domain sizes ($F = 4$ and $F = 1$). In all cases, the solid regions are nearly isothermal, as expected. As the gas pressure or the accommodation coefficient is decreased, the gas temperature field becomes more uniform. This is related to the fact that the heat transfer coefficient decreases as the pressure or the accommodation coefficient is decreased: it becomes harder to transfer heat from the solid to the gas and vice versa than it is to transfer heat through the gas itself. As expected, the influence of the finite domain on the temperature field decreases as the domain size is increased.

Figures 3.12 and 3.13 quantify the effect of the domain scale factor on the heat flux for the pressures and accommodation coefficients of Figures 3.10 and 3.11. Here, Q is the total heat flow or power (in watts) from the full microbeam (i.e., double that from the half-microbeam domain in Figure 3.8), and $L = 1\text{ }\mu\text{m}$ is the domain extent in the third dimension. The Q/L values from the $F = 1$ domain are 15-25% lower than the values from the $F = 16$ domain (essentially infinite), whereas the values from the $F = 4$ domain are only a few percent lower. Thus, a half domain of $48 \times 64\text{ }\mu\text{m}$ ($F = 4$) or larger is needed for minimal influence of domain size. However, for comparing Calore, FIDAP, and DSMC (rather than for obtaining infinite-domain results), the $12 \times 16\text{ }\mu\text{m}$ ($F = 1$) half domain is acceptable.

Figure 3.14 shows the microbeam heat flow per unit length from the Calore, FIDAP, and DSMC simulations. In all cases, the Calore and FIDAP values are in excellent agreement (typically to three significant figures), verifying the correctness of the implementation. However, the model systematically overpredicts the heat flow per unit length relative to the DSMC method. Although the difference is quite small for large pressures and for small accommodation coefficients, the model predicts values that are approximately double the DSMC values for low pressures and order-unity accommodation coefficients. While relatively large, this discrepancy is small in an absolute sense (i.e., two orders of magnitude smaller than the continuum value).

The good agreement between the Calore, FIDAP, and DSMC microbeam results at atmospheric and higher pressures indicates that the noncontinuum gas-phase heat transfer model in Calore can be used with confidence to predict gas-phase heat transfer for microscale devices in ambient air. This extends the range of applicability from the simple microgap geometry to the more complex geometries often encountered in microsystems (Sniegowski and de Boer, 2000). The causes of the discrepancy observed at low pressures and order-unity accommodation coefficients and possible ways to improve the model in this regime are discussed in the following section.

3.5. Model Improvements

The cause of the above discrepancies can be understood by comparing model results to known results from the Boltzmann equation (BE) in the free-molecular (FM) and near-continuum limits. So-called NSSJ-FM results are obtained from the limit of the model solution for a particular geometry as the heat transfer coefficient becomes small so that the gas temperature becomes independent of position. Exact BE-FM results are obtained for particular geometries by equating the incident and reflected molecule fluxes at one or more impermeable solid boundaries and determining the heat flux from the difference between the corresponding incident and reflected energy fluxes (Bird, 1976).

For motionless gas confined between two parallel solid surfaces at temperatures $T_A < T_B$ (essentially the geometry of Figure 3.1), the BE and NSSJ results for the FM gas temperature T and heat flux q have closed-form expressions (Gallis et al., 2005):

$$\frac{T}{\sqrt{T_A T_B}} = \frac{\left(\frac{2-\sigma_B}{\sigma_B}\right)\sqrt{T_A} + \left(\frac{2-\sigma_A}{\sigma_A}\right)\sqrt{T_B}}{\left(\frac{2-\sigma_A}{\sigma_A}\right)\sqrt{T_A} + \left(\frac{2-\sigma_B}{\sigma_B}\right)\sqrt{T_B}} \quad \{\text{BE-FM}\}, \quad (3.12)$$

$$q = \frac{\left(1 + \frac{\zeta}{4}\right)\left(\frac{p\bar{c}}{\sqrt{T}}\right)(T_B - T_A)}{\left(\frac{T}{\sqrt{T_A T_B}}\right)\left\{\left(\frac{2-\sigma_A}{\sigma_A}\right)\sqrt{T_A} + \left(\frac{2-\sigma_B}{\sigma_B}\right)\sqrt{T_B}\right\}} \quad \{\text{BE-FM}\}; \quad (3.13)$$

$$T = \frac{\left(\frac{2-\sigma_B}{\sigma_B}\right)T_A + \left(\frac{2-\sigma_A}{\sigma_A}\right)T_B}{\left(\frac{2-\sigma_A}{\sigma_A}\right) + \left(\frac{2-\sigma_B}{\sigma_B}\right)} \quad \{\text{NSSJ-FM}\}, \quad (3.14)$$

$$q = \frac{\left(1 + \frac{\zeta}{4}\right)\left(\frac{p\bar{c}}{\sqrt{T}}\right)(T_B - T_A)}{\left\{\left(\frac{2-\sigma_A}{\sigma_A}\right)\sqrt{T} + \left(\frac{2-\sigma_B}{\sigma_B}\right)\sqrt{T}\right\}} \quad \{\text{NSSJ-FM}\}. \quad (3.15)$$

The NSSJ-FM heat flux approaches the BE-FM heat flux in the limits that the temperature difference and/or exactly one accommodation coefficient becomes small. For temperature ratios in the range $1/4 \leq T_B/T_A \leq 4$ with arbitrary accommodation coefficients, the NSSJ-FM heat flux is always within 5% of the BE-FM heat flux. These observations explain the good agreement observed in Figures 3.4, 3.5, 3.6, and 3.7 for the microgap at low pressures.

