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ANALYSIS OF MEASURING TECHNIQUES OF SUPERLATTICES THERMAL CONDUCTIVITY

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Abstract

It has been reported in a number of publications that measured values of superlattice thermal conductivities, for example, GaAs/AlAs, Si/Ge, InAs/AlSb, etc., do not compare well with expected or modeled values. There are questions about measurement techniques that are used and some improvements are being made. One of the used techniques is the 3(omega) measurement of thermal conductivity of superlattices. Some of these issues will be addressed in our work. The full two-scale heat transport and electrodynamics governing equations are used to achieve understanding of the possible mechanisms that play a role in shaping the effective (measured) coefficients of thermal and electrical conductivities in superlattices. It is shown that the issues of simulation or measurement of the effective coefficients at the upper scale are essentially the same as simulation of the complete two-scale problem in its complexity. Some of these concerns have been dealt with elsewhere. Here we will contribute to understanding of surficial transport and its inclusion into simulation procedures on the upper scale, and the problem of interaction of charge carriers transport and heat transport on both scales. Possible improvements of techniques for measuring superlattices conductivities will be suggested.

NOMENCLATURE

c_p - specific heat $[J/(kg \cdot K)]$
ds - interface differential area in porous medium $[m^2]$
∂S_{12} - internal surface in the REV $[m^2]$
$\mathbf{D}$ - electric flux density $[C/m^2]$
$\mathbf{E}$ - electric field $[V/m]$
$\widetilde{f_i} \equiv \{f_i\}_i$- VAT intrinsic phase averaged over $\Delta\Omega_i$ value f
$< f >_f$ - VAT phase averaged value f, averaged over $\Delta\Omega_i$ in a REV
$\hat{f}$ - VAT morpho-fluctuation value of f in a Ω_i
$\mathbf{j}$ - current density $[A/m^2]$
$< f >_t$ - time averaged value f
$k_1 = k_f$ - fluid phase thermal conductivity $[W/(mK)]$
$k_2 = k_s$ - homogeneous effective thermal conductivity of solid phase $[W/(mK)]$
$\mathbf{H}$ - magnetic field $[A/m]$
$\langle m \rangle$ - averaged porosity [-]
$\langle s_2 \rangle$ - solid phase fraction [-]

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S_{12} - specific surface of a porous medium $\partial S_{12}/\Delta\Omega$ [1/m]

T - temperature [K]

Subscripts $f \equiv 1$ - phase 1 or fluid phase

$s \equiv 2$ - solid phase

c - charge

Superscripts $\sim$- value in phase averaged over the phase $\Delta\Omega_n$

$*$ - complex conjugate variable

Greek letters $\varepsilon -$ dielectric permittivity [Fr/m]

μ - magnetic permeability [H/m]

ρ - electric charge density [C/m^3]

σ - medium specific electric conductivity [A/V/m]

Φ - electric scalar potential [V]

$\Delta\Omega$- representative elementary volume (REV) [m^3]

$\Delta\Omega_1 = \Delta\Omega_f$ - pore or phase 1 volume in a REV [m_3]

$\Delta\Omega_2 = \Delta\Omega_s$- second or phase 2 volume in a REV [m_3]

INTRODUCTION

The mathematical description of the coupled thermal transport and electromagnetic wave propagation fields for heterogeneous media were developed recently using spatial non-local theorems from volume averaging theory (VAT) as a method for accounting for multiple scale characteristics and their interactions. The VAT approach has been successfully applied during the past ten years to a number of difficult problems in the fluid mechanics and thermal physics of heterogeneous media, specifically of porous media. The main idea of performing transport and field description of electrodynamics problems in heterogeneous media through the spatial non-local theorems of the volume averaging theory (VAT) is to provide the means to account for local and non-local, phase and interface phenomena and requirements.

The vast majority of experimental methods are designed for homogeneous processes or like homogeneous,

making it difficult to assess the impact of heterogeneities. Meanwhile, it is the only major feature in the nature which causes the very different behavior and properties of matter or substances. The VAT provide the tools of doing analysis of the heterogeneous experimental data on the basis of heterogeneous theory based on heterogeneous versions of Ostrogradsky-Gauss theorem - not homogeneous classical mathematical models and equations.

Analysis of few problems in electrodynamics in terms of VAT was given in Ryvkina et al., (1998), Travkin et al., (1999,2000), Ponomarenko et al., (1999a,b), and Travkin and Catton, (2001), and there was shown that what is calculated as effective coefficients in many cases - as transient, nonlinear, interface dependent, with non-constant characteristics on the lower level components (dependents on temperature, or acoustical waves, or level of EM propagation) - they are not the conventional effective characteristics. They are effective ones, but in the form not conventionally formulated. First initial steps were made toward development heterogeneous media experimental approaches in thermal physics, fluid mechanics and electrodynamics based on the VAT tools Ponomarenko et al., 1999b; Ryvkina et al., 1998,1999; Travkin et al., 2001a,b).

Volume Averaging Theory Derivations and Theorems

The basic idea of hierarchical medium description is that the physical phenomena, mathematical presentation of those phenomena, and their models can be very different and in most of situations are different even if phenomena itself are identical, but the scales are different and the lower scale features should be transported to the upper level of description in such a mode that useful information would be added to the characteristics on the upper level.

