

Heat Transfer Regimes in Microstructures

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Submicron dimensions are the hallmark of integrated electronic circuits, photovoltaic cells, sensors, and actuators. The design of these devices requires heat transfer analysis. Often it is not known to the designer whether a given microstructure can be analyzed using macroscale heat transfer theory, i.e., a method not considering the size dependence of a transport property such as thermal conductivity. This study develops regime maps showing the boundary between the macroscale and microscale heat transfer regimes. The maps relate the geometric dimension separating the two regimes to temperature for conduction in solids, to temperature, pressure, and Reynolds number for convection in gases, and to the temperature of the emitting medium for radiative transfer. The material purity and defect structure strongly influence the regime boundaries. Microstructures pertaining to a given technology are marked on these maps to determine whether macroscale heat transfer theory is applicable. By marking regions on the maps for the expected future development of microtechnologies, research needs in microscale heat transfer can be anticipated.

1 Introduction

Structures with dimensions between $100\text{ }\mu\text{m}$ and $50\text{ }\text{\AA}$ can be fabricated with modern film deposition and patterning techniques. These microstructures are the basis of integrated electronic circuits, photovoltaic cells, sensors, and actuators. The analysis of heat transfer in these devices is essential for their successful design and fabrication. Often it is not known whether heat transfer in microstructures can be analyzed with *macroscale* theories, i.e., methods that do not consider the size dependence of a transport property such as thermal conductivity or thermal radiation reflectance.

If macroscale heat transfer theory is applied to a microstructure in a situation for which it is inappropriate, then a significant error in the calculated heat transfer rate or temperature distribution can result. Such an error can cause the device to be designed to perform in a suboptimal manner or prevent it from being able to function. In electronic devices, microscale effects in a thin layer can inhibit the flow of heat from hotspots within the layer, such as the channel of a MOSFET in silicon-on-insulator electronics, resulting in peaks of temperature of a magnitude greater than those predicted by macroscale analysis (Goodson and Flik, 1992). These temperature peaks can affect the performance of the device and reduce the mean time to failure of an electronic circuit. If the influence of the film thickness on the absorptance of an infrared radiation detector element is not considered, then the detector sensitivity is different from the design value. A pyrometric measurement of the substrate temperature during film deposition is in error if the emissivity variation with the film thickness is neglected, resulting in poor temperature control (Flik et al., 1992). The designer of microstructures must have a criterion with which to decide whether macroscale heat transfer theory can be applied to a given device or whether *microscale* theory must be used. Microscale theory determines the effect of the structure dimensions on a transport property by considering the physical mechanism of transport, e.g., electron conduction or electromagnetic wave propagation.

Fundamentals and applications were presented for microscale thermal conduction by Ziman (1960), Devienne (1965), and Tien et al. (1969), and for microscale thermal radiation by Yeh (1988), Cravalho et al. (1967), Armaly and Tien (1970),

and Chen and Tien (1991). Recently, microscale heat transfer phenomena have received intensive interest due to the emergence of thermal microsensors (Udell et al., 1990) and high- T_c superconducting films (Flik and Tien, 1990; Goodson and Flik, 1991). None of these studies presented the boundary of the microscale heat transfer regime for a given transport mechanism in terms of parameters available to the microstructure designer, i.e., the structure dimensions and the operating temperature. Hence, based on these works it is not immediately possible to decide whether macroscale theory is applicable for a microstructure or not.

The present study develops heat transfer *regime maps* for microstructures relating a geometric length scale to temperature. The boundary between the microscale and macroscale regimes is determined as a function of temperature by the requirement that the application of macroscale theory yields an error in the transport property not exceeding 5 percent. Through the mechanistic length scale governing the transport process, this functional relation depends on the material properties, i.e., the scattering mechanisms for electron and phonon heat conduction in solids, and the electromagnetic dispersion relations for thermal radiation absorption. The geometric lengthscale is the smallest structure dimension, except for conduction in rapidly moving gases, where it is given by the boundary-layer thickness. Previous regime maps delineating boundaries between applicable theories of transport phenomena were published for rarified gas dynamics by Tsien (1946) and for thermal radiation in packed beds by Tien (1988). Recently, Majumdar (1991) illustrated the analogy between microscale conduction in dielectrics and radiative transfer, and presented a regime map for diamond films similar to the one in the present study.

The impact of these regime maps is twofold. First, specific microdevices can be represented with a region in a regime map, showing immediately whether or not a certain transport process in a given device can be analyzed with macroscale theory. Second, demands for future research in microscale heat transfer can be anticipated by marking regions in the regime maps that correspond to the expected development of a given microtechnology. This work does not present new physics information. It relies on known physical foundations of transport phenomena. But this knowledge has not been applied to date in thermal analysis and design. By providing regime maps, this work attempts to aid in the development of microscale thermal analysis and experimentation.

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2 Mechanistic Length Scales

2.1 Thermal Conduction. Mean Free Path. In solids, heat is carried by electrons and lattice waves, whose quanta are phonons. In pure metals, the electron contribution is dominant. In dielectrics and semiconductors, the phonon contribution is dominant. In gases, heat is carried by molecules.

Kinetic theory yields the thermal conductivity (Rohsenow and Choi, 1961):

$$k = \frac{1}{3} C v \Lambda. \quad (1)$$

For gas conduction, the specific heat $C = C_m$ is that of the gas at constant volume per unit volume, $v = v_m$ is the average molecular velocity, and $\Lambda = \Lambda_m$ is the molecular mean free path. For thermal conduction in metals, $C = C_e$ is the electron specific heat, $v = v_e$ is the electron Fermi velocity (Kittel, 1986), and $\Lambda = \Lambda_e$ is the electron mean free path. For conduction in dielectrics and semiconductors, $C = C_s$ is the phonon specific heat, $v = v_s$ is the average speed of sound, and $\Lambda = \Lambda_s$ is the phonon mean free path. The specific heat C to be used in Eq. (1) is only that portion of the total specific heat which is due to the energy carrier.