For the above situation but in the near-continuum limit, the level of agreement depends on the values of the accommodation coefficients. When one or both accommodation coefficients are small, the BE and NSSJ results are given by the small-accommodation-coefficient-limit versions of Equations (3.12), (3.13), (3.14), and (3.15). As indicated above, these limiting versions agree exactly in the limits that the temperature difference or exactly one accommodation coefficient becomes small and are quite close when both accommodation coefficients are small even for large temperature differences. The situation is different when both accommodation coefficients are near unity because the gas properties are now neither spatially uniform nor approximately equilibrium near the surface. These regions (Knudsen layers) are affected by collision parameters like ω , α , ζ , and Z (Bird, 1994). The heat transfer coefficient in Equation (3.8) does not account for the fact that molecular collisions in the Knudsen layer alter the distribution of the incident molecules to something other than an equilibrium distribution. These observations explain the good agreement between the NSSJ and DSMC heat-flux values in Figures 3.4, 3.5, 3.6, and 3.7 for the microgap at pressures between 10^4 - 10^5 Pa with small accommodation coefficients as well as the slight but noticeable degradation of agreement in this pressure range for near-unity accommodation coefficients.

For an isolated finite convex object in an infinite gas region, the BE and NSSJ results for the FM heat flux have closed-form expressions:

$$q = \left(1 + \frac{\zeta}{4}\right) \left(\frac{\sigma}{2}\right) \left(\frac{p\bar{c}}{T}\right) \Delta T \quad \{\text{BE-FM}\}; \quad (3.16)$$

$$q = \left(1 + \frac{\zeta}{4}\right) \left(\frac{\sigma}{2 - \sigma}\right) \left(\frac{p\bar{c}}{T}\right) \Delta T \quad \{\text{NSSJ-FM}\}. \quad (3.17)$$

The NSSJ-FM heat flux is thus larger than the BE-FM heat flux by a constant factor of $2/(2 - \sigma)$. This factor approaches 1 as σ becomes small but approaches 2 as σ approaches unity. These observations explain the general form of the discrepancy between the NSSJ and DSMC heat fluxes in Figure 3.14 for the microbeam at FM conditions (pressures below 10^3 Pa). More specifically, the NSSJ heat fluxes are about twice the DSMC heat fluxes for order-unity accommodation coefficients but are only slightly larger for small accommodation coefficients.

The NSSJ expression for the heat transfer coefficient h , namely Equation (3.8), is reasonably accurate or exact for some situations but is rather inaccurate for others. For gas contained between two parallel solid surfaces (commonly encountered in microsystems), Equation (3.8) is exact in many limiting regimes (e.g., continuum conditions, one small accommodation coefficient, free-molecular conditions with small temperature differences) and is reasonably accurate, although not exact, for all other conditions in this geometry. Since Equation (3.8) is reasonably accurate, although not exact, for near-continuum conditions with planar surfaces, it should also be comparably accurate for near-continuum conditions with curved surfaces or surfaces of finite extent, where in this context “near-continuum” means that the mean free path is small compared to the surface’s radius of curvature or lateral extent. However, Equation (3.8) is potentially inaccurate when the mean free path is large compared to the surface’s radius of curvature or lateral extent. One example of this is the isolated finite convex object in an infinite gas region, for

which Equation (3.8) is too large by a factor of $2/(2 - \sigma)$. It is in this situation (large mean free path relative to surface curvature or lateral extent) that the heat-transfer-coefficient expression in Equation (3.8) needs to be modified.

These issues are clarified by application to the microbeam geometry. Figure 3.15 shows schematic diagrams of the microbeam geometry for near-continuum conditions (high pressure) and near-free-molecular conditions (low pressure). In each schematic diagram, regions with continuum behavior are blue, whereas regions with strong noncontinuum effects are red (these colors do not refer to temperature). In the high-pressure situation, noncontinuum effects appear only in thin, essentially planar layers adjacent to solid surfaces (Knudsen layers). Inaccuracies arise from two sources in this situation. First, as discussed above, although it is reasonably accurate, Equation (3.8) is not exact even for planar near-continuum conditions. Second, although corner regions occupy only a small fraction of the region with strong noncontinuum effects, the Knudsen layers around corners probably differ from planar Knudsen layers. Both sources of inaccuracy are small, so Equation (3.8) should be reasonably accurate for the microbeam at near-continuum conditions. In the low-pressure situation, the microbeam is embedded in a near-free-molecular region that is bounded by ambient gas and the substrate, both of which are at the ambient temperature and both of which are of large extent compared to the microbeam. This situation is similar to the isolated finite convex object, so Equation (3.8) is probably too large by a factor on the order of $2/(2 - \sigma)$.

It is desirable to modify Equation (3.8) so that it correctly represents the situation of an isolated finite convex object. More specifically, the factor $\sigma/(2 - \sigma)$ should be replaced by $\sigma/2$ when the mean free path λ becomes large compared to the “diameter” D of the object. For a solid object with large thermal conductivity relative to the gas (e.g., the microbeam), it is possible that a single value of D could be used to represent the object and that a function of λ/D could be used to transition smoothly between the factors $\sigma/(2 - \sigma)$ and $\sigma/2$ in h . For a particular geometry such as the microbeam, the “best” diameter and the “best” function could be determined by comparing NSSJ and DSMC heat fluxes at low pressures. The utility of such an approach remains a subject for future research.

Table 3.1: Gas properties for simulations.