Five types of two-phase medium averaging over the REV function f are defined by the following averaging operators arranged in the order of seniority (Whitaker, 1977, 1997; Primak et al., 1986, Travkin and Catton 1998)

$$\langle f \rangle = \langle f \rangle_1 + \langle f \rangle_2 = \langle s_1 \rangle \, \widetilde{f_1} + (1 - \langle s_1 \rangle) \, \widetilde{f_2},$$

where the phase averages are given by

$$\langle f \rangle_1 = \langle s_1 \rangle \frac{1}{\Delta \Omega_1} \int\limits_{\Delta \Omega_1} f\left(t, \vec{x}\right) d\omega = \langle s_1 \rangle \, \widetilde{f_1},$$

$$\langle f \rangle_2 = \langle s_2 \rangle \frac{1}{\Delta \Omega_2} \int\limits_{\Delta \Omega_2} f\left(t, \vec{x}\right) d\omega = \langle s_2 \rangle \, \widetilde{f_2},$$

and the internal phases are given by

$$\{f\}_1 = \widetilde{f_1} = \frac{1}{\Delta \Omega_1} \int\limits_{\Delta \Omega_1} f\left(t, \vec{x}\right) d\omega,$$

$$\{f\}_2 = \widetilde{f_2} = \frac{1}{\Delta \Omega_2} \int\limits_{\Delta \Omega_2} f\left(t, \vec{x}\right) d\omega, \qquad (1)$$

where $\widetilde{f_1}$ is an average over the space of phase one $\Delta \Omega_1$ in the REV, $\widetilde{f_2}$ is an average over the second phase volume $\Delta \Omega_2 = \Delta \Omega - \Delta \Omega_1$, and $\langle f \rangle$ is an average over the whole REV. There are also important heterogeneous averaging theorems for averaging of the spacial ∇ operator - analogs of Ostrogradsky-Gauss theorem. The few of them that are needed to average the field equations are

$$\{\nabla f\}_1 = \nabla \widetilde{f} + \frac{1}{\Delta \Omega_1} \int\limits_{\partial S_{12}} \widehat{f} \, \vec{ds_1}, \qquad (2)$$

$$\widehat{f} = f - \widetilde{f}, \quad f \, \forall \, \Delta \Omega_1, \qquad (3)$$

$$\langle \nabla f \rangle_1 = \nabla \langle f \rangle_1 + \frac{1}{\Delta \Omega} \int\limits_{\partial S_{12}} f \, \vec{ds_1}, \qquad (4)$$

The following averaging theorem is found for the rot operator

$$\langle \nabla \times \mathsf{f} \rangle_1 = \nabla \times \langle \mathsf{f} \rangle_1 + \frac{1}{\Delta \Omega} \int\limits_{\partial S_{12}} \vec{ds_1} \times \mathsf{f}, \qquad (5)$$

and as a consequence, the theorem for the intraphase average of $\nabla \times \mathsf{f}$ is found to be

$$\{\nabla \times \mathsf{f}\}_1 = \nabla \times \{\mathsf{f}\}_1 + \frac{1}{\Delta \Omega_1} \int\limits_{\partial S_{12}} \vec{ds_1} \times \widehat{\mathsf{f}}. \qquad (6)$$

These theorems applied to the physical processes in heterogeneous media completely change the simulation governing equations. More detail on the non-local VAT procedures and governing equations for different physical problems modeled in homogeneous media by linear and nonlinear mathematical physics equations can be found in Travkin and Catton (1998, 2001).

Experimental Observations of Scaled Transport in Superlattices

At present time the effort to advance the theory and models of heterogeneous media based on VAT description into experimental practice is in the very initial stage and actually does not exist as a field. Only few studies exist in this area. In the recent studies (Ryvkina et al., 1998; Ponomarenko et al., 1999a,b; Ryvkina et al., 1999) was outlined few of the VAT most frequently addressed issues in application to the heterogeneous ferrite media experiment as, effective conductivities and permittivities in singled and composite medium. Next are studies on optimization of semiconductor chip heat sink by Travkin and Catton (2000), Travkin et al., (2001b, 2001d), Rizzi et al. (2001) in which scaled approach allows the connection of the homogeneous lower scale heat transfer and convection inside the heat sink and upper scale bulk (actually averaged) fields of momentum, energy transport and general characteristics of effectiveness of the device.

As it appears due to application of VAT models the issues of effective coefficients in heterogeneous media are multivariant. Unlike in homogeneous medium, there are few coefficients can be derived for heterogeneous medium transport coefficients which have effective characteristics. The challenge at present moment is for experimentalists to begin to realize the difference in data obtained when medium is heterogeneous in essence.

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It is well known that the scale of measurements and of the modeling must correspond one to another. This obvious and simple principle is violated when what is clearly a two scale physical problem is described on the upper (measurement) scale with the same kind homogeneous mathematics as is used for the lower scale. Substitution of effective coefficients into models of this type is the primary question that must be dealt with.

Most of the additional terms in the VAT equations are terms which based on effects of interface phenomena and field fluctuations acting in the phase. There is, however, a lack of experimental results and data reduction procedures particularly developed for the purpose of experimental closure or verification of VAT semiconductor heat sink governing equations.

A majority of thermal conduction experiments are based on a constant heat flux through the experimental specimen and measurement of interface temperatures (Figs. 1-2). Data reduction is accomplished using

$$K = \frac{QL}{A\Delta T}, \qquad (7)$$

where Q is the electrical power from heater dissipated through the specimen, L is the distance used to measure the temperature difference, A is the uniform cross-sectional area of the sample.

Effective Coefficients Modeling

Starting, we choose the conductivity problem and first will be treating the example of constant phase conductivity coefficient conventional equations for the heterogenous medium.