Solids. Figure 1 illustrates that for a thin layer, the importance of boundary scattering increases with the ratio Λ/d , where Λ is the bulk value of the mean free path of the dominant carriers of heat, and d is the layer thickness. Scattering on the boundaries of the layer reduces the carrier mean free path from its bulk value, reducing the thermal conductivity according to Eq. (1). For $\Lambda \ll d$, this reduction may be neglected, but for $\Lambda \sim d$ and $\Lambda > d$, the effect of boundary scattering must be considered. For this case, the effective thermal conductivity even in an isotropic film depends on the direction of energy flow. In what follows, the effective thermal conductivity along the layer is the absolute value of the ratio of the heat flux to the temperature gradient along the layer. The effective thermal

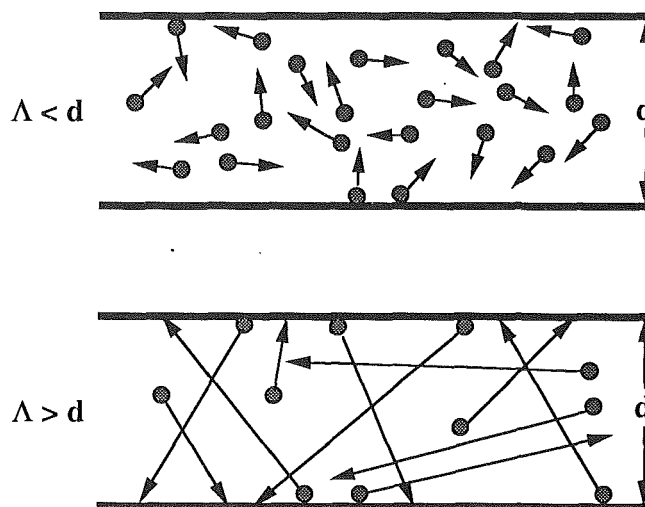


Fig. 1 Thermal conduction in a thin layer

conductivity normal to the layer is the product of the heat flux normal to the layer and the layer thickness divided by the temperature difference between the top and bottom surfaces of the layer.

Fuchs (1938) and Sondheimer (1952) determined the effect of the boundary scattering of electrons on the effective electrical conductivity along thin metal films by solving the Boltzmann equation. Tien et al. (1969) and Kumar and Vradis (1991) showed that this result may be used with little error up to room temperature to determine the effective thermal conductivity along thin metal films. Majumdar (1991) developed the equation of phonon radiative transfer from the Boltzmann equation to determine microscale phonon conduction in dielectrics. This equation considers the variation of the phonon free paths about the mean free path and the dependence of the phonon mean

Nomenclature

C = specific heat at constant volume per unit volume, $\text{J m}^{-3} \text{K}^{-1}$
 D = molecular diameter, m
 d = smallest dimension, m
 e = electron charge = $-1.60 \times 10^{-19} \text{ C}$
 h = heat transfer coefficient, $\text{W m}^{-2} \text{K}^{-1}$
 i = $(-1)^{1/2}$
 i'_λ = directional spectral intensity, $\text{W m}^{-2} \mu\text{m}^{-1} \text{sr}^{-1}$
 k = thermal conductivity, $\text{W m}^{-1} \text{K}^{-1}$
 k_B = Boltzmann constant = $1.38 \times 10^{-23} \text{ J K}^{-1}$
 L = smallest streamwise dimension, m
 M = Mach number
 m_e = electron mass = $9.11 \times 10^{-31} \text{ kg}$
 m_e^* = effective electron mass, kg
 Nu = Nusselt number = hL/k
 $\bar{n}$ = complex refractive index = $n + ik$
 n = real part of complex refractive index = refractive index
 n_e = electron number density, m^{-3}
 n_m = molecule number density, m^{-3}

Pr = Prandtl number = ν/α
 p = pressure, N m^{-2}
 R = reflectance
 Re = Reynolds number = LV_∞/ν
 R_I = reflectance calculated considering interference
 R_N = reflectance calculated not considering interference
 T = temperature, K
 T_r = reference temperature, K, Eqs. (11), (13), and (14)
 t = time, s
 V_∞ = free-stream velocity, m s^{-1}
 v = average carrier velocity, m s^{-1}
 α = thermal diffusivity, $\text{m}^2 \text{s}^{-1}$
 γ = Sommerfeld parameter, $\text{J m}^{-3} \text{K}^{-2}$
 δ = boundary layer thickness, m; oxygen content parameter of $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$
 ϵ = dielectric function
 ϵ_0 = electric permittivity of vacuum = $8.85 \times 10^{-12} \text{ C}^2 \text{N}^{-1} \text{m}^{-2}$
 ϵ_∞ = high-frequency dielectric constant
 θ = Debye temperature, K
 κ = imaginary part of complex refractive index = extinction coefficient

Λ = carrier mean free path, m
 λ = wavelength in vacuum, m
 ν = kinematic viscosity, $\text{m}^2 \text{s}^{-1}$
 ρ = electrical resistivity, Ωm
 σ = Stefan-Boltzmann constant = $5.67 \times 10^{-8} \text{ W m}^{-2} \text{K}^{-4}$
 τ = relaxation time = Λ/v , s
 ϕ = phase difference = $4\pi nd/\lambda$
 ω = frequency, rad s^{-1}
 ω_p = plasma frequency, rad s^{-1}

Subscripts

A = I or N , Eq. (5)
 e = electron property
 e,i = electron property limited by scattering on imperfections
 e,s = electron property limited by scattering on phonons
 m = molecular property
 p = photon property
 s = phonon property
 s,e = phonon property limited by scattering on electrons
 s,i = phonon property limited by scattering on imperfections
 s,s = phonon property limited by scattering on phonons
 tot = total property

free path on the phonon frequency. Chen and Tien (1992) solved the equation of radiative transfer considering the transmission of carriers through the film boundaries to determine the effective thermal conductivity normal to and along GaAs films in a GaAs-AlGaAs multilayer structure. Because of the complexity of solutions to this equation and the uncertainty in the frequency dependence of the mean free path, the equation of phonon radiative transfer is not used to determine regime boundaries in the present work.

Flik and Tien (1990), by assuming that all carrier free paths are equal to the mean free path in the absence of boundary scattering, obtained approximate closed-form solutions for the effective electron or phonon conductivity along or normal to a film. The result for conduction along a film agrees within 20 percent with that of Fuchs (1938) and Sondheimer (1952). For $d > \Lambda$, the analysis of Flik and Tien (1990) yielded $k_{\text{eff}}/k = 1 - \Lambda/(3d)$ for the effective conductivity normal to the layer, and $k_{\text{eff}}/k = 1 - 2\Lambda/(3\pi d)$ for the effective conductivity along the layer, where k and Λ are the isotropic bulk values of the conductivity and the mean free path. The use of the bulk value of k rather than k_{eff} results in an error greater than 5 percent for $d < 7\Lambda$ for conduction normal to the layer, and for $d < 4.5\Lambda$ for conduction along the layer. These inequalities determine the microscale regimes in the present analysis.