Quantity	Symbol	Argon Value	Nitrogen Value	Unit
Boltzmann constant	k_B	1.380658×10^{-23}	1.380658×10^{-23}	J/K
Ref. temperature	T_{ref}	273.15	273.15	K
Ref. pressure	p_{ref}	101,325	101,325	Pa
Ref. number density	n_{ref}	2.687×10^{25}	2.687×10^{25}	$\#/\text{m}^3$
Molecular mass	m	66.3×10^{-27}	46.5×10^{-27}	kg
Ref. mass density	ρ_{ref}	1.781	1.249	kg/m^3
Ref. mean molec. speed	$\bar{c}_{\text{ref}}$	380.6	454.5	m/s
Ref. molec. mean free path	λ_{ref}	0.0624×10^{-6}	0.0583×10^{-6}	m
Ref. viscosity	μ_{ref}	2.117×10^{-5}	1.656×10^{-5}	Pa·s
Ref. thermal conductivity	K_{ref}	0.01641	0.02426	W/(m·K)
Specific heat const. pres.	C_p	520.6	1039.2	J/(kg·K)
Specific heat ratio	γ	5/3	7/5	pure
Visc. temp. exponent	ω	0.81	0.74	pure
Ang. scatt. exponent	α	1.40	1.36	pure
Int. en. mode no.	ζ	0	2	pure
Int. en. relax. coll. no.	Z	irrelevant	5	pure

Table 3.2: Silicon properties at 300 K for simulations.

Quantity	Symbol	Value	Unit
Density	ρ_s	2329	kg/m^3
Specific heat constant pressure	$C_{p,s}$	712.1	J/(kg·K)
Thermal conductivity	K_s	148	W/(m·K)

Figure 3.1. Microgap domain with three layers of material: silicon, gas, silicon.

Figure 3.2. Microgap computational mesh showing the three layers.

Figure 3.3. Microgap temperature fields: argon and nitrogen, walls 285 K and 315 K.

Argon: 1 μm , 285–315 K

Figure 3.4. Microgap heat flux vs. pressure: argon, 1- μm gap, walls 285 K and 315 K.

Nitrogen: 1 μm , 285–315 K

Figure 3.5. Microgap heat flux vs. pressure: nitrogen, 1- μm gap, walls 285 K and 315 K.

Argon: 1 μm , 150–450 K

Figure 3.6. Microgap heat flux vs. pressure: argon, 1- μm gap, walls 150 K and 450 K.

Nitrogen: 1 μm , 150–450 K

Figure 3.7. Microgap heat flux vs. pressure: nitrogen, 1- μm gap, walls 150 K and 450 K.

Figure 3.8. Microbeam computational domain and mesh (dimensions in microns).

Figure 3.9. Microbeam continuum and noncontinuum temperature fields at same power.

Figure 3.10. Microbeam temperature fields: effects of pressure and accommodation.

Figure 3.11. Microbeam temperature fields: effect of domain size.

Figure 3.12. Microbeam heat flow per unit length vs. domain size: low pressure.

Figure 3.13. Microbeam heat flow per unit length vs. domain size: ambient pressure.

Figure 3.14. Microbeam heat flow vs. pressure: baseline domain.

Figure 3.15. Microbeam continuum (blue) and noncontinuum (red) regions.

4. Calore Microscale Heat Transfer Simulation

4.1. Overview

In this section, the previously described models for solid-phase and gas-phase noncontinuum heat transfer are exercised together on a three-dimensional problem involving steady heat conduction along a microbeam and through the surrounding gas to the adjacent substrate. The problem is intended to be representative of a moderately challenging analysis that could confront a microsystem designer.

4.2. Problem Description

The problem chosen for this demonstration simulation is a three-dimensional I-beam suspended above a substrate. The beam cross-section and height above the substrate ($2\text{ }\mu\text{m}$) are consistent with the SUMMIT V process and identical to the two-dimensional examples presented in earlier sections (see Figure 3.8). The length of the microbeam along the third dimension is $120\text{ }\mu\text{m}$. Taking advantage of symmetry, only one quarter of the beam is represented in the computational domain.

Figure 4.1 shows a cross section of the computational mesh that is used to perform the three-dimensional simulations. The beam cross section is discretized into nearly uniform elements. The gas grid is nonuniform, with finer elements near the beam and substrate and progressive coarsening toward the far field. Both grids are uniform along the beam axis. The combined element count is 1,037,760.

Volumetric heating is applied uniformly within the microbeam to produce a temperature gradient. Physically, such heating can be produced via Joule heating by passing an electric current through the beam. The beam end, the gas occupying the end plane, and the substrate are held at the ambient temperature, namely 298 K. The remaining domain boundaries are adiabatic (insulating).

The solid-phase and gas-phase material properties are as discussed in previous chapters. More specifically, solid properties for bulk and polycrystalline silicon (see Chapter 2) and gas properties for nitrogen (see Chapter 3, Table 3.1) are used.

4.3. Calore Implementation

The heat transfer code Calore (Bova et al., 2005) is used to perform all simulations. The subroutines implementing the solid-phase and gas-phase models discussed in the preceding chapters are used. Details of these subroutines can be found in Appendix A.

Calculations are performed in parallel on Myrinet-connected LINUX-based computer clusters. Using eight processors with clock speeds near 3 GHz, a simulation can be completed in approximately fifteen minutes.

4.4. Simulation Results

Temperature fields from two simulations with volumetric heating rates of $1 \times 10^{13} \text{ W/m}^3$ are compared in Figure 4.2. In both cases, the solid is silicon, and the gas is nitrogen at a pressure of $p = 10^5 \text{ Pa}$. The simulation on the left employs a solid bulk thermal conductivity from Holland (1963), a gas bulk thermal conductivity from Sutherland's law, and a zero thermal resistance (infinite heat transfer coefficient) at the gas-solid interface. The simulation on the right employs the polycrystalline-silicon thermal-conductivity model with a grain size of $d_{\text{grain}} = 500 \text{ nm}$ and a film thickness of $l = 2.25 \text{ }\mu\text{m}$ together with a nonzero thermal resistance corresponding to a finite heat transfer coefficient appropriate to nitrogen at the indicated pressure with an accommodation coefficient of $\sigma = 0.5$ (i.e., Equation (3.8)).

It is immediately evident that the beam temperatures are significantly higher in the noncontinuum case than in the continuum case. The maximum temperature rise in the noncontinuum case, 361 K, is approximately 2.6 times the maximum temperature rise in the continuum case, 138 K. These higher temperatures are a result of the lower thermal conductivity in the beam, which impedes heat flow to the cool ends, as well as the insulating effect at the gas-solid interface, which impedes heat flow through the surrounding gas.