As shown elsewhere (see, for example, Travkin and Catton, (2001) this mathematical statement is incorrect when the equation applied to the volume containing both phases, even when coefficient $k(\mathsf{r})$ is taken as random scalar or tensorial function. The reason for that is incorrect averaging over the media which have discontinuities. Conventional theories of treatment of this problem do not specify what is the meaning of the field T, assuming that it is the local variable, or - $T = T(\mathsf{r})$, where at the point r there is the point value of potential T exists.

Standard definition of effective (macroscopic) conductivity tensor determines from the following equation

$$\langle \mathsf{j} \rangle = -k_{ij}^* \langle \nabla T \rangle, \qquad (8)$$

in which assumed that

$$\langle \mathsf{j} \rangle = -k_1 \langle \nabla T \rangle_1 - k_2 \langle \nabla T \rangle_2 = -k_{ij}^* \langle \nabla T \rangle = -k_{ij}^* \nabla \langle T \rangle =$$

$$= -k_{ij}^* [\langle \nabla T \rangle_1 + \langle \nabla T \rangle_2] = -k_{ij}^* \langle \nabla T \rangle_1 - k_{ij}^* \langle \nabla T \rangle_2, \qquad (9)$$

so, for usually assumed an interface ∂S_{12} physics the effective coefficient determines

$$k_{ij}^* = \left[k_1 \nabla \left(\langle m_1 \rangle \widetilde{T}_1 \right) + k_2 \nabla \left(\langle m_2 \rangle \widetilde{T}_2 \right) + \right.$$

$$\left. + (k_2 - k_1) \frac{1}{\Delta\Omega} \int_{\partial S_{12}} T_2 \vec{ds_2} \right] \langle \nabla T \rangle^{-1}, \qquad (10)$$

involving knowledge of three different functions $\widetilde{T}_1$, $\widetilde{T}_2$, $T_{2|\partial S_{12}}$ in the volume Ω. This formula for the steady state effective conductivity can be shown is equal to the known expression

$$k_{ij}^* \langle \nabla T \rangle = k_2 \nabla \langle T \rangle + (k_1 - k_2) \frac{1}{\Delta\Omega} \int_{\Delta\Omega_1} \nabla T \, d\omega =$$

$$= k_2 \nabla \langle T \rangle + (k_1 - k_2) \langle \nabla T \rangle_1. \qquad (11)$$

It is worth to note here that the known formulae for the effective heat conductivity (or dielectric permittivity) of the layered medium

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$$k_e^* = \sum_{i=1} \langle m_i \rangle k_i, \ i = 1, 2, \qquad (12)$$

for field applied in parallel to interface of layers, and

$$k_e^* = \left[\sum_{i=1} \frac{\langle m_i \rangle}{k_i} \right]^{-1}, \qquad (13)$$

when the heat flux is perpendicular to the interface, are easily derived from the general expression (10).

Two-Scale Measurements of Heat and Charge Conductivities in Superlattices

To measure and model a multilayer films as scaled hierarchical objects we will discuss here the two possible techniques. One is when the Scanning Laser Thermoelectric Microscope (SLTM) technique (see, for example, the recent experiments performed by Borca-Tasciuc and Chen, 1997, 1998; Borca-Tasciuc, 2000) used for measurement of thermal conductivity and diffusivity of thin films - Fig. 3. The equation of heat conduction in a homogeneous film used for data reduction

$$\frac{\partial T_i}{\partial t} = a_i \nabla^2 T_i + S_{ihm}, \qquad (14)$$

should be changed for the heterogeneous VAT heat conduction equation with the corresponding VAT boundary conditions. Some more simple morphologies can be addressed easier than other. For example, the columnar 2D grains structure of one layer film on Fig. (3) with the straight vertical intergrain boundaries can supply needed morphological information for the closure of the VAT's equations on both scales. The same is to be said about closure of the heterogeneous VAT equations for the superlattice film as in Figs. (3-4). Knowing the period, thicknesses of 2-, 3-, or 4 component structure makes closure of governing equations available.

After transformation of the equation (14) to the moving system of coordinates with scanning coordinate $x_2 = x - Ut$, this equation becomes

$$\frac{\partial T_i}{\partial t} = U \frac{\partial T_i}{\partial x_2} + a_i \nabla^2 T_i + S_{ihm}. \qquad (15)$$

and used actually in modeling and data reduction of these experiments. Meanwhile, the non-local temperature equation which actually corresponds to the local equation (15) and corresponds to the scale of observation and measurements, can be written as

$$\langle m_i \rangle \frac{\partial T_i}{\partial t} = \langle m_i \rangle U \frac{\partial \widetilde{T_i}}{\partial x_2} + \frac{U}{\Delta \Omega} \int\limits_{\partial S_w} T_i \cdot \vec{ds_1} +$$

$$+ a_1 \nabla \cdot \left(\nabla \left(\langle m \rangle \widetilde{T_i} \right) \right) +$$

$$+ a_1 \nabla \cdot \left[\frac{1}{\Delta \Omega} \int\limits_{\partial S_w} T_i \vec{ds_1} \right] + \frac{a_1}{\Delta \Omega} \int\limits_{\partial S_w} \frac{\partial T_i}{\partial x_j} \cdot \vec{ds_1}. (16)$$

This is the equation which should be used in superlattice effective conductivity coefficient data reduction procedures when measurements done with SLTM. Exploring further the equation of heat transfer in each i-th layer of superlattice as one with the ohmic heat source due to impact of EM fields one can gets

$$c_{pi} \rho_i \frac{\partial T_i}{\partial t} = \nabla \cdot (k_i (T_i) \nabla T_i) + \sigma_i E_i^2. \qquad (17)$$

When one needs to study the more complete model of heat transport using the features of ohmic as well as dipolar heating the equations in each layer the set of governing equations for temperature and polarization field P in a Debye material becomes

$$c_{pi} \rho_i \frac{\partial T_i}{\partial t} = \nabla \cdot (k_i (T_i) \nabla T_i) +$$

$$+ \sigma_i (T_i) E_i^2 - \mathsf{P}_i \frac{\partial \mathsf{E}_i}{\partial t},$$

$$\frac{\partial \mathsf{E}_i}{\partial t} + r_{\tau i} (T_i) \mathsf{P}_i = \beta_i (T_i) \mathsf{E}_i, \qquad (18)$$

where $r_{\tau i}$ and β_i are the relaxation rates.