These criteria determine whether the microscale effect increases the volume resistance of the film. They do not consider the thermal boundary resistance, which can cause the effective conductivity normal to multilayer structures to vary with the layer thicknesses. If the temperature difference across the interface is small and the temperature is below about 30 K, the thermal boundary resistance at a dielectric-dielectric or metal-dielectric interface is governed by the acoustic mismatch between the materials and is inversely proportional to the third power of the lower temperature (Swartz and Pohl, 1989). At temperatures above 100 K, the boundary resistance is between 10^{-7} and 10^{-8} m² K W⁻¹ (Swartz and Pohl, 1989). The partial transmission of carriers through the boundaries, which is limited by the boundary resistance, is not considered in the present analysis. Partial transmission increases the free path of some carriers, and can reduce the dimension separating the microscale and macroscale regimes for conduction normal to a film. Chen and Tien (1992) showed that if the conduction in the bounding media is neglected and carrier transmission through the boundaries is diffuse, the effective phonon conductivity along a dielectric layer does not depend on the phonon transmission coefficients at the boundaries.

The hyperbolic heat conduction equation considers the finite propagation speed of energy and was proposed for use when the duration of a thermal disturbance is very small (Joseph and Preziosi, 1989, 1990), i.e., in a temporal microscale situation. For conduction in the absence of a heat source, the hyperbolic conduction equation is

$$\frac{\tau}{\alpha} \frac{\partial^2 T}{\partial t^2} + \frac{1}{\alpha} \frac{\partial T}{\partial t} = \nabla^2 T, \quad (2)$$

where α is the thermal diffusivity and τ is the relaxation time. The relaxation time is the average time a carrier travels between collisions and is given by $\tau = \Lambda/v$. Majumdar (1991) showed that Eq. (2) can be derived from the Boltzmann equation for dielectric films only if the film thickness is much larger than the phonon mean free path. Equation (2) reduces to the macroscale heat conduction equation if the second term on the left is much larger than the first term. Order-of-magnitude analysis yields the criterion $(\tau/\alpha)(\Delta T/\Delta t^2) \ll (1/\alpha)(\Delta T/\Delta t)$ for the macroscale regime, where Δt is the characteristic time scale of the heat transfer process and ΔT is the characteristic temperature difference. If for a thin layer of thickness d the characteristic time scale Δt is given by diffusion across the layer, then it satisfies $d \sim (\alpha \Delta t)^{1/2}$, and the macroscale criterion is $d^2 \gg \alpha \tau$. Using Eq. (1), the thermal diffusivity can be ex-

pressed as $\alpha = k/C \sim v\Lambda$. Since $\tau = \Lambda/v$, the final criterion for macroscale conduction is $d^2 \gg \Lambda^2$. If no time scales shorter than d^2/α are present, then the Fourier equation is valid for conduction across a thin film as long as carrier boundary scattering is not important. For shorter time scales, or if d is of the order of or smaller than Λ , the Fourier equation is not valid. Vedavarz et al. (1991) prepared a regime map for hyperbolic heat conduction, but their use of Eq. (2) in the regime of $d^2 \sim \Lambda^2$ requires further examination.

Moving Gases. The case of laminar gas convection from a surface with a large radius of curvature and $Re_L > 1$, where L is the streamwise dimension, is considered in the present analysis. For this case, the microscale regime is governed by the ratio of the molecular mean free path to the boundary layer thickness, Λ_m/δ . Tsien (1946) derived a regime map for this case, separating the macroscale regime from the slip-flow regime by the criterion $\Lambda_m/\delta = 0.01$. To obtain a more precise criterion in the present analysis, the result of Rohsenow and Choi (1961) is used for the average Nusselt number for slip-flow convection from a flat plate of length L in terms of the Mach number, M , the Reynolds number, Re_L , and the Prandtl number, Pr . In the macroscale limit, this solution approaches $Nu = 1.13 (Re_L Pr)^{1/2}$. For air convection with $Pr = 0.72$, this macroscale approximation exceeds the exact result by more than 5 percent for $Re_L^{1/2}/M < 55$. Tsien (1946) derived the relationship $L \sim (Re_L/M)\Lambda_m$, yielding the microscale criterion $L < 55 Re_L^{1/2} \Lambda_m$, which is used in the present analysis.

In a gas and a solid, heat transfer is modeled using carriers that move independently of one another between scattering events. Their interactions are characterized simply by the mean free path. In a liquid, transport phenomena cannot be explained by such ideal carriers. Cohesive forces between liquid molecules, such as van der Waals forces and those due to hydrogen bonds, are sufficiently strong to prevent random motion (Moore, 1972). Thus, a mechanistic length scale delineating the regime boundary for liquids may not be defined in the same way as for gases and solids, and further study is necessary for understanding microscale convection in liquids. Bankoff (1990) stated that the behavior of thin liquid films thinner than 100 nm is influenced by van der Waals forces. The flow of liquid in small channels has been studied by several groups. Experimental work provided conflicting results. Israelachvili (1986) measured the apparent viscosity of tetradecane, $CH_3(CH_2)_{12}CH_3$, and water flowing through a very thin gap. The apparent viscosities of the liquids did not depend on the gap size and were within 10 percent of their bulk values even for a gap thinner than 5 nm. This result is made plausible by classical theories for the viscosity and thermal conductivity of liquids (Bird et al., 1960), which are based on nearest-neighbor interactions between molecules, resulting in a mechanistic lengthscale of the order of the molecular size. Pfahler et al. (1991) measured the friction coefficients of silicon oil flowing in microchannels. In contrast to the observations of Israelachvili (1986), the apparent viscosities were smaller than the bulk viscosity and decreased with decreasing channel dimension. The study of liquid convection in microchannels is a fruitful field with technical impact.

2.2 Thermal Radiation. For thermal radiation, there are two mechanistic lengthscales, the photon mean free path and the wavelength within the medium of propagation. The two lengthscales are illustrated in Fig. 2 for a free-standing film. For normal incidence, the interference of light in a film is governed by the phase difference acquired upon traversing the film, $4\pi nd/\lambda$. The attenuation of the intensity of radiation in an absorbing medium is governed by the ratio of the film thickness to the photon mean free path, $\Lambda_p = \lambda/(4\pi\kappa)$.