Figure 4.3 shows the effects of the noncontinuum solid and gas models on the maximum beam temperature for various volumetric heating rates. In this figure, “on” denotes using the model (i.e., noncontinuum effects included), and “off” denotes not using the model (i.e., noncontinuum effects ignored). Thus, the curve denoted “gas off, solid off” indicates values that would be obtained from the conventional continuum representations of the gas and the solid, whereas the curve denoted “gas on, solid on” includes the gas and solid noncontinuum effects discussed in the preceding chapters. The other two curves show the effect of incorporating noncontinuum effects for only one of the materials while neglecting the noncontinuum effects for the other.

From this figure, the maximum beam temperature is seen to be dominated by noncontinuum effects in the solid, namely the grain-induced reduction in the silicon thermal conductivity at the conditions chosen for this test problem. Lowering the pressure would increase the importance of noncontinuum effects in the gas, and reducing the grain size would increase the importance of noncontinuum effects in the solid. Under all conditions, both models have an increasingly strong effect on the maximum beam temperature as the volumetric heating rate is increased.

It is noted in passing that the effect of the finite size of the domain also increases as the volumetric heating rate is increased. At the largest heating rate, the temperature of the gas in the upper right corner of the domain (see Figure 4.1) can rise by as much as 200 K above the ambient temperature. This phenomenon increases the maximum temperature of the microbeam slightly and can be mitigated by increasing the domain size.

Figure 4.1. Grid cross section for three-dimensional heated microbeam.

heating = $1.000\text{e}+13$ W/m³

temperature

$6.590\text{e}+02$
 $5.687\text{e}+02$
 $4.785\text{e}+02$
 $3.882\text{e}+02$
 $2.980\text{e}+02$

Figure 4.2. Comparison of continuum and noncontinuum results.

Figure 4.3. Maximum beam temperature vs. volumetric heating rate.

5. Conclusions

The use of the Sierra code Calore to simulate microscale heat transfer problems is discussed. Microscale heat transfer differs from macroscale heat transfer in that noncontinuum processes that are not significant for macroscale geometries can become important for microscale geometries. Two classes of noncontinuum processes are considered: phonon processes in thin films of polycrystalline silicon and gas-molecule processes adjacent to gas-solid interfaces. Noncontinuum effects in the solid are described in terms of a thermal conductivity that depends on the film thickness, the surface roughness, and the grain size. The model compares reasonably well to available experimental data. Noncontinuum effects in the gas are described in terms of a heat transfer coefficient at the gas-solid interface, which is the constant of proportionality that relates the normal heat flux to the temperature difference between the solid and the gas.

Calore subroutines implementing these models are developed, entered into Sandia's SourceForge server, and applied to a thermal-actuator microbeam. The Calore results indicate that failure to use the noncontinuum models results in a significant underprediction of the temperature rise produced by a prescribed heating rate. Since the temperature rise in the microbeam is directly related to the thermal stress and the resulting displacement, it is important to use the noncontinuum models in such simulations.

Future efforts will focus on improving the models describing noncontinuum heat transfer effects in the solid and in the gas. For example, the solid thermal-conductivity model can be extended to include the effect of having a distribution of grain sizes as opposed to only a single grain size. Similarly, the model for the heat transfer coefficient at a gas-solid interface can be extended to include the effects of the distance to the nearest surface and of the lateral extent of the solid body. After development and testing, the subroutines incorporating these extensions can be routinely archived into Sandia's SourceForge server and thereby made readily available to the Calore user community.

Appendix A: Calore Subroutines

A.1. Obtaining Subroutines

The subroutines developed for this work are located on Sandia's SourceForge server under the project name "SIERRA User Subroutines." They may therefore be obtained through the URL

<https://sourceforge.sandia.gov/horde/chora/cvs.php/sierrausersub/calore/src>

by clicking on the desired subroutine and then clicking "Download" from the upper right hand corner of the frame in which the source code appears.

A.2. Solid Model

The user subroutines that implement the model for conduction in the solid described in Chapter 2 are provided below. These subroutines are contained in the file `kpolysi.f`.

```
C   Subroutine to calculate thermal conductivity based on
C   the empirical formula.
C   Please note that the unit of k is W/m.K

      subroutine kpolysi ( objid,
&   n,
&   nint,
&   coords,
&   temperature,
&   cond,
&   ierror)

      implicit none

      integer n
      integer nint
      integer objid(n)
      double precision coords(3, n, nint)
      double precision temperature(n, nint)
      double precision cond(3,3,n, nint)
      integer ierror

      integer idop, numipt

      integer ln

      integer i, j, k, q

      real wtfn(3), ddx, hcce, sfrms, dgrx, sdvgrx, tp, dgrn

C   Initialization
```

```

        hcce = 0.0                ! Zero out thermal conductivity
C
C   Set default value
        ddx = 2.25e-6            ! Film thickness
        sfrms = 1.0e-10          ! Surface sfrmsness (asperity: rms~0.1nm)
        dgrx = 500e-9            ! Mode Grain size = 0.1 um = 100 nm
        sdvgrx = 250e-9! Standard deviation for size distribution

C   Weighting function for grain scattering rate
C   to capture the grain size distribution
C   In this case, a symmetric distribution is assumed.
        wtfm(1) = 0.25
        wtfm(2) = 0.50
        wtfm(3) = 0.25

        dgrn = 1 / (2*(wtfm(1)/(dgrx-sdvgrx/2) + wtfm(2)/dgrx
&          + wtfm(3)/(dgrx+sdvgrx/2)))

        do q = 1, nint
            do i = 1, n

                do j = 1, 3
                    do k = 1, 3
                        cond(k,j,i, q) = 0.0D00
                    end do
                end do
            end do
        end do

        do q = 1, nint
            do i = 1, n
                tp = temperature(i,q)
                call effk(tp, hcce, ddx, sfrms, dgrn)
                cond(1,1, i, q) = hcce
                cond(2,2, i, q) = hcce
                cond(3,3, i, q) = hcce

            end do
        end do

        return
    end

```

This subroutine functions within the property specification for material facility. The subroutine name is given for the thermal conductivity of a given material, within the property specification for material block, with the line command:

```
thermal conductivity subroutine = <subroutine_name>
```

Due to an inability, as of this writing, to store instance data within a property specification for a material block, a uniquely-named subroutine is required for each material in the simulation, where the grain size and other distinguishing parameters are specified within the subroutine itself.