Derivation of dc VAT effective coefficients models shows that the conditions for the upper and lower

boundaries in effective composite medium approximations as the boundaries of laminated medium assumed are usually not met. There is no surprise that in many experiments (Ryvkina et al., 1998; Ponomarenko et al., 1999a,b; Ryvkina et al., 1999) the effective coefficients exceeded the parallel layers medium upper boundary values.

Heat conductivity coefficient in superlattice structures

using the 3ω technique Another method used for assessment of heat conductivity coefficient in superlattice structures is the 3ω technique (Cahill et al. 1989; Cahill, 1990; Cahill et al., 1992). Equations of heat transfer in each i-th layer used

$$\rho_i c_{pi} \frac{\partial T_i}{\partial t} = \nabla \cdot \left[(k_i) \nabla T_i \right],$$

with IVth kind boundary conditions between them. To take into account the a.c. electric field the equation in each of the layers of superlattice can be used in two forms (with the constant coefficients, taken here for simplicity)

$$\nabla^2 \mathsf{E} - \mu\sigma \frac{\partial \mathsf{E}}{\partial t} - \mu\varepsilon \frac{\partial^2 \mathsf{E}}{\partial t^2} = \boldsymbol{\nabla}\left(\frac{\rho_c}{\varepsilon} \right), \qquad (19)$$

$$\nabla^2 \left(\mathsf{E}\left(x, y, z \right) \right) + \omega^2 \mu\overline{\varepsilon}\mathsf{E} = \mathsf{e}^{-\mathsf{i}\omega\mathsf{t}} \frac{1}{\varepsilon} \boldsymbol{\nabla}\left(\rho_c \right), \quad (20)$$

$$\varepsilon = \mathsf{const}, \sigma = \mathsf{const},$$
$$\mu = const, \overline{\varepsilon} = \left(\varepsilon - i\frac{\sigma}{\omega} \right) const.$$

Non-local form of the electric field wave equation becomes for layers (type m, main)

$$\nabla^2 \left(\langle s_m \rangle \widetilde{\mathsf{E}}_m \right) + \nabla \cdot \left[\frac{1}{\Delta\Omega} \int\limits_{\partial S_{ms}} \mathsf{E}_m \overrightarrow{ds_m} \right] +$$

$$+ \frac{1}{\Delta\Omega} \int\limits_{\partial S_{ms}} \nabla \mathsf{E}_m \cdot \overrightarrow{ds_m} =$$

$$= \mu_m \sigma_m \frac{\partial \langle \mathsf{E} \rangle_m}{\partial t} + \mu_m \varepsilon_m \frac{\partial^2 \langle \mathsf{E} \rangle_m}{\partial t^2} +$$

$$+ \frac{1}{\varepsilon_m} \nabla \left(\langle s_m \rangle \widetilde{\rho}_{cm} \right) + \frac{1}{\varepsilon_m \Delta\Omega} \int\limits_{\partial S_{ms}} \rho_{cm} \overrightarrow{ds_m}. \qquad (21)$$

As it can be observed the most advantages feature of the heterogenous media electrodynamics equations is the inclusion of terms reflecting phenomena on the interface surface ∂S_{ms}, and that fact can be used to incorporate morphologically precisely multiple effects occurring at the interfaces.

In a quasistatic form the VAT equation of electric field is in a semiconductor layered component 1 (or m) looks (Travkin and Catton, 2001)

$$\nabla^2 \left(\langle m_1 \rangle \widetilde{\mathsf{E}}_1 \right) + \nabla \cdot \left[\frac{1}{\Delta\Omega} \int\limits_{\partial S_{12}} \mathsf{E}_1 \overrightarrow{ds_1} \right] +$$

$$+ \frac{1}{\Delta\Omega} \int\limits_{\partial S_{12}} \nabla \mathsf{E}_1 \cdot \overrightarrow{ds_1} =$$

$$\mathsf{e}^{-\mathsf{i}\omega\mathsf{t}} \left[\frac{1}{\varepsilon_1} \nabla \left(\langle m_1 \rangle \widetilde{\rho}_1 \right) + \frac{1}{\varepsilon_1 \Delta\Omega} \int\limits_{\partial S_{12}} \rho_1 \overrightarrow{ds_1} \right], \ \varepsilon_1 = const,$$
$$(22)$$

plus the similar equation of electric field in a quasistatic form in a dielectric layered component 2. There are two dependencies usually used for assessing, for example, the effective permittivity in a bulk material

$$\langle \mathsf{D} \rangle = \varepsilon_{eff} \langle \mathsf{E} \rangle, \ \ \langle \mathsf{E} \rangle = \langle m_1 \rangle \left\{ \mathsf{E}_1 \right\}_1 + \langle m_2 \rangle \left\{ \mathsf{E}_2 \right\}_2,$$
$$(23)$$

with the averaged volumetrically fields $\left\{ \mathsf{E}_1 \right\}_1$ and $\left\{ \mathsf{E}_2 \right\}_2$ used in this formula. Also

