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A COMPACT ENHANCED FOURIER LAW FOR NEXT-GENERATION DEVICE THERMAL MODELLING

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ABSTRACT In light of the findings of Johnson *et al.* that ballistic phonons with mean-free paths upto 500 microns carry a significant fraction of the total heat-flux in silicon at room temperature, it has become imperative to include ballistic transport effects in electronic and optoelectronic device thermal simulations even in the microscale. It would be impractical, in the short run at least, to shift to a fully numerical solution of the Boltzmann transport equation (BTE) for phonon transport. Coupling such a numerical solver with electron distributions and optical fields will be very time consuming, over and above the demanding computational requirements of the BTE solution itself. We present here an alternative, the "enhanced Fourier law", which retains the mathematical brevity and simplicity of the Fourier law while including important ballistic transport effects. Rigorous derivation starting from the BTE lends clear physical meanings to various parameters in our equations, as opposed to so-called "phenomenological" models containing large numbers of essentially numerical fitting parameters. Two illustrative applications are considered: (a) deviations from the Fourier law reported by Johnson *et al.* using the transient gratings experiment, and (b) a serious difficulty in extracting the mean-free path accumulation function from frequency-domain thermoreflectance experiments - a difficulty that has not been pointed out until now. The enhanced Fourier law is expected to be of great promise to industrial device simulation because of the detailed information it yields about the heat-flux resolved according to the mean-free path, or in other words, according to the length scale of scattering.

NOMENCLATURE

q = the net heat-flux.

q^{LF} = the LF-mode contribution to the heat-flux

q^{HF} = the HF-mode contribution to the heat-flux

$S^{HF}(x,t)$= external heat source term

T = local temperature of HF modes

v = group-velocity magnitude.

$\boldsymbol{v}$ = group velocity

$\boldsymbol{k}$ = LF-mode wave-vector

GREEK SYMBOLS

κ = the net bulk thermal conductivity

κ^{HF} = the contribution of HF modes to the bulk thermal conductivity

κ^{LF} = the contribution of LF modes to the bulk thermal conductivity

Λ^{LF} = the MFP of the LF modes

τ = LF mode lifetime

$\omega(k)$ = frequency of LF mode of wave-vector $\boldsymbol{k}$

While the phenomenological Fourier law adequately explains heat transfer in the macroscale (generally > 10 micron at 300 K), its applicability is seriously limited at short length-scales, due to its incomplete treatment of heat transport by low-frequency (LF) phonons with mean-free paths (MFPs) of the same order as the length scale of interest [1][2][3]. Self-heating is becoming an increasing concern in high-frequency and high-power electronic devices [4], and in optoelectronic devices [5][6]. In these devices, the length-scales are short enough that low-frequency components of the heat-flux deviate seriously from the Fourier law, yet too long for it to be computationally practical to entirely abandon the Fourier law. Despite the fact that the Fourier law is known to dramatically overestimate the heat flux [7] due to ballistic transport, it continues to be used in device thermal analysis, occasionally even in cases where it is patently inappropriate to use (e.g. filaments a few nanometers in diameter [8][9]). It is therefore highly timely to develop a model that goes beyond the Fourier law, for the thermal analysis of highly scaled electronic and optoelectronic devices, and for enabling interpretation of transient grating [10], transient thermoreflectance [11] and other experiments. For such a model to permit of the aforementioned applications, it must (a) maintain as far as possible the mathematical simplicity afforded us by the usual heat equation based on the Fourier law, and (b) identify the important correction terms engendered by the highly non-equilibrium LF modes. We have previously derived such an enhanced Fourier law from the Boltzmann transport equation (BTE) [20].

A recent experiment by Johnson *et al.* [10] has revealed important information about the breakdown of the Fourier law in silicon at length scales much longer than expected on the basis of simple kinetic theory arguments [12]. Details of the transient gratings experiment can be found in Ref. [10]. Johnson *et al.* found that the grating decay rate starts deviating from the linear as a function of inverse square grating period – a clear indication of the breakdown of Fourier law - at a grating period (of the order of 1 micron) that is much larger than that expected from kinetic theory considerations (on the order of tens of nm).