Several supporting subroutines are required within the same file to enable them to function, which are listed below. Only one copy of these subroutines is required, regardless of how many materials are present. The last subroutine is a numerical integration routine from the SLATEC library (Fong, et al., 1993). Any reasonable numerical integration routine can be substituted.

```

C23456789012345678901234567890123456789012345678901234567890123456789012
C
C Subroutine to predict thermal conductivity using the semi-classical theory
C (ref. Callaway 1959, Holland 1963)
C Multiple-mode Holland model - phonon transport in microscale structures
C Included the thin film surface effect; grain bound. scatter.
C use the sound speed (weighted average) as the propagation group velocity
C Units are in SI

C Developed by C. Channy Wong on 10/1/2002
C Revised to be user-subroutine for Calore: ccw 09/21/2004
C
C hcce: heat conductivity in W/m.K
C tp: temperature in K (default: 300K)
C dd: characteristic length in m, (default: 100um)
C vs: sound speed
C vl: phonon propagating group velocity in ith mode
C dgrn: size of grain in m (default: film thickness ~100um)

C23456789012345678901234567890123456789012345678901234567890123456789012
C
  subroutine effk(tp, hcce, ddx, sfrmx, dgrx)

    common ee, tau0, vs, vl, dd, tp2, tp4, tp5, psrc, alpha1, beta1
    *          , sfrms, dgrn, ptrm

    common jmode

    real x0,x1,funxx,smx
    real c11, c22
    external funxx

    real v11(3), xx0(3), xx1(3), b1(3), hcc(3)

    integer ifact(3)

    dd = ddx
    sfrms = sfrmx
    dgrn = dgrx

C set constants

    pi = 3.141592654
    ee = 2.718281828

C Boltzmann constant = bzm*1.e-23
C h-bar = hb*1.e-34

```

```

      bzm = 1.380658
      hb = 1.05457266

C Boltzmann const./h-bar = c1 * 1.0e+11

      c1 = bzm/hb
      c11 = c1**3

C Boltzmann const./(2*pi**2) = c22 * 1.0e-23

      c22 = bzm/(2*pi*pi)

C initialize variables

      smx = 0.

      tp2 = tp**2
      tp3 = tp**3
      tp4 = tp**4
      tp5 = tp**5

      do 10 i=1,3
          ifact(i) = 1
10      continue

C Modified Holland Model with multiple phonon propagation modes
C 1 for longitudinal, 2 for transverse lower, 3 for transverse upper
C data for PolySilicon
C dtmp in K, vss in m/s
C aal unit in e-44 sec**3, bbl unit in e-22 sec. deg**-3

      mxmode = 3

      aal = 0.132

      b1(1) = 0.020 * c1**2
      v11(1) = 8480.
      xx0(1) = 0.0
      dtmp = 570.
      xx1(1) = dtmp/tp

      b1(2) = 9.3e-2 * c1
      v11(2) = 5860.
      xx0(2) = 0.0
      dtmp = 180.
      xx1(2) = dtmp/tp
      ifact(2) = 2

      b1(3) = 5.5e+4 * c1**2
      v11(3) = 2000.
      xx0(3) = dtmp/tp      ! Use Debye temp. from lower mode
      dtmp = 210.
      xx1(3) = dtmp/tp
      ifact(3) = 2

```



```

C   Sound speed as an averaged phonon group velocity
      vs = 3 / (2/v11(2) + 1/v11(1))

C   Constant for Probability of specular reflection
      pcst = 4 * pi * c1**2 * tp2 / vs**2
      psrc = pcst * (sfrms*1.0e+11)**2

C   Roughness of grain boundary is same as film layer surface
C   relating the surface character to the grain size
C
      coefx = 1.0e-15
      sfixx = coefx / dgrn
      ptrm = pcst * (sfixx*1.0e+11)**2

C   Coeff. constant for impurity scattering
      alpha1 = aal * c1**4

C      print *, tp, c1, c11, c22, alpha1, beta1, psrc

      hcce = 0.0

      do 600 jm=1,mxmode

C   Coeff. constant for Umklapp and N-process
      beta1 = b1(jm)

      vl = v11(jm)

C      vs = v11(jm)

      ifact0 = ifact(jm)

C   set integral limits

      x0 = xx0(jm)
      x1 = xx1(jm)

      jmode = jm

      call qnc79(funxx,x0,x1,1e-5,smx,ierr,ik)

C      print *, 'Integral of function is ', smx

      hcc0 = c11 * tp3 * c22 * smx / 3
      hcc(jm) = ifact0* hcc0 * 1.e+10
      hcce = hcce + hcc(jm)
600  continue

C      print *, tp, hcce

      return
      end