$$\langle \mathsf{D} \rangle = \langle m_1 \rangle \left\{ \varepsilon_1 \mathsf{E}_1 \right\}_1 + \langle m_2 \rangle \left\{ \varepsilon_2 \mathsf{E}_2 \right\}_2 =$$

$$= \langle m_1 \rangle \left[\left\{ \widetilde{\varepsilon}_1 \widetilde{\mathsf{E}}_1 \right\}_1 + \left\{ \widehat{\varepsilon}_1 \widehat{\mathsf{E}}_1 \right\}_1 \right] +$$
$$+ \langle m_2 \rangle \left[\left\{ \widetilde{\varepsilon}_2 \widetilde{\mathsf{E}}_2 \right\}_2 + \left\{ \widehat{\varepsilon}_2 \widehat{\mathsf{E}}_2 \right\}_2 \right],$$

which becomes for $\varepsilon_1 = const$, $\varepsilon_2 = const$

$$\langle \mathsf{D} \rangle = \langle m_1 \rangle \, \varepsilon_1 \, \{\mathsf{E}_1\}_1 + \langle m_2 \rangle \, \varepsilon_2 \, \{\mathsf{E}_2\}_2 . \qquad (24)$$

Using these equalities the effective permittivity coefficient field for superlattice can be presented for constant phase components as

$$\varepsilon_{eff} = \frac{\langle \mathsf{D} \rangle}{\langle \mathsf{E} \rangle} = \frac{\langle m_1 \rangle \, \varepsilon_1 \, \{\mathsf{E}_1\}_1 + \langle m_2 \rangle \, \varepsilon_2 \, \{\mathsf{E}_2\}_2}{\langle m_1 \rangle \, \{\mathsf{E}_1\}_1 + \langle m_2 \rangle \, \{\mathsf{E}_2\}_2}. \qquad (25)$$

In spite that this formula is based on the constant phase permittivity coefficients it is still needs to incorporate the fields of averaged variables of electric field in both phases $\{\mathsf{E}_1\}_1$, $\{\mathsf{E}_2\}_2$. These functions are not merely statistically (ensemble) or volumetrically averaged E_1 and E_2. They should be found through the properly constructed sets of models for upper $\{\mathsf{E}_1\}_1$, $\{\mathsf{E}_2\}_2$ and often lower E_1 and E_2 scales (Travkin and Catton, 1998,1999, 2001a; Travkin et al., 1999). Also, the effective coefficients would be different for stationary and time-dependent fields.

As the number of layers in superlattice can be substantial then the actual response of superlattice and it's temperature, heat conductivity, and electromagnetic microscale effective coefficients become a bulk (averaged) quantities. The volume of averaging can reach a proportion of a superlattice thickness in a cross-section Figs. 3-4. Then, the number of mathematical consequences and non-local models can be derived, with the simplest set of governing equations for the two-component superlattice.

Heat conductivity in plane and in cross section in a superlattice

The case of parallel plates (2 kinds of layers) with temperature field applied parallel to the boundary surfaces: 2 alternating kind of plates the effective coefficient is simple for analysis

$$k_{\shortparallel 2}^* (\mathsf{r}) = \left[k_1 \langle \nabla T (\mathsf{r}) \rangle_1 + k_2 \langle \nabla T (\mathsf{r}) \rangle_2 \right] / \langle \nabla T (\mathsf{r}) \rangle =$$

$$= \left[k_1 \nabla \left(\langle m_1 \rangle \widetilde{T}_1 \right) + k_2 \nabla \left(\langle m_2 \rangle \widetilde{T}_2 \right) + \right.$$

$$\left. + (k_2 - k_1) \frac{1}{\Delta \Omega} \int\limits_{\partial S_{12}} T_2 \vec{ds_2} \right] /$$

$$/ \left[\langle \, \nabla T \rangle_1 + \langle \, \nabla T \rangle_2 \right] =$$

$$= \left(k_1 \langle m_1 \rangle \nabla \widetilde{T}_1 (\mathsf{r}) + k_2 \langle m_2 \rangle \nabla \widetilde{T}_2 (\mathsf{r}) \right) /$$

$$/ \left(\langle m_1 \rangle \nabla \widetilde{T}_1 (\mathsf{r}) + \langle m_2 \rangle \nabla \widetilde{T}_2 (\mathsf{r}) \right), \qquad (26)$$

from which it is obvious that because the fields $\widetilde{T}_1 (\mathsf{r})$ and $\widetilde{T}_2 (\mathsf{r})$ are not equal generally, then the problem of finding the solutions for both are inevitable. Analysis shows that the lower scale linear function known solutions averaging do not correspond to the stated problem on the upper scale. This finding changes the approach for treatment of this problem.

Upper scale conventional equation of temperature field for which coefficient (26) was found as

$$\nabla \cdot \left(k_{\shortparallel 2}^* (\mathsf{r}) \nabla \langle T (\mathsf{r}) \rangle \right) = 0, \ \mathsf{r} \in \Omega,$$
$$\langle T (\mathsf{r}) \rangle = \langle m_1 \rangle \widetilde{T}_1 + \langle m_2 \rangle \widetilde{T}_2,$$

with the boundary conditions (BC) which are not analogous to the homogeneous heat transfer BC. That is all in the case when we want to analyze and simulate the problem on the upper scale (measurement scale) and, at the same time, just want to use only effective coefficient $k_{\shortparallel 2}^*$.

