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Prediction and measurement of thermal transport across interfaces between semiconductor and adjacent layers

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ABSTRACT

The thermal boundary conductance between multilayer structures including Al film, semiconductors with high Debye temperatures (GaN, AlN, Si, diamond) and dielectric substrates (sapphire) has been measured using a two-color femtosecond laser pump-probe system (a variation of transient time-domain thermoreflectance, TDTR). The thermal boundary conductance for the combinations of semiconductors and dielectrics falls within a relatively narrow range, 10–20 MW m^{-2} K^{-1}, at room temperature. The measured thermal boundary conductance between Al film and semiconductor or dielectric substrates is one order of magnitude larger than that between semiconductor and dielectric substrates. A modified diffuse mismatch model (DMM) is used to interpret the data and extract the phonon transmissivity at the interface. The predicted results of the DMM corrected by attenuation constant agree well with the experimental values. Over a wide phonon velocity, both the measured and predicted results decrease with the increasing average phonon velocity. Both the vibration mismatch and changes in the localized phonon transport near the interface contribute to the reduction in thermal boundary conductance. Other scattering mechanisms are discussed which may explain the failure of the DMM at room temperature.

1. Introduction

Semiconductor interfaces are pervasive in advanced technological devices. For example, the active region in a quantum cascade laser, a light-emitting diode or micro-electromechanical system (MEMS) contains films of large band gap semiconductors such as GaN, AlN and diamond in semiconductor multilayer structures [1–3]. Because thermal transport in large band gap semiconductors is dominated by phonons (i.e., quantized lattice vibrations) with bulk mean free paths that exceed the characteristic scale of microstructures (roughness, dislocation) at interfaces, the phonon transport is significantly impeded due to scattering at the high density of material interfaces [4]. This impediment, which is quantified by the thermal boundary resistance, can lead to thermal management challenges due to its adverse effect on device performance and reliability. In some applications, however, the impediment of the thermal transport resulting from phonon scattering at semiconductor interfaces is desirable. This effect is used, for example, to improve the effectiveness of thermoelectric materials, and thus, increase the efficiency of thermoelectric energy conversion devices. The structures encountered in many applications, however, often contain more than one or two interfaces. In these cases it is important to be able to estimate and measure the local thermal boundary resistance.

Since the primary heat carriers in insulating materials are phonons, the metal-semiconductor and semiconductor-dielectric interfacial properties are related to the phonon transmission probability and the effects of scattering at the interface. The classical approach has been suggested to neglect scattering at the interface and use continuum acoustical theory to calculate the transmission probability. Recently, Hopkins et al. [5] developed an analytical model for phonon transport at rough interfaces based on a diffusive scattering assumption and phonon attenuation. The functional dependence of thermal boundary conductance (TBC) with rms surface roughness reveals a trend that suggests that both vibration mismatch and changes in the localized phonon transport near the interface contribute to the reduction in TBC.

Experimental investigation on TBC still remains a challenging work and only several methods have been used to characterize it.

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Nomenclature

d	thickness of the media m
D	phonon density of states per unit volume s m^{-3}
f	phonon distribution function
h	thermal boundary conductance W/m^2 K
k	thermal conductivity W/mK
l	length or depth m
q	heat flux W/m^2
Q	heat flux power of pump beam W/m^2
R	thermal resistance m^2 K/W
R_0	radius of pump beam m
R_1	radius of probe beam m
T	temperature K
Z	lock-in transfer function

Greek letters

α	thermal diffusivity m^2/s
θ	temperature oscillation K
θ_D	Debye temperature K
v	phonon group velocity m/s
β	attenuation constant
ζ	phonon transmission coefficient
ω	angular frequency or phonon frequency s^{-1}
τ	time s

Subscript

BD	boundary
e	value for emitted phonons
L	longitudinal
pd	penetration depth
T	transverse