The present discussion is limited to thin films. Microscale criteria for small particles and their agglomerates were reviewed by Tien (1988). The regime boundary was represented in terms of the particle size and the particle volume fraction. Chen and

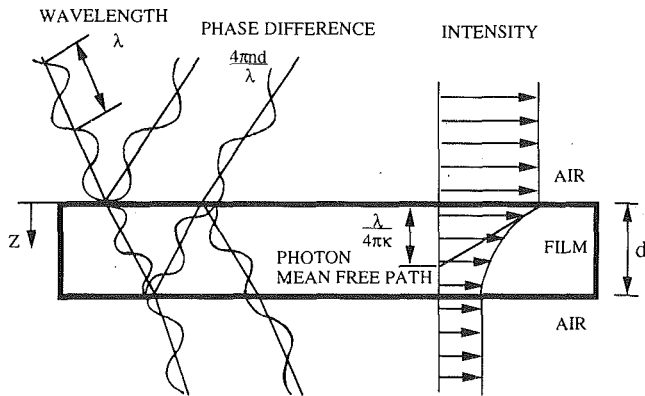


Fig. 2 Wave interference and attenuation in a thin layer

Tien (1991) discussed the regimes for thin-film optics and for geometric optics using the partial coherence theory. They obtained regime boundaries for a nearly monochromatic wave without considering dispersion. The finite bandwidth of the monochromatic wave produces incoherence and the regime boundary was expressed in terms of the product of the phase difference and the relative bandwidth of the wave. In the present study, the microscale regime boundary is determined considering radiation having the Planck energy distribution, and the frequency dependence of optical constants is considered. The regime maps for thin layers presented here are different from those of Chen and Tien (1991) because the current maps concern thermal radiation with a large bandwidth. Chen and Tien (1991) applied the partial coherence theory only to nearly monochromatic fields. However, the partial coherence formulation can be applied to thermal radiation with a large bandwidth if the film refractive index is independent of wavelength within the bandwidth.

Nonabsorbing Materials. If the film thickness is much larger than the wavelength, the reflectance can be predicted correctly by ray tracing. If the film thickness is less than or comparable to the wavelength in the film, the interference of waves has a measurable influence on the reflectance. The radiative transfer of nonabsorbing layers is defined to be microscale if the reflectance predicted by ray tracing differs by more than 5 percent from that predicted by accounting for interference. The light source is assumed to emit polychromatic thermal radiation. The microscale criterion is applied to the total normal reflectance for radiation having the spectral distribution of blackbody radiation.

The normal spectral reflectance of a single nonabsorbing layer considering interference, R_I , is given by thin-film optics (Yeh, 1988),

$$R_I = \frac{(n^2 - 1)^2 \left[1 - \cos\left(\frac{4\pi nd}{\lambda}\right) \right]}{n^4 + 6n^2 + 1 - (n^2 - 1)^2 \cos\left(\frac{4\pi nd}{\lambda}\right)}, \quad (3)$$

where n is the refractive index. The normal spectral reflectance without interference, R_N , is (Siegel and Howell, 1981)

$$R_N = \frac{(n - 1)^2}{n^2 + 1}. \quad (4)$$

The total normal reflectance for radiation having the spectral distribution of blackbody radiation at temperature T is

$$R_{A,tot} = \frac{\int_{\lambda_1}^{\lambda_2} R_A e_b(\lambda, T) d\lambda}{\sigma T^4}, \quad A = I \text{ or } N \quad (5)$$

where e_b is the blackbody emissive power. The numerical in-

tegration covers the spectral range from $\lambda_1 = 1666.7/T$ to $\lambda_2 = 16666.7/T$, which includes 95 percent of the total blackbody energy. As the film thickness is increased, the spacing of interference fringes decreases and the difference between $R_{N,tot}$ and $R_{I,tot}$ becomes smaller. The boundary between the microscale and the macroscale regimes is the film thickness for which the relative difference between $R_{N,tot}$ and $R_{I,tot}$ is equal to 5 percent. Equation (4) shows that in the macroscale regime, the reflectance does not depend on the film thickness. For a given nonabsorbing material, the regime boundary thickness is expressed in terms of the temperature of the emitting blackbody.

Absorbing Materials. Absorbing thin-film materials are technically important for application in radiation detectors. The radiative properties depend on the film thickness if it is smaller than the photon mean free path, Λ_p . The intensity of radiation at a depth z normal to the film surface is (Siegel and Howell, 1981)

$$i'_\lambda(z) = i'_\lambda(0) \exp\left(\frac{-z}{\Lambda_p}\right) = i'_\lambda(0) \exp\left(\frac{-4\pi\kappa z}{\lambda}\right) \quad (6)$$

where i'_λ is the directional spectral intensity and κ is the extinction coefficient. If the film thickness is greater than the photon mean free path, the absorption strongly reduces the intensity of the wave reflected at the second interface. If the film thickness is much greater than the photon mean free path, $d \gg \Lambda_p$, radiative properties can be obtained considering only the air-film interface and do not depend the film thickness, i.e., the film acts as a semi-infinite medium.

The boundary between the microscale and macroscale regimes is defined based on the total normal reflectance. The normal spectral reflectance, R_I , considering interference is given by Yeh (1988),

$$R_I = \left| \frac{1 - \exp\left(i \frac{4\pi \bar{n} d}{\lambda}\right)}{\frac{1 + \bar{n}}{1 - \bar{n}} - \frac{1 - \bar{n}}{1 + \bar{n}} \exp\left(i \frac{4\pi \bar{n} d}{\lambda}\right)} \right|^2, \quad (7)$$

where $\bar{n}$ is the complex refractive index of the film material. The normal spectral reflectance of a semi-infinite medium, R_N , is

$$R_N = \frac{(n - 1)^2 + \kappa^2}{(n + 1)^2 + \kappa^2}. \quad (8)$$

The total normal reflectances, $R_{N,tot}$ and $R_{I,tot}$, are calculated from Eq. (5). The boundary between the microscale and the macroscale regimes is the film thickness for which the relative difference between $R_{N,tot}$ and $R_{I,tot}$ is equal to 5 percent.

3 Material Properties

3.1 Thermal Conduction. Metals. The theory of thermal conduction in metals was summarized by Wilson (1953) and Ziman (1960). The electron mean free path may be obtained from experimental values of the thermal conductivity using Eq. (1), the electron specific heat, C_e , and the Fermi velocity, v_e . The thermal conductivity of metals was given by Touloukian et al. (1970). The Fermi velocities of electrons in metals are of the order of 10^6 m s⁻¹ and were tabulated by Kittel (1986). The volumetric specific heat of electrons, C_e , is proportional to temperature,

$$C_e = \gamma T, \quad (9)$$

The Sommerfeld parameter, γ , was tabulated for metals by Kittel (1986) and is of the order of 100 J m⁻³ K⁻².