In all of the above only after acceptance of the idea of temperature equilibrium $\widetilde{T}_1 = \widetilde{T}_2$ in both phases, the known conventional formula for the effective conductivity will work

$$k_{\shortparallel 2}^* = \sum_{i=1} \langle m_i \rangle \, k_i, \ i = 1, 2. \qquad (27)$$

In the case when temperature field applied perpendicular to the boundary surfaces: 2 alternating kind of microscale sublayers (Figs. 3-4) one can get the similar model

$$k^*_{\perp 2} = \left[k_1 \left\langle \nabla T\left(x\right) \right\rangle_1 + k_2 \left\langle \nabla T\left(x\right) \right\rangle_2 \right] / \left\langle \nabla T\left(x\right) \right\rangle =$$

$$= \left[k_1 \nabla \left(\left\langle m_1 \right\rangle \widetilde{T}_1 \right) + k_2 \nabla \left(\left\langle m_2 \right\rangle \widetilde{T}_2 \right) + \right.$$

$$\left. + \left(k_2 - k_1\right) \frac{1}{\Delta \Omega} \int\limits_{\partial S_{12}} T_2 \vec{ds}_2 \right] /$$

$$/ \left(\left\langle m_1 \right\rangle \nabla \widetilde{T}_1\left(x\right) + \left\langle m_2 \right\rangle \nabla \widetilde{T}_2\left(x\right) \right). \qquad (28)$$

The key element to obtain the simplified formula is the recognition that the traversing heat flux at steady state conditions is the same for both phases $k_1 \nabla T_1 = k_2 \nabla T_2$. That formula may be used for substitution as $\nabla T_2 = \left(k_1 / k_2\right) \nabla T_1$, and the specific assumption for this morphology is that the averaged variables can be used in this equality (meaning that $k_1 \nabla \widetilde{T}_1 = k_2 \nabla \widetilde{T}_2$), then following the above procedure one can obtain

$$k^*_{\perp 2} = \left[\left(\left\langle m_1 \right\rangle + \left\langle m_2 \right\rangle \right) k_1 \nabla \widetilde{T}_1 \right] /$$

$$/ \left[\left(\left\langle m_1 \right\rangle + \left(k_1 / k_2\right) \left\langle m_2 \right\rangle \right) \nabla \widetilde{T}_1 \right] =$$

$$= \left[\left(\left\langle m_1 \right\rangle + \left\langle m_2 \right\rangle \right) k_1 \right] / \left[\left(\frac{\left\langle m_1 \right\rangle}{k_1} + \frac{\left\langle m_2 \right\rangle}{k_2} \right) \sigma_1 \right] =$$

$$= \left[\sum_{i=1} \frac{\left\langle m_i \right\rangle}{k_i} \right]^{-1}, i = 1, 2, \qquad (29)$$

because as it is assumed that the values $T_2(\partial S_{12})$ on both surfaces are very close then

$$\left(k_2 - k_1\right) \frac{1}{\Delta \Omega} \int\limits_{\partial S_{12}} T_2 \vec{ds}_2 \cong 0. \qquad (30)$$

This integral term (30) is never shown up in the homogeneous heat transfer treatment of this problem. We must to recognize that the assumption $k_1 \nabla \widetilde{T}_1 = k_2 \nabla \widetilde{T}_2$ is generally not correct, but the equality

$$k_1 \left\langle \nabla T\left(x\right) \right\rangle_1 = k_2 \left\langle \nabla T\left(x\right) \right\rangle_2 ,$$

is correct for simple situations. Then, as long as for the problem the heat fluxes in each of two phases formulates as

$$k_1 \left\langle \nabla T\left(x\right) \right\rangle_1 = k_2 \left\langle \nabla T\left(x\right) \right\rangle_2 ,$$

or

$$k_1 \nabla \left(\left\langle m_1 \right\rangle \widetilde{T}_1 \right) + k_1 \frac{1}{\Delta \Omega} \int\limits_{\partial S_{12}} T_1 \vec{ds}_1$$

$$= k_2 \nabla \left(\left\langle m_2 \right\rangle \widetilde{T}_2 \right) + k_2 \frac{1}{\Delta \Omega} \int\limits_{\partial S_{12}} T_2 \vec{ds}_2, \qquad (31)$$

meaning that the nominator in the effective coefficient formula can be written as

$$k_1 \left\langle \nabla T\left(x\right) \right\rangle_1 + k_2 \left\langle \nabla T\left(x\right) \right\rangle_2 =$$

$$= 2k_2 \left\langle m_2 \right\rangle \nabla \widetilde{T}_2 + 2k_2 \frac{1}{\Delta \Omega} \int\limits_{\partial S_{12}} T_2 \vec{ds}_2 =$$

$$= 2k_2 \left\langle m_2 \right\rangle \nabla \widetilde{T}_2 + 2k_2 \left[\left(T_{2(21)} - T_{(12)2} \right) \frac{1}{\Delta x_{REV}} \right] =$$

$$= 2k_2 \left\langle m_2 \right\rangle \nabla \widetilde{T}_2 + 2k_2 A, \qquad (32)$$

where

$$A = \frac{1}{\Delta \Omega} \int\limits_{\partial S_{12}} T_2 \vec{ds}_2 = \left[\left(T_{2(21)} - T_{(12)2} \right) \frac{1}{\Delta x_{REV}} \right], \quad (33)$$

where $T_{2(21)}$ means the value T_2 on the boundary surface where phase 2 changes to phase 1 (holding the phase 1 at the right, so the flux is going from left to right side), and vice versa for the $T_{(12)2}$ in the same REV.

This relationship could be an equality for the certain REV but could change in another REV - the simulation is needed to provide an answer to this question.