```

```

C23456789012345678901234567890123456789012345678901234567890123456789012
C
      Function funxx(x)

      common ee, tau0, vs, vl, dd, tp2, tp4, tp5, psrc, alpha1, betal
*          , sfrms, dgrn, ptrm

      common jmode

      real funxx, fxx, x

      tau0r = 0.0

      if (x.eq.0.0) then
        funxx=0
        return
      endif

C relaxation time for boundary scattering
C tau0r1 = sound speed / length / factor
      psr = exp(-psrc * x**2)
      rfbndy = (1-psr) / (1+psr)
      tau0r = tau0r + vs / dd * rfbndy

C relaxation time for grain boundary scattering
C tau0r1 = sound speed / length / factor
      if (dgrn .lt. dd) then
        ptr = exp(-ptrm * x**2)
        grainbdy = (1-ptr) / (1+ptr)
        vvs = vl
        tau0r = tau0r + grainbdy*vvs/dgrn
      endif

C relaxation time for scattering with point defect
C tau0r2 = A*omega**4
      tau0r = tau0r + alpha1 * tp4 * x**4

C relaxation time for normal process (low temperature)
C tau0r3 = Bi * temp**5 * x**2 (longitudinal mode)
C tau0r3 = Bi * temp**5 * x      (transverse mode)

C relaxation time for umklapp process
C tau0r3 = Bt * temp**5 * x**2 (longitudinal mode)
C tau0r3 = 0                    (transverse mode; low freq.)
C tau0r3 = Bt * temp**2 * x**2 / sinh x (transverse wave; high freq.)

      go to (110, 120, 130) jmode
110      tau0r = tau0r + betal * tp5 * x**2 ! combine N & U
          go to 140

120      tau0r = tau0r + betal * tp5 * x      ! only N
          go to 140

```

```

130      tau0r = tau0r + betal * tp2 * x**2 / sinh(x)

140  continue

      if (tau0r.eq.0) then
        pause 'Error: 1/tau0 is zero.'
      else
        tau0 = 1/tau0r
      endif
C

      tau = tau0
      fxx = x**4 * ee**x / (ee**x-1)**2
      funxx = fxx * tau / vl

      return
      end

      SUBROUTINE QNC79 (FUN, A, B, ERR, ANS, IERR, K)
C***BEGIN PROLOGUE  QNC79
C***PURPOSE  Integrate a function using a 7-point adaptive Newton-Cotes
C             quadrature rule.
C***LIBRARY    SLATEC
C***CATEGORY   H2A1A1
C***TYPE       SINGLE PRECISION (QNC79-S, DQNC79-D)
C***KEYWORDS   ADAPTIVE QUADRATURE, INTEGRATION, NEWTON-COTES
C***AUTHOR    Kahaner, D. K., (NBS)
C             Jones, R. E., (SNLA)
C***DESCRIPTION
C
C   Abstract
C
C     QNC79 is a general purpose program for evaluation of
C     one dimensional integrals of user defined functions.
C     QNC79 will pick its own points for evaluation of the
C     integrand and these will vary from problem to problem.
C     Thus, QNC79 is not designed to integrate over data sets.
C     Moderately smooth integrands will be integrated efficiently
C     and reliably. For problems with strong singularities,
C     oscillations etc., the user may wish to use more sophis-
C     ticated routines such as those in QUADPACK. One measure
C     of the reliability of QNC79 is the output parameter K,
C     giving the number of integrand evaluations that were needed.
C
C   Description of Arguments
C
C   --Input--
C     FUN - name of external function to be integrated. This name
C           must be in an EXTERNAL statement in your calling
C           program. You must write a Fortran function to evaluate
C           FUN. This should be of the form
C
C             REAL FUNCTION FUN (X)
C
C             C
C             C      X can vary from A to B

```

```

C          C      FUN(X) should be finite for all X on interval.
C          C
C          FUN = ...
C          RETURN
C          END
C      A      - lower limit of integration
C      B      - upper limit of integration (may be less than A)
C      ERR    - is a requested error tolerance.  Normally, pick a value
C              0 .LT. ERR .LT. 1.0E-3.
C
C      --Output--
C      ANS    - computed value of the integral.  Hopefully, ANS is
C              accurate to within ERR * integral of ABS(FUN(X)).
C      IERR   - a status code
C              - Normal codes
C                1  ANS most likely meets requested error tolerance.
C               -1  A equals B, or A and B are too nearly equal to
C                   allow normal integration.  ANS is set to zero.
C              - Abnormal code
C                2  ANS probably does not meet requested error tolerance.
C      K      - the number of function evaluations actually used to do
C              the integration.  A value of K .GT. 1000 indicates a
C              difficult problem; other programs may be more efficient.
C              QNC79 will gracefully give up if K exceeds 2000.
C
C***REFERENCES  (NONE)
C***ROUTINES CALLED  I1MACH, R1MACH, XERMSG
C***REVISION HISTORY  (YYMMDD)
C  790601  DATE WRITTEN
C  890531  Changed all specific intrinsics to generic.  (WRB)
C  890531  REVISION DATE from Version 3.2
C  891214  Prologue converted to Version 4.0 format.  (BAB)
C  900315  CALLs to XERROR changed to CALLs to XERMSG.  (THJ)
C  920218  Code and prologue polished.  (WRB)
C***END PROLOGUE  QNC79
C      .. Scalar Arguments ..
C      REAL A, ANS, B, ERR
C      INTEGER IERR, K
C      .. Function Arguments ..
C      REAL FUN
C      EXTERNAL FUN
C      .. Local Scalars ..
C      REAL AE, AREA, BANK, BLOCAL, C, CE, EE, EF, EPS, Q13, Q7, Q7L,
+      SQ2, TEST, TOL, VR, W1, W2, W3, W4
C      INTEGER I, KML, KMX, L, LMN, LMX, NBITS, NIB, NLMN, NLMX
C      LOGICAL FIRST
C      .. Local Arrays ..
C      REAL AA(40), F(13), F1(40), F2(40), F3(40), F4(40), F5(40),
+      F6(40), F7(40), HH(40), Q7R(40), VL(40)
C      INTEGER LR(40)
C      .. External Functions ..
C      REAL R1MACH
C      INTEGER I1MACH
C      EXTERNAL R1MACH, I1MACH