The mean free path of electrons in metals is limited by scattering on imperfections and phonons. Imperfections include impurity atoms and lattice defects. Matthiessen's rule

breaks the inverse electron mean free path, $1/\Lambda_e$, into components due to imperfection scattering, $1/\Lambda_{e,i}$, and phonon scattering, $1/\Lambda_{e,s}$,

$$\frac{1}{\Lambda_e} = \frac{1}{\Lambda_{e,i}} + \frac{1}{\Lambda_{e,s}} \quad (10)$$

The imperfection-limited mean free path $\Lambda_{e,i}$ is independent of temperature, while the phonon-limited mean free path $\Lambda_{e,s}$ decreases with increasing temperature. At very low temperatures, $T \ll \theta$, where θ is the Debye temperature, the absence of phonon scattering allows $\Lambda_{e,i}$ to be determined.

The scattering of electrons on phonons dominates over the scattering of electrons on imperfections above a temperature near 50 K. When phonon scattering dominates, $\Lambda_{e,s}$ can be determined from thermal conductivity data using Eq. (1). The value of $\Lambda_{e,s}$ may be extrapolated to lower temperatures using the formula of Wilson (1953) for electron thermal conduction limited by scattering on phonons. At temperatures below a low reference temperature, $T < T_r < \theta/10$, this formula may be simplified with less than 10 percent error in metals to $k_{e,s}(T)/k_{e,s}(T_r) = (T_r/T)^2$. This result and Eqs. (1) and (9) yield the mean free path for $T < T_r$,

$$\frac{\Lambda_{e,s}(T)}{\Lambda_{e,s}(T_r)} = \left(\frac{T_r}{T}\right)^3, \quad T_r < \theta/10. \quad (11)$$

Dielectrics and Semiconductors. Phonon conduction in dielectrics and semiconductors was reviewed by Ziman (1960). The phonon mean free path in dielectrics is calculated from experimental conductivity data using Eq. (1), the phonon specific heat, C_s , and the average speed of sound in the material, v_s . The specific heats of dielectrics and semiconductors were given by Touloukian and Buyco (1970a, 1970b).

Phonon conduction in dielectrics is limited by scattering on other phonons and on imperfections, which include lattice defects and isotopes. In doped semiconductors, the free carriers also scatter phonons. Matthiessen's rule yields (Ziman, 1960)

$$\frac{1}{\Lambda_s} = \frac{1}{\Lambda_{s,i}} + \frac{1}{\Lambda_{s,s}} + \frac{1}{\Lambda_{s,e}}, \quad (12)$$

where Λ_s is the phonon mean free path, $\Lambda_{s,i}$ is the phonon mean free path limited by scattering on imperfections, $\Lambda_{s,s}$ is the phonon mean free path limited by scattering on phonons, and $\Lambda_{s,e}$ is the phonon mean free path limited by scattering on free carriers in semiconductors. The third term on the right of Eq. (12) is zero for dielectrics.

Below a reference temperature, $T < T_r \ll \theta$, the phonon mean free path limited by scattering on phonons is approximately

$$\frac{\Lambda_{s,s}(T)}{\Lambda_{s,s}(T_r)} = \exp\left[\frac{\theta}{2}\left(\frac{1}{T} - \frac{1}{T_r}\right)\right]. \quad (13)$$

At low temperatures, the phonon mean free path in undoped crystals is limited by scattering on isotopes and point imperfections. When this mechanism is dominant and $T < T_r \ll \theta$, the phonon mean free path is well approximated by (Berman et al., 1956)

$$\frac{\Lambda_s(T)}{\Lambda_s(T_r)} = \left(\frac{T_r}{T}\right)^4. \quad (14)$$

Gases. Rohsenow and Choi (1961) derived an approximate expression for the mean free path of a gas molecule,

$$\Lambda_m = \frac{1}{n_m \pi D^2}, \quad (15)$$

where n_m is the number density of molecules. The molecular diameter D was tabulated for technically important gases by Hirschfelder et al. (1954). Values of D include 0.2789 nm for neon, 0.3617 nm for air, and 0.4055 nm for xenon. The values of D for xenon and neon bound those for the most important gases.

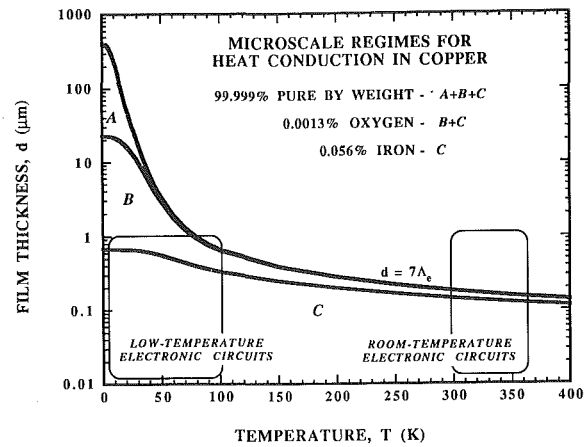


Fig. 3 Regime map for thermal conduction normal to copper films

If the gas is ideal, the molecular number density is related to the pressure, p , and temperature, T , by $p = n_m k_B T$, where $k_B = 1.38 \times 10^{-23} \text{ J K}^{-1}$ is the Boltzmann constant. Using Eq. (15), the mean free path is

$$\Lambda_m = \frac{k_B T}{\pi D^2 p}. \quad (16)$$

3.2 Thermal Radiation. The optical behavior of materials is governed by the complex refractive index, $n + ik$. In doped semiconductors, the imaginary part increases with the carrier number density. The optical properties of doped semiconductors are described by the Drude model (Senitzky and Weeks, 1981). The dielectric function is

$$\epsilon = \epsilon_\infty + \frac{i\omega_p^2}{\omega(1/\tau - i\omega)}, \quad (17)$$

where ω is the frequency, ω_p is the plasma frequency, and ϵ_∞ is the high-frequency dielectric constant. The plasma frequency is $\omega_p = (n_e e^2 / m_e^* \epsilon_0)^{1/2}$, where m_e^* is the electron effective mass and ϵ_0 is the vacuum electrical permittivity.

The optical properties of the high-temperature superconductor $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ vary dramatically with varying oxygen content ($6.0 < 7-\delta \leq 7.0$) (Kamaras et al., 1989; Bozovic, 1990). The optical properties of $\text{YBa}_2\text{Cu}_3\text{O}_6$ are important for the thermal analysis of the film deposition process (Flik et al., 1992). Choi et al. (1991) obtained the optical constants of $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ films with varying oxygen content by fitting the measured reflectance to the Drude-Lorentz model. An $\text{YBa}_2\text{Cu}_3\text{O}_7$ film has a highly metallic behavior. As the oxygen content of the film decreases, the film becomes more transparent.