That means also that the field $\left\langle m_1 \right\rangle \nabla \widetilde{T}_1\left(x\right)$ in the denominator can be substituted by using $\left\langle \nabla T\left(x\right) \right\rangle_2$ in the equality (31) or

$$\langle m_1 \rangle \nabla \widetilde{T_1} (x) = \frac{1}{k_1} \left[k_2 \langle m_2 \rangle \nabla \widetilde{T_2} + k_2 \frac{1}{\Delta \Omega} \int\limits_{\partial S_{12}} T_2 \vec{ds_2} - \right.$$

$$\left. - k_1 \frac{1}{\Delta \Omega} \int\limits_{\partial S_{12}} T_1 \vec{ds_1} \right] =$$

$$= \frac{1}{k_1} \left[k_2 \langle m_2 \rangle \nabla \widetilde{T_2} + (k_1 + k_2) \frac{1}{\Delta \Omega} \int\limits_{\partial S_{12}} T_2 \vec{ds_2} \right] =$$

$$= \frac{1}{k_1} \left[k_2 \langle m_2 \rangle \nabla \widetilde{T_2} + (k_1 + k_2) A \right]. \qquad (34)$$

Now, the whole expression for the $k^*_{\perp 2}$ becomes clear

$$k^*_{\perp 2} = \left[k_1 \langle \nabla T (x) \rangle_1 + k_2 \langle \nabla T (x) \rangle_2 \right] / \langle \nabla T (x) \rangle =$$

$$= \left[k_1 \nabla \left(\langle m_1 \rangle \widetilde{T_1} \right) + k_2 \nabla \left(\langle m_2 \rangle \widetilde{T_2} \right) + \right.$$

$$\left. + (k_2 - k_1) \frac{1}{\Delta \Omega} \int\limits_{\partial S_{12}} T_2 \vec{ds_2} \right] /$$

$$/ \left(\langle m_1 \rangle \nabla \widetilde{T_1} (x) + \langle m_2 \rangle \nabla \widetilde{T_2} (x) \right) =$$

$$= \frac{2 k_2 \langle m_2 \rangle \nabla \widetilde{T_2} + 2 k_2 A}{\frac{1}{k_1} \left[k_2 \langle m_2 \rangle \nabla \widetilde{T_2} + (k_1 + k_2) A \right] + \langle m_2 \rangle \nabla \widetilde{T_2} (x)} =$$

$$= \frac{2 \left(\langle m_2 \rangle + A/ \left(\nabla \widetilde{T_2} \right) \right)}{\left[\frac{1}{k_1} \langle m_2 \rangle + \frac{1}{k_2} \langle m_2 \rangle + \frac{(k_1 + k_2)}{k_1 k_2} A/ \left(\nabla \widetilde{T_2} \right) \right]}. \qquad (35)$$

Now, let's present the A value, which is the surface integral over the singled out and bounded by ∂S_{12} phase 2, as

$$A = \frac{1}{\Delta \Omega} \int\limits_{\partial S_{12}} T_2 \vec{ds_2} = \left(T_{2(21)} - T_{(12)2} \right) \frac{1}{\Delta x_{REV}} \cong$$

$$\cong \nabla T_2 \left(\frac{\Delta m_2}{\Delta m_1 + \Delta m_2} \right) = \langle m_2 \rangle \nabla T_2, \qquad (36)$$

where Δm_1 and Δm_2 are sub-volumes of the each phase, and which is just the consequence of the homogeneous Ostrogradsky-Gauss theorem for a single domain (layer). Because we accepted in this substitution the idea of negligible influence of lateral (in coordinates (y, z) closing surfaces, this won't be the exact equality, but sufficiently close). When there are only two different kinds of layers and thicknesses are maintained as constants then this expression can be valid for almost the whole superlattice (excluding close to the boundary volumes). The accuracy of this substitution can be verified by numerical simulation. Next, after substitution of this expression into the formula for $k^*_{\perp 2}$ one gets

$$k^*_{\perp 2} = \frac{2 \left(\langle m_2 \rangle + \langle m_2 \rangle \nabla T_2 / \left(\nabla \widetilde{T_2} \right) \right)}{\left[\frac{1}{k_1} \langle m_2 \rangle + \frac{1}{k_2} \langle m_2 \rangle + \frac{(k_1 + k_2)}{k_1 k_2} \langle m_2 \rangle \nabla T_2 / \left(\nabla \widetilde{T_2} \right) \right]} =$$

$$= \frac{2 \left(1 + \nabla T_2 / \left(\nabla \widetilde{T_2} \right) \right)}{\left[\frac{1}{k_1} + \frac{1}{k_2} + \frac{(k_1 + k_2)}{k_1 k_2} \nabla T_2 / \left(\nabla \widetilde{T_2} \right) \right]}. \qquad (37)$$

This formula presents the chance for development of the experimental procedure for assessment of effective conductivity coefficient of the layer through the solution of the problem for the only one phase or the measurement of the only one phase temperature field properties.

When there are three or more phases are combined in the superlattice then the sequence would play a significant role and each morphology can change the data reduction procedures.

The thermal flux directions and the polarizations of electromagnetic fields can have a number of key combinations. This situation also needed to be accounted when the experimental set-up and data reduction are

planned for semiconductor, magnetic etc. media. Directing a study to include more then 2 scales of superlattice physics as the nanoscale and atomic scale is the challenging but treatable task in brackets of scaled VAT approach. Some of considerations pertinent to nanoscale transport and coefficients given in Travkin and Catton (2001b).