```

```

C    .. External Subroutines ..
    EXTERNAL XERMSG
C    .. Intrinsic Functions ..
    INTRINSIC ABS, LOG, MAX, MIN, SIGN, SQRT
C    .. Save statement ..
    SAVE NBITS, NLMX, FIRST, SQ2, W1, W2, W3, W4
C    .. Data statements ..
    DATA KML /7/, KMX /2000/, NLMN /2/
    DATA FIRST /.TRUE./
C***FIRST EXECUTABLE STATEMENT   QNC79
    IF (FIRST) THEN
        W1 = 41.0E0/140.0E0
        W2 = 216.0E0/140.0E0
        W3 = 27.0E0/140.0E0
        W4 = 272.0E0/140.0E0
C        NBITS = R1MACH(5)*I1MACH(11)/0.30102000E0
        NBITS = 24
        NLMX = MIN(40,(NBITS*4)/5)
        SQ2 = SQRT(2.0E0)
    ENDIF
    FIRST = .FALSE.
    ANS = 0.0E0
    IERR = 1
    CE = 0.0E0
    IF (A .EQ. B) GO TO 260
    LMX = NLMX
    LMN = NLMN
    IF (B .EQ. 0.0E0) GO TO 100
    IF (SIGN(1.0E0,B)*A .LE. 0.0E0) GO TO 100
    C = ABS(1.0E0-A/B)
    IF (C .GT. 0.1E0) GO TO 100
    IF (C .LE. 0.0E0) GO TO 260
    NIB = 0.5E0 - LOG(C)/LOG(2.0E0)
    LMX = MIN(NLMX,NBITS-NIB-4)
    IF (LMX .LT. 2) GO TO 260
    LMN = MIN(LMN,LMX)
100  TOL = MAX(ABS(ERR),2.0E0**(5-NBITS))
C    IF (ERR .EQ. 0.0E0) TOL = SQRT(R1MACH(4))
    EPS = TOL
    HH(1) = (B-A)/12.0E0
    AA(1) = A
    LR(1) = 1
    DO 110 I = 1,11,2
        F(I) = FUN(A+(I-1)*HH(1))
110  CONTINUE
    BLOCAL = B
    F(13) = FUN(BLOCAL)
    K = 7
    L = 1
    AREA = 0.0E0
    Q7 = 0.0E0
    EF = 256.0E0/255.0E0
    BANK = 0.0E0
C

```

```

C      Compute refined estimates, estimate the error, etc.
C
120 DO 130 I = 2,12,2
      F(I) = FUN(AA(L)+(I-1)*HH(L))
130 CONTINUE
      K = K + 6
C
C      Compute left and right half estimates
C
      Q7L = HH(L)*((W1*(F(1)+F(7))+W2*(F(2)+F(6)))+
+      (W3*(F(3)+F(5))+W4*(F(4))))
      Q7R(L) = HH(L)*((W1*(F(7)+F(13))+W2*(F(8)+F(12)))+
+      (W3*(F(9)+F(11))+W4*(F(10))))
C
C      Update estimate of integral of absolute value
C
      AREA = AREA + (ABS(Q7L)+ABS(Q7R(L))-ABS(Q7))
C
C      Do not bother to test convergence before minimum refinement level
C
      IF (L .LT. LMN) GO TO 180
C
C      Estimate the error in new value for whole interval, Q13
C
      Q13 = Q7L + Q7R(L)
      EE = ABS(Q7-Q13)*EF
C
C      Compute nominal allowed error
C
      AE = EPS*AREA
C
C      Borrow from bank account, but not too much
C
      TEST = MIN(AE+0.8E0*BANK,10.0E0*AE)
C
C      Don't ask for excessive accuracy
C
      TEST = MAX(TEST,TOL*ABS(Q13),0.00003E0*TOL*AREA)
C
C      Now, did this interval pass or not?
C
      IF (EE-TEST) 150,150,170
C
C      Have hit maximum refinement level -- penalize the cumulative error
C
140 CE = CE + (Q7-Q13)
      GO TO 160
C
C      On good intervals accumulate the theoretical estimate
C
150 CE = CE + (Q7-Q13)/255.0
C
C      Update the bank account.  Don't go into debt.
C

```

```

160 BANK = BANK + (AE-EE)
    IF (BANK .LT. 0.0E0) BANK = 0.0E0
C
C    Did we just finish a left half or a right half?
C
    IF (LR(L)) 190,190,210
C
C    Consider the left half of next deeper level
C
170 IF (K .GT. KMX) LMX = MIN(KML,LMX)
    IF (L .GE. LMX) GO TO 140
180 L = L + 1
    EPS = EPS*0.5E0
    IF (L .LE. 17) EF = EF/SQ2
    HH(L) = HH(L-1)*0.5E0
    LR(L) = -1
    AA(L) = AA(L-1)
    Q7 = Q7L
    F1(L) = F(7)
    F2(L) = F(8)
    F3(L) = F(9)
    F4(L) = F(10)
    F5(L) = F(11)
    F6(L) = F(12)
    F7(L) = F(13)
    F(13) = F(7)
    F(11) = F(6)
    F(9) = F(5)
    F(7) = F(4)
    F(5) = F(3)
    F(3) = F(2)
    GO TO 120
C
C    Proceed to right half at this level
C
190 VL(L) = Q13
200 Q7 = Q7R(L-1)
    LR(L) = 1
    AA(L) = AA(L) + 12.0E0*HH(L)
    F(1) = F1(L)
    F(3) = F2(L)
    F(5) = F3(L)
    F(7) = F4(L)
    F(9) = F5(L)
    F(11) = F6(L)
    F(13) = F7(L)
    GO TO 120
C
C    Left and right halves are done, so go back up a level
C
210 VR = Q13
220 IF (L .LE. 1) GO TO 250
    IF (L .LE. 17) EF = EF*SQ2
    EPS = EPS*2.0E0