The optical constants are assumed to be independent of the film thickness. When the electron mean free path or the radius of an electron-hole pair is comparable to the film thickness, then the optical constants depend on the film thickness. The present study does not account for the influence of the film thickness on n and κ .

4 Regime Maps

4.1 Thermal Conduction. Figure 3 shows the regimes for thermal conduction in annealed, polycrystalline copper. The mean free path is given by Eq. (10). Above 30 K, $\Lambda_{e,s}$ is obtained using Eqs. (1) and (9) and values of the thermal conductivity recommended by Touloukian et al. (1970). Below 30 K, $\Lambda_{e,s}$ is obtained using Eq. (11) with $T_r = 30 \text{ K}$. Based on Eqs. (1) and (9) and low-temperature thermal conductivity data from the following sources, the imperfection-limited mean free path for copper at least 99.999 percent pure by weight is $\Lambda_{e,i} = 57 \mu\text{m}$

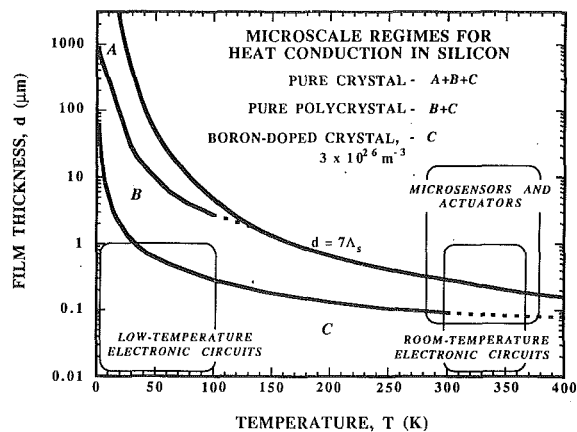


Fig. 4 Regime map for thermal conduction normal to silicon films

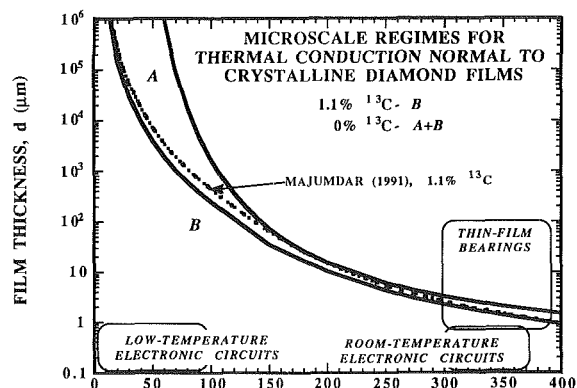


Fig. 5 Regime map for thermal conduction normal to diamond films

(White and Tainsh, 1960), for copper containing 0.0013 percent oxygen it is $\Lambda_{e,i} = 3.2 \mu\text{m}$ (Powell et al., 1957), and for copper containing 0.056 percent iron it is $\Lambda_{e,i} = 0.096 \mu\text{m}$ (White and Woods, 1954). Below 30 K, the film thickness denoting the microscale regime boundary varies by three orders of magnitude depending on the purity. In cryogenic electronics applications, the effective thermal conductivity of almost all copper films is size dependent, while at room temperature films of thickness greater than about $0.1 \mu\text{m}$ belong to the macroscale regime.

Figure 4 is a regime map for thermal conduction normal to silicon layers. The average speed of sound is $v_s = 6500 \text{ m s}^{-1}$ (McSkimin, 1953) and the values of the pure crystalline thermal conductivity are those recommended by Touloukian et al. (1970). The mean free path is extrapolated to low temperatures for an infinite crystal using Eq. (14) with $T_r = 25 \text{ K}$. The data of Rosenberg (1954) are employed for the thermal conductivity of polycrystalline silicon below 100 K. The dashed curve section in the left of Fig. 4 indicates that the mean free paths for the crystal and polycrystal must approach one another with increasing temperature and is not supported by experimental data. Slack (1964) gave the thermal conductivity of a boron-doped silicon crystal from which the dashed curve section on the right of Fig. 4 is extrapolated. The dimension bounding the microscale regime is highly dependent on the carrier concentration, and at low temperatures it is reduced by grain boundary scattering in a polycrystalline specimen compared to a crystal. Silicon microstructures used in the majority of room-temperature sensors and actuators do not exhibit a size-dependent thermal conductivity, in contrast to films in low-temperature electronic circuits. The doping level determines whether a silicon film is in the microscale conduction regime at room temperature.

Regimes for conduction normal to type IIa diamond films

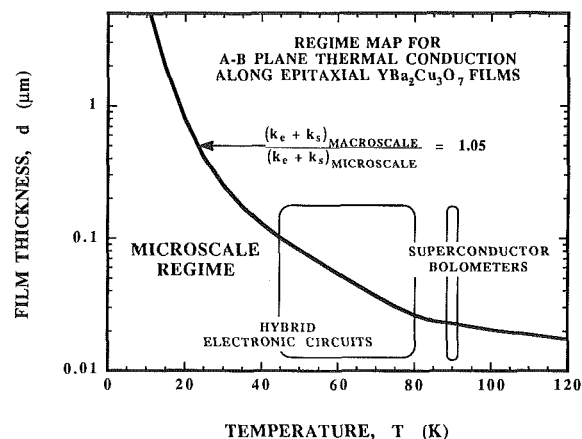


Fig. 6 Regime map for thermal conduction along epitaxial films of the high- T_c superconductor $\text{YBa}_2\text{Cu}_3\text{O}_7$

are shown in Fig. 5. The thermal conductivity was given by Berman et al. (1956) and the average speed of sound, $v_s = 13,500 \text{ m s}^{-1}$, by McSkimm and Andreatch (1972). Equation (14) determines the imperfection-limited mean free path at temperatures where boundary scattering was important. The reference temperature is $T_r = 100 \text{ K}$, which satisfies $T_r \ll \theta$ because the Debye temperature of diamond is $\theta = 1880 \text{ K}$. Although the primary constituent of diamond is the ^{12}C atom, naturally occurring diamond contains 1.1 percent of the isotope ^{13}C . At low temperatures, scattering on this isotope limits the thermal conductivity of natural diamond. Majumdar (1991) presented an algorithm to determine the regime boundary for diamond as a function of the fraction of ^{13}C . In Fig. 5, the regime boundary for diamond with a ^{13}C content of 1.1 percent calculated using his algorithm is shown to be in agreement with the regime boundary of the present analysis.