SUMMARY

The fundamental peculiarities of interface transport and hierarchical mathematical coupling for measurements of heat conductivity in superlattices bring together issues that have never actually been addressed as a scaled phenomena. It is shown that accurate accounting for scale interactions and, as is inevitable in scaled problems, application of fundamental heterogeneous theorems to a scaled description of the Laplace and ∇ operators bring to the upper scales completely different mathematical governing equations and models. We have conducted some assessment of the differences between the static upper scale and transient nanoscale transport coefficients and show how the lattice morphology and its irregularities influence the effective conductivities.

Developed scaled concepts to address the issues of nanoscale multiphysics heat conductivity measurement techniques in electronic materials. The two methods usually applied toward these tasks are approached in terms of hierarchical scaled theory of VAT.

It's shown a number of situations when the two scale VAT numerical simulation effort should be used to address issues of coupled thermal - electrodynamic response in a superlattice when effective conductivity is studied.

There is also outlined a need to consider more appropriately the scales of measurements and the models used for a data reduction. Their correspondence is a key issue when more then one scale heterogeneous material is under investigation.

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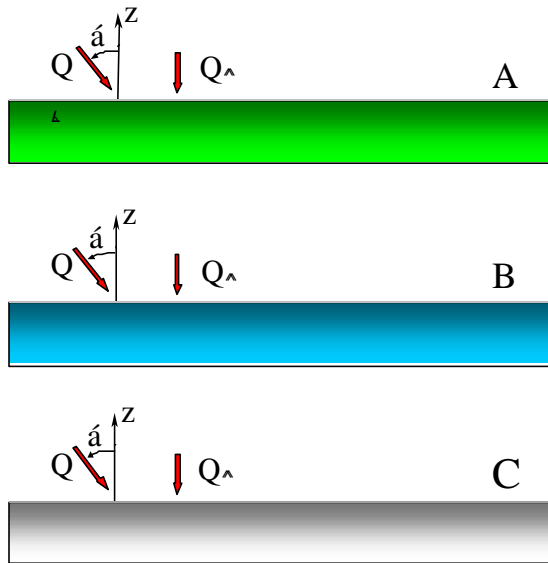
Fig. 1   Layer 1D on the top of medium, common ground
homogeneous description upper hierarchical scale
effective conductivity coefficient determination
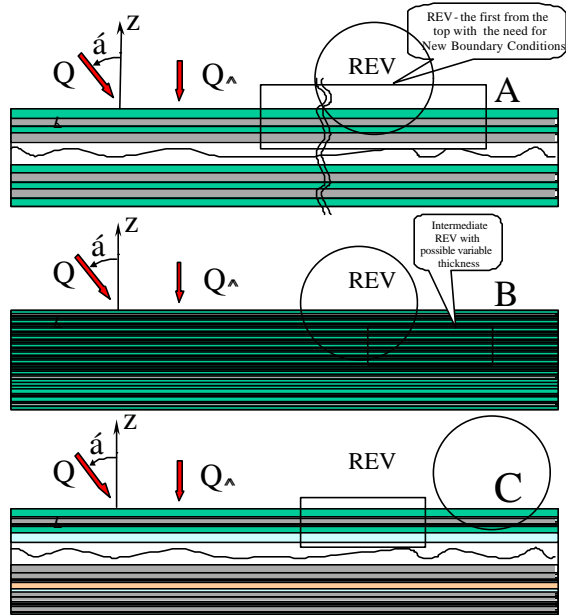- perfect (A) and imperfect (B, C) interface conductance

Fig. 2   Layered 1D medium upper hierarchical scale
effective conductivity coefficient determination
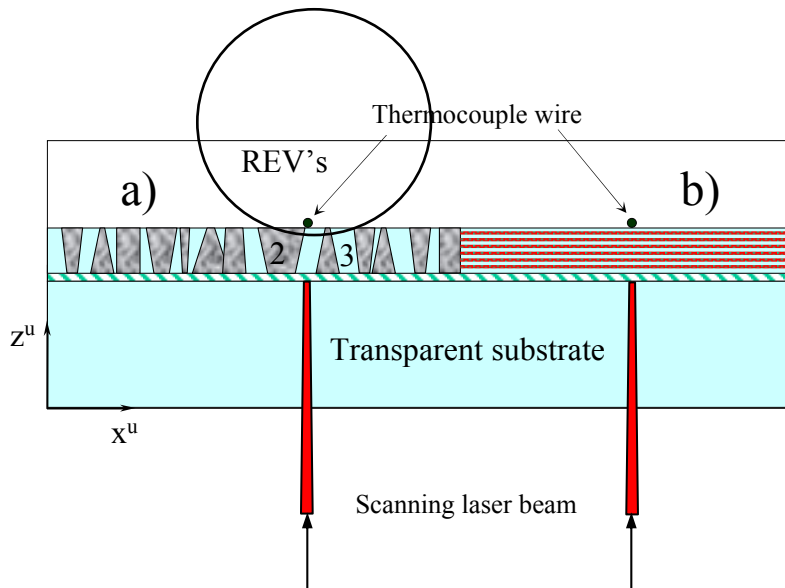- perfect (A) and imperfect (B, C) interface conductance

Fig. 3 The schematic of the SLTM measurement area with the one layer of 2D
lower scale column grains – (a), and the superlattice film on the substrate (b);

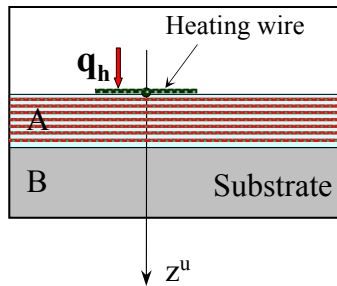x^u and z^u are upper scale coordinate axes unit vectors

Fig. 4 Heat conductivity 3T method measurement physical model
for multilayred film or superlattice A on the substrate B