One technique is the steady-state resistance-based techniques (two microbridges and 3ω method) which are based on the fact that the electrical resistivity of a sample or test strip is related to the temperature change; therefore, by monitoring the change in electrical resistivity of a reference, the change in temperature can be determined. Swartz and Pohl [6,7] utilize two thin-film microbridges deposited close to one another on a dielectric substrate. One microbridge is used as both a heat source and thermal sensor on the metal side and the other microbridge is a thermal sensor for the dielectric side. This technique requires that the mean-free path of the phonon is larger than the spacing between the microbridges, and is therefore only applicable at low temperatures. The 3ω method uses an ac hot-wire setup to measure apparent thermal conductivity of a film and interface system. The TBC is extracted from data taken on a series of films while varying thickness [8,9] or using reference sample [10]. The disadvantages, however, in addition to the potential uncertainty in sample geometries, are that these techniques require intimate contact between the electrical leads and the sample platform of interest. Inherent in these contacts are both electrical and thermal contact resistances that must be accounted for [11]. In addition to these measurement difficulties, direct measurement of the TBC between two materials of interest is very difficult without the use of multiple samples. For example, if one were to use a steady-state or frequency domain (such as 3ω) electrical resistivity technique to measure the thermal properties of a two-layer sample, the measured data would represent the total thermal resistance of the sample. Although the individual film properties could be inferred from multilayer thermal modeling [12], a heat capacity-less thin interface could not be differentiated from the individual layers.

A second technique, called modulated thermoreflectance microscopy, examines the propagation of thermal waves generated by a laser pulse [13,14]. The wave propagation is determined by measuring the reflectance of a probe beam that is rastered around the heating location. The phase of the probe is measured and compared to a thermal model where the thermal boundary resistance is treated as a free parameter [15,16].

A third technique is the Micro-Raman Thermometry where the temperature rises across the interface are measured by Raman spectroscopy. By contrast, direct access to the full temperature distribution in three dimensions can be provided by Raman spectroscopy, giving the possibility of a much more direct experimental determination of the thermal boundary resistance (TBR) and thermal resistances of each layer. This technique has proved to be a very effective tool to obtain the temperature rises during operation in semiconductor devices with high spatial resolution [17–19]. A disadvantage is that the influence of TBR on temperature increase is much smaller for devices on low thermal conductivity substrate (sapphire).

A forth technique is the transient time-domain thermoreflectance (TDTR) technique where a short-pulsed laser beam is used to heat a thin metal film. The thin metal film is then probed with a weaker laser pulse after a known time delay in order to measure the transient temperature change of the metal film. This technique was used by Smith et al. [20], Stoner and Maris [21], Stevens et al. [22], Hopkins et al. [23] and Cahill et al. [24] to measure the TBR of metal films and dielectric substrates. One distinct advantage of this technique is the ability to directly measure the thin film TBC of films with thicknesses on the order of the optical penetration depth. Time domain techniques for measuring the thermal transport of materials have proven invaluable for monitoring the thermal conductivity and TBC of multilayer structures due to the fact that the thermal effusivity or thermal diffusivity of a material responds differently than the thermal transport across an interfacial region in the time domain.

Up to now, most of the TBC measurements by single-color TDTR systems have been made on samples with only one interface [20–25]. Stoner and Maris [21] reported some of the first measurements of TBR on a range of acoustically mismatched solid–solid metal/dielectric interfaces. Their results showed that the diffuse mismatch model (DMM) underpredicted the measured TBR by over an order of magnitude for interfaces that were heavily mismatched. Norris and Hopkins [25] reported the compared results between the measured TBC by TDTR and predicted ones by DMM. The assumption that phonons can only transmit energy across the interface by elastic scattering can lead to underpredictions by almost an order of magnitude. For the metal/dielectric interfaces, the general trend shows that the DMM underpredicts measurements on acoustically mismatched samples and overpredicts measurements on acoustically matched samples. Conventional single-color laser pump–probe methods for measuring thermal properties are limited by perfect isolation of the pump beam from the detector, large deformation of the laser profile, sample requirements that arise from considerations of surface roughness and compatible thermoreflectance transducers. Nearly all the above TDTR measurements apply a one dimensional thermal model neglecting the radial heat conduction and are limited to films with nanoscale thickness.