Maznev *et al.* [13] explained this phenomenon starting from a "two-fluid" model described later. However, their analysis was restricted to spatially sinusoidal dependences of variables, as was appropriate for the experiment under their study. Collins *et al.* [14] confirmed the decay rates of Maznev *et al.* by exactly solving the full spectral Boltzmann transport equation; however their solution was largely numerical. Another approach [15] that is used for analyzing transient thermoreflectance experiments assumes that the LF modes are characterized by a local temperature just like the high-frequency (HF) modes, which is questionable since LF modes are frequently far out of thermal equilibrium.

Working within the two-fluid model, we have developed [20] new equations resembling the Fourier law for describing heat transport. To this end, we derived general expressions for the heat-flux and temperature by means of spherical harmonic expansions (SHEs) of the distribution functions for the HF and LF components. For bulk electron transport, even low-order SHE – based BTE solutions are known to give excellent agreement with experimental results [16][17][18]. Our procedure results in an analytical model for heat transport that eschews the notion of a local temperature for the LF modes. The enhanced Fourier law reads as follows:

$$\frac{\partial q}{\partial x} = -C\frac{\partial T}{\partial t} + S^{HF}(x,t) \qquad (1)$$

$$q = \frac{3}{5}(\Lambda^{LF})^2\frac{\partial^2 q}{\partial x^2} + \frac{3}{5}\kappa^{HF}(\Lambda^{LF})^2\frac{\partial^3 T}{\partial x^3} - \kappa\frac{\partial T}{\partial x} \qquad (2)$$

Here, the net heat-flux q= q^{LF}+q^{HF},q^{LF}= the LF-mode contribution to the heat-flux, q^{HF}= the HF-mode contribution to the heat-flux; $S^{HF}(x,t)$= external heat source term; T = local temperature of HF modes; κ is the net bulk thermal conductivity; $\kappa = \kappa^{LF} + \kappa^{HF}$, κ^{HF}= the contribution of HF modes to the bulk thermal conductivity, κ^{LF}= the contribution of LF modes to the bulk thermal conductivity; and Λ^{LF}= the MFP of the LF modes =$v\tau$ where v is the group-velocity magnitude of all LF modes and τ = LF mode lifetime. We assume that each and every LF mode has the same lifetime τ, as well as the same group-velocity magnitude v. The frequency of an LF mode of wave-vector $\boldsymbol{k}$, denoted by $\omega(k)$ is permitted to vary with k. We also assume isotropic phonon dispersion.

We state equations for the LF mode and HF mode heat-fluxes q^{HF} and q^{LF}separately:

$$q^{LF} = \frac{3}{5}(\Lambda^{LF})^2\frac{\partial^2 q^{LF}}{\partial x^2} - \kappa^{LF}\frac{\partial T}{\partial x} \qquad (3)$$

$$q^{HF} = -\kappa^{HF}\frac{\partial T}{\partial x} \qquad (4)$$

Length-scale dependence of thermal conductivity is a signature feature of nondiffusive heat transport. As an application exemplifying the utility of our model, we have specialized our equations to the spatially sinusoidal conditions of the transient gratings experiment. We have compared the effective thermal conductivity (ETC) of silicon versus length-scale as predicted by our model with the transient gratings experiment (Fig. 1), and therefrom extracted the following bound on the mean-free path of LF phonon modes in silicon: Λ^{LF} = 200 – 900 nm, with a best-fit value of 400 nm, consistent with [19].