```

```

        L = L - 1
        IF (LR(L)) 230,230,240
230  VL(L) = VL(L+1) + VR
        GO TO 200
240  VR = VL(L+1) + VR
        GO TO 220
C
C      Exit
C
250  ANS = VR
        IF (ABS(CE) .LE. 2.0E0*TOL*AREA) GO TO 270
        IERR = 2
C      CALL XERMSG ('SLATEC', 'QNC79',
C      + 'ANS is probably insufficiently accurate.', 2, 1)
        write(*,*) "SLATEC:QNC79: ANS is probably insufficiently
1 accurate."
        GO TO 270
260  IERR = -1
C      CALL XERMSG ('SLATEC', 'QNC79',
C      + 'A and B are too nearly equal to allow normal integration. $$'
C      + '// 'ANS is set to zero and IERR to -1.', -1, -1)
270  RETURN
        END

```


A.3. Gas Model

The user subroutines that implement the gas model described in Chapter 3 are provided below. These subroutines are contained in the file `gasnoncon.f`.

```
      subroutine conhot(faceid, nelemf, nint, coords, t, cond,ierror)
c
c  calculate contact conductance as a function of hot wall temperature
c
      integer faceid, nelemf, nint, ierror
      integer ie, ii
      double precision coords,t,cond,rdata(5)
      double precision  sigma, press, kb, pi, m, c, gamma, twall
      dimension faceid(nelemf)
      dimension coords(3,nelemf,nint)
      dimension t(nelemf,nint),cond(nelemf,nint)
c
      pi = 4.0*DATAN(dble(1.0))
c
c  get instance data for conductance calculation
      call acal_get_region_real_data(5,rdata)
c
c  gas pressure
      press = rdata(1)
c  accomodation coefficient
      sigma = rdata(2)
c  Boltzmann constant
      kb = rdata(3)
c  molec. mass
      m = rdata(4)
c  specific heat ratio
      gamma = rdata(5)
c
c  use hot wall temperature for h calc
      twall = MAX(t(1,nint), t(2,nint))
c
      c = DSQRT(8.0*kb*twall/pi/m)
c
      do ii = 1, nint
        do ie = 1, nelemf
          cond(ie,ii)= 0.25*(gamma+1.0)/(gamma-1.0)*
1          (sigma/(2.0-sigma))*press*c/twall
        end do
      end do
c
      return
      end
c
      subroutine concold(faceid, nelemf, nint, coords, t, cond,ierror)
c
c  calculate contact conductance as a function of cold wall temperature
c
```

```

integer faceid, nelemf, nint, ierror
integer ie, ii
double precision coords,t,cond,rdata(5)
double precision sigma, press, kb, pi, m, c, gamma, twall
dimension faceid(nelemf)
dimension coords(3,nelemf,nint)
dimension t(nelemf,nint),cond(nelemf,nint)
C
    pi = 4.0*DATAN(dble(1.0))
C
C   get instance data for conductance calculation
    call acal_get_region_real_data(5,rdata)
C
C   gas pressure
    press = rdata(1)
C   accomodation coefficient
    sigma = rdata(2)
C   Boltzmann constant
    kb = rdata(3)
C   molec. mass
    m = rdata(4)
C   specific heat ration
    gamma = rdata(5)
C
C   use cold wall temperature for h calc
    twall = MIN(t(1,nint), t(2,nint))
C
    c = DSQRT(8.0*kb*twall/pi/m)
C
    do ii = 1, nint
        do ie = 1, nelemf
            cond(ie,ii)= 0.25*(gamma+1.0)/(gamma-1.0)*
1              (sigma/(2.0-sigma))*press*c/twall
        end do
    end do
C
    return
end

subroutine conconst(faceid, nelemf, nint, coords, t, cond,ierror)
C
C   calculate convection coefficient as a function of constant wall temperature
C
integer faceid, nelemf, nint, ierror
integer ie, ii
double precision coords,t,cond,rdata(5)
double precision sigma, press, kb, pi, m, c, gamma, twall
double precision coef
dimension faceid(nelemf)
dimension coords(3,nelemf,nint)
dimension t(nelemf,nint),cond(nelemf,nint)
C
    pi = 4.0*DATAN(dble(1.0))

```

```

C
C      get region data for conductance calculation
C      call acal_get_region_real_data(5,rdata)
C
C      gas pressure
C      press = rdata(1)
C      accomodation coefficient
C      sigma = rdata(2)
C      Boltzmann constant
C      kb = rdata(3)
C      molec. mass
C      m = rdata(4)
C      specific heat ration
C      gamma = rdata(5)

C      get the wall temperature from instance data
C      call acal_get_instance_real_data(1,rdata)
C      twall = rdata(1)
C
C      c = DSQRT(8.0*kb*twall/pi/m)
C
C      coef = 0.25*(gamma+1.0)/(gamma-1.0)*(sigma/(2.0-sigma))*
1      press*c/twall

      do ii = 1, nint
        do ie = 1, nelemf
          cond(ie,ii) = coef
        end do
      end do
C
      return
      end

```

The first two subroutines are used in conjunction with the contact capability in Calore. The subroutine name is given within the contact enforcement block with the line command:

```
coefficient subroutine = <subroutine_name>
```

Use of the first subroutine, `conhot`, is indicated if the solid is hotter than the adjacent air. The second subroutine, `concold`, is used in the converse situation.

The final subroutine, `conconst`, is used in conjunction with the convective boundary condition in Calore. This subroutine enables a constant-temperature solid that is not included in the simulation to be represented. In this case, the subroutine name is given within a convective flux boundary condition block with the line command:

```
convective coefficient subroutine = conconst
```

Because, as of this writing, user subroutines do not have access to the reference temperature on a convective flux boundary condition, the reference temperature must be specified as real data within the block.

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