Anthony et al. (1990) achieved a ^{13}C content of 0.07 percent in a synthetic diamond crystal and showed that its thermal conductivity at room temperature was 50 percent greater than that measured previously for diamond. Based on this result, the mean free path of a hypothetical crystal containing no isotopes or lattice defects is estimated using Eq. (13) with $T_r = 300 \text{ K}$. The microscale regime for this case is shown in Fig. 5 and indicates the largest value of d for a given temperature at which microscale conduction may ever occur in diamond. The regime map shows that it is not possible to achieve in thin diamond films in electronic circuits the same high thermal conductivities measured in bulk crystals. Because of the low coefficient of friction between diamond surfaces, diamond films possess great potential for application as bearing materials (Guyer and Koshland, 1990). Figure 5 shows that for room-temperature applications, the thermal conductivity of bearing films thinner than $3 \mu\text{m}$ is size dependent. This fact can strongly affect the temperature fields existing in such bearings due to dissipation.

Figure 6 concerns thermal conduction along epitaxial films of the high-temperature superconductor $\text{YBa}_2\text{Cu}_3\text{O}_7$. The orthorhombic, nearly tetragonal crystal structure of this material results in similar thermal conductivities in the a and b crystal axis directions, but a different thermal conductivity in the c direction. The films with the best superconducting properties are deposited epitaxially with the c axis normal to the film surface, such that conduction along the films occurs in the a - b plane. Goodson and Flik (1991) determined the contribution of each carrier to energy transport and its mean free path as functions of temperature. The thinnest high- T_c superconductor films will exhibit microscale conduction in detectors and electronic circuits. Flik and Hijikata (1990) demonstrated that thermal conduction in hybrid superconducting-semiconducting electronic circuits results in a packing limit.

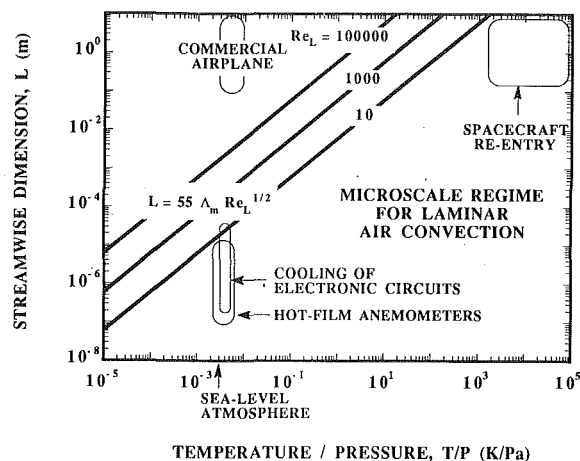


Fig. 7 Approximate regime map for air convection

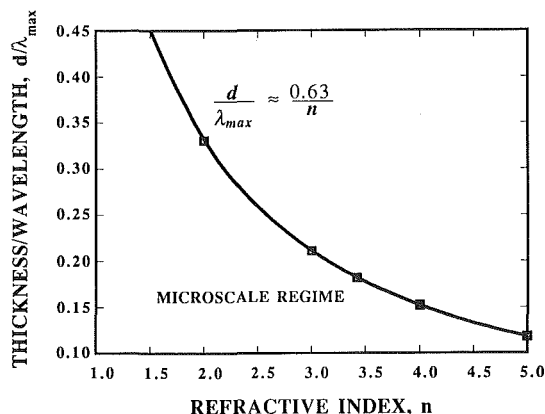


Fig. 8 General regime map for reflection from nonabsorbing films

Air convection regimes are shown in Fig. 7. The regime maps for other gases can be constructed from the air regime map by substituting the mean free path of the particular gas, which depends on the molecular diameter. Convective heat transfer from individual electronic devices and from hot-film mass-flow sensors does not follow the continuum theory. Commercial airplanes fall well within the continuum regime, in contrast to convection from spacecraft re-entering the atmosphere of the earth.

4.2 Thermal Radiation. Figure 8 displays the microscale regime for reflection from nonabsorbing materials. The film thickness is normalized by the wavelength where blackbody radiation has the maximum spectral energy for a given temperature, $\lambda_{\max}$, which is given by Wien's displacement law, $\lambda_{\max} T = 2897.8 \mu\text{m K}$. The refractive index is assumed to be constant over the total spectral range. For materials used for windows and filters, generally the refractive index does not change strongly within the transparent spectral range. Pure silicon has a refractive index close to 3.42 for the whole infrared range (Edwards, 1985). ZnS has $2.1 \leq n \leq 2.4$ for $0.5 \mu\text{m} \leq \lambda \leq 14 \mu\text{m}$ and ZnSe has $2.3 \leq n \leq 2.7$ for $0.55 \mu\text{m} \leq \lambda \leq 18 \mu\text{m}$ (Li, 1984). For all materials whose refractive indices vary little with wavelength, the generalized regime map of Fig. 8 can be used.

The boundary between the microscale and macroscale regimes can be approximated as $d/\lambda_{\max} \approx 0.63/n$. Since the mechanistic lengthscale associated with the wave interference is $\lambda/4\pi n$, the film thickness denoting the regime boundary decreases as the refractive index increases. As the refractive index approaches unity, the reflectance of the film approaches zero. In this limit, even a small difference between $R_{N,\text{tot}}$ and $R_{I,\text{tot}}$ produces a large relative error and the film thickness that

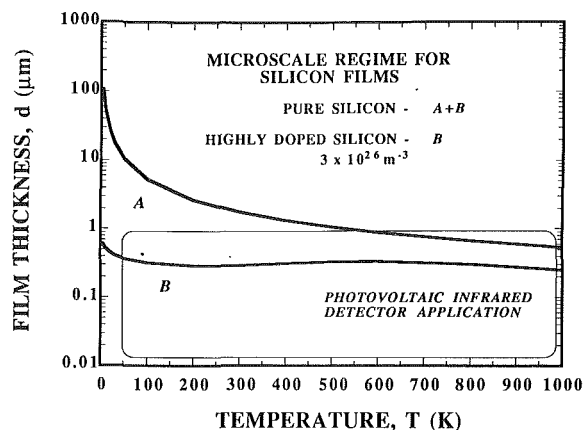


Fig. 9 Regime map for reflection from silicon films

separates the regimes increases dramatically. In contrast, for large n the reflectance is close to unity, and the film must be very thin to exhibit a size-dependent reflectance. If the partial coherence theory presented by Chen and Tien (1991) is used, the regime boundary between partial coherence and incoherence is $d/\lambda_{\max} = 0.40/n$. The regime boundary is based on the mutual coherence function and the relative error between $R_{N,\text{tot}}$ and $R_{I,\text{tot}}$ is between 10 and 20 percent. This error is larger than 5 percent, which is used to determine the regime boundary of the present study. The present regime boundary is more stringent.