As another application, we study the mean-free path accumulation function (MFPAF) introduced by Dames and Chen [21], a powerful tool in studying ballistic phonon transport. The MFPAF at a given mean-free path Λ is defined as the effective thermal conductivity (ETC) of all phonons with mean-free paths less than or equal to Λ. The utility of the MFPAF lies in that it explains within a unified framework[22] diverse experiments, like the transient gratings[13], time-domain thermoreflectance (TDTR)[23][24] and frequency domain thermoreflectance (FDTR)[25] experiments, that probe heat transport on length scales comparable to the phonon mean-free path. The thermoreflectance class of measurements was invented by Paddock and Easley [26]. The FDTR experiment is especially well suited to the determination of the MFPAF. We have shown that the choice of the thermal penetration depth (TPD) as the cutoff between ballistic and diffusive modes in FDTR experiments is intrinsically arbitrary and leads to significant error in the extracted MFPAF especially in the low MFP regime. The most serious source of error lies in that phonons with MFP equal to the TPD contribute significantly (roughly 42% at 88 MHz in silicon at 300 K) to the net heat-flux. Clearly, ignoring phonon modes with this MFP as fully ballistic (instead of quasi-ballistic) leads to erroneous conclusions about the MFPAF.

We set the criterion for the cut-off as the mean-free path at which the HF-mode heat-flux contribution (q^{HF} of Eq. (4)) drops to the point where it equals the LF-mode contribution (q^{LF} of Eq. (3)). Fig. 6 compares the MFPAF derived from our model to that from the TPD-cutoff model. Our model clearly shifts the MFPAF derived from the TPD cut-off model to the right. This is to be expected, since quasi-ballistic phonon heat-fluxes which decay slower than diffusive fluxes are accounted for in our model. We note here that unlike Regner *et al.*[26] whose MFPAF extraction is based on the TPD model, our MFPAF is inconsistent with ab-initio calculations of Esfarjani *et al*. [27]. Further exploration of this discrepancy is indicated.
With the above-mentioned capabilities demonstrated, we may expect that the enhanced Fourier law will adequately address the needs of next-generation device thermal simulators.

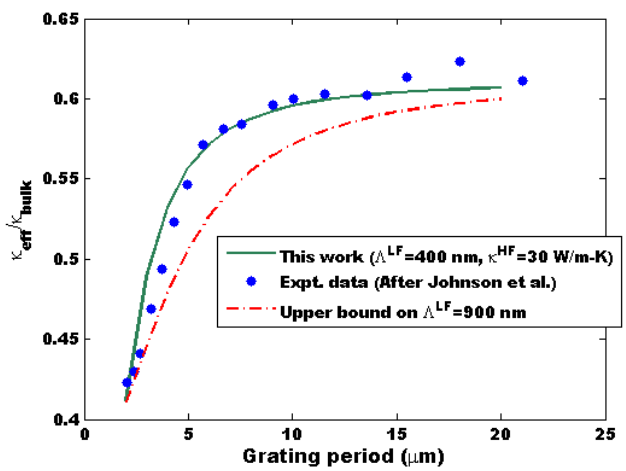

Fig. 1. Comparison of the ETC with experimental data after Johnson *et al.* [10]. The best fit to experiment is obtained with LF phonon MFP Λ^{LF}=400 nm, and κ^{HF}=30 W/m-K.

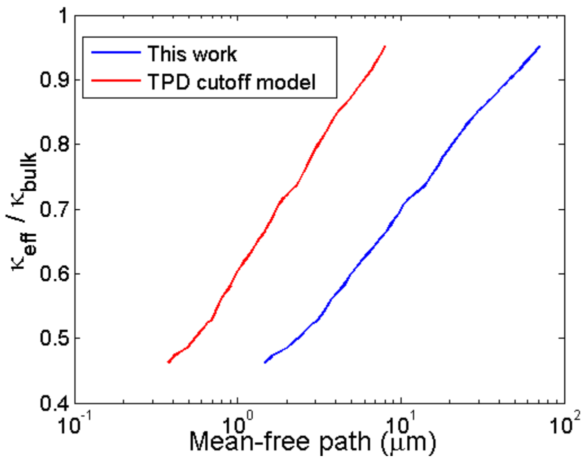

Fig. 2: The mean-free path accumulation function; red solid curve is after Regner *et al.* [25]. Our values (blue solid curve) are shifted considerably to the right due to contributions from quasi-ballistic LF-mode phonons.

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