In pure silicon, the imaginary part of the complex refractive index is extremely small in the whole infrared range (Edwards, 1985). For highly doped silicon, the optical constants are calculated from Eq. (17). The high-frequency dielectric constant and effective mass were given as $\epsilon_{\infty} = 11.7$ and $m_e^* = 0.26 m_e$ by Spitzer and Fan (1957). The plasma frequency and relaxation time are (Senitzky and Weeks, 1981),

$$(\omega_p/\omega) = (5.87 \times 10^{-14} \mu\text{m}^{-1} \text{m}^3)^{1/2} \lambda (n_e)^{1/2}, \quad (18)$$

$$(1/\tau\omega) = [5.74 \times 10^{-23} \mu\text{m}^{-1} \text{m}^3 (\Omega\text{m})^{-1}] \lambda n_e \rho, \quad (19)$$

where λ is the wavelength in a vacuum and ρ is the d-c electrical resistivity. The dependence of the d-c resistivity of doped silicon on the carrier density was given by Irvin (1962). The refractive index is obtained from the relation $n + ik = \epsilon^{1/2}$.

The regime map for pure and highly doped silicon films is shown in Fig. 9. The region below each curve is the microscale regime. The temperature denotes that of the blackbody emitting the radiation, which is reflected by the room-temperature film. When the film temperature differs from room temperature, a new regime map must be constructed using the optical properties at that temperature. The regime boundary for pure silicon is derived from the results of Fig. 8 using $n = 3.42$. Since the highly doped silicon film has a high density of free carriers, it shows metallic optical behavior. For highly doped silicon films, the boundary of the microscale regime is determined by the attenuation criterion. The photon mean free path of doped silicon is found to be nearly wavelength independent for wavelengths up to $30 \mu\text{m}$ because the extinction coefficient increases proportional to the wavelength. The regime boundary of the doped silicon film is independent of temperature above 100 K. In photovoltaic infrared detector applications, doped silicon films with thicknesses less than $0.3 \mu\text{m}$ are in the microscale regime.

Figure 10 shows the regime map for $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ films with three different oxygen contents. The oxygen content has a similar influence on the reflectance as the doping level of a semiconductor. The films with oxygen contents of 7.0 and 6.6 are highly absorbing and the boundary between the microscale and macroscale regimes is determined by the attenuation cri-

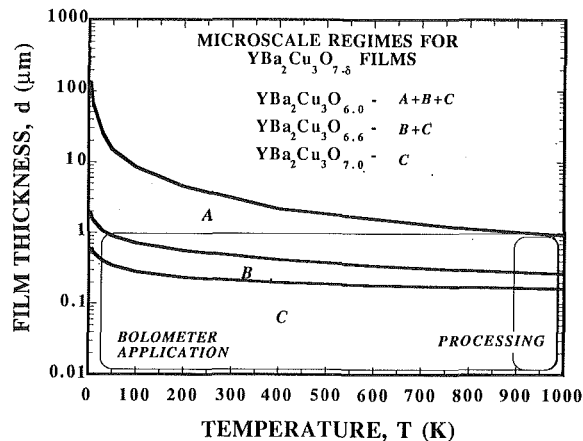


Fig. 10 Regime map for reflection from superconducting $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$ films

terion. The $\text{YBa}_2\text{Cu}_3\text{O}_6$ film has the optical properties of a dielectric material and the boundary of the microscale regime is determined by the interference criterion. It is shown in Fig. 10 that in bolometer applications of $\text{YBa}_2\text{Cu}_3\text{O}_7$ and during the film deposition process ($\text{YBa}_2\text{Cu}_3\text{O}_6$), thin films of this superconductor exhibit strong microscale behavior. The emittance change with the growth of the film is a major process control problem (Flik et al., 1992).

5 Concluding Remarks

The criteria developed for microscale conduction, convection, and radiation are summarized in Table 1.

5.1 Thermal Conduction. For thermal conduction in solids, the dimension that separates the microscale and macroscale regimes is related to the carrier mean free path and depends strongly on the purity and microstructure of the solid. The present regime maps do not consider the effect of the transmission of carriers through interfaces, which was accounted for by Chen and Tien (1992) in an analysis of the thermal conductivity of multiple quantum wells.

For gas convection, the streamwise length denoting the microscale regime boundary is linearly related to $\text{Re}^{1/2}T/p$. No simple regime maps may be constructed for liquid convection, due to the complexity of the intermolecular and surface forces. Investigations of the microscale regime boundary for liquid convection are particularly warranted in view of the results of Pfahler et al. (1991).

5.2 Thermal Radiation. Regime maps for thermal radiation must consider the entire spectral region of the Planck energy distribution and account for the spectral variation of optical constants. The microscale regime boundary is determined by two mechanistic length scales: the wavelength in the medium for nonabsorbing materials and, in addition, the photon mean free path for absorbing materials. For nonabsorbing materials, the regime boundary is $d = 0.63 \lambda_{\max}/n$ if n is independent of wavelength.

The optical constants n and κ of the microstructures are assumed to be the same as those of the bulk materials. They may change, however, if the size of the microstructures approaches the electron mean free path or the exciton radius. Further study is required to determine size effects on optical constants.

5.3 Property Measurements. The present state of research in microscale heat transfer displays an imbalance between theoretical and experimental achievements. In the area of thermal conduction in solids, several excellent computational studies were presented recently (Majumdar, 1991; Ku-

Table 1. Summary of microscale regime criteria

	MICROSCALE CRITERION	REFER TO THESE EQUATIONS
Thermal Conduction: Metal Films	$d < 7\Lambda_e$	(1), (9), (10), (11)
Thermal Conduction: Semiconducting and Dielectric Films	$d < 7\Lambda_s$	(1), (12), (13), (14)
Thermal Convection: Air	$L < 55 \text{ Re}_L^{1/2} \Lambda_m$	(1), (15), (16)
Thermal Radiation: Reflection From Non-absorbing Films	$d < 0.63 \lambda_{\max}/n$	(3), (4), (5)
Thermal Radiation: Reflection From Absorbing Films	No explicit form	(6), (7), (8), (17), (18), (19)

mar and Vradis, 1991). But it was not possible to verify these predictions experimentally. More experiments on microscale heat conduction must be performed. In the area of microscale radiation, experiments are needed on the size dependence of the optical constants of microstructures, such as multiple quantum wells, quantum wires, and quantum dots.

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