Proceedings of
2001 ASME International Mechanical Engineering Congress and Exposition
November 11-16, 2001, New York, NY

HEAT AND CHARGE CONDUCTIVITIES IN SUPERLATTICES - TWO-SCALE MEASURING AND MODELING

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Abstract

Conventional reasoning and established procedures for measurement of heat and charge conductivities at the continuum micrometer scale, or higher scales, results in a number of variables and physical entities being the subject of measurement. These variables themselves are not point values if to define them with the lower scale concepts. When the media overall properties are sought, their dependence on lower (smaller) scale physical phenomena and their mathematical descriptions need to be considered and incorporated into the higher (larger) scale description and mathematical modeling. This is not a new problem. How to treat or solve multi-scale problems is the issue. Effective scaled heat and charge conductivity are studied for a morphologically simple 1D layered heterostructure with the number of components being $n \geqslant 2$, the effective scaled heat and charge conductivities. It is a two-scale media with the lower scale physics of energy and charge carriers being described by commonly used models. A continuum $\leftrightarrow$ continuum description of $\eta m \leftrightarrow \mu m$ transport of electron - phonon energy fields, as well as the electromagnetic and temperature fields for ηm scale coupled with the microscale (μm) mathematical models are studied. The medium is heterogeneous because it has multiple phases, volumetric phases 1, 2, 3 .... and (n+m) phases that are the interfaces between volumetric phases. The fundamental peculiarities of interface transport and hierarchical mathematical coupling bring together issues that have never actually been addressed correctly. It is shown that accurate accounting for scale interactions and, as is inevitable in scaled problems, application of fundamental 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 and report some preliminary quantitative 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.

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 $[m^2]$

D - electric flux density [C/m^2]
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
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 $[W/(mK)]$
$\langle m \rangle$ - averaged porosity [-]
$\langle s_2 \rangle$ - solid phase fraction [-]
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 fluid 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

In a heterogeneous medium the phenomena in each of a two- (or more) phases are considered as a major with physical impacts. The great number of facts evidence in a favor of interface physical processes are being the important component of a process or transport. There is the need to understand the physics and to model multiscale characteristics in heterogeneous media.

The suggested study is pointing out on using the very established in thermophysics and fluid mechanics theoretical tools of heterogeneous media scaled description - volume averaging theory (VAT), to address the problem of multilayer bulk cross-section and in-plane properties. Multiscale problems of this type have mostly been solved using ensemble averaging to couple the phenomena at the different scales, a correct procedure for variables and fields of homogeneous nature (excluding dynamics and other features involving differential operators). The focus of this work is transport phenomena in media having distinctive heterogeneous characteristics consisting of two or more phases at the upper scale in an area of promising application. The VAT provides the tools of doing analysis of the heterogeneous experimental data on the basis of heterogeneous theory - not homogeneous classical mathematical models and equations.

The main point in this - if at any scale there is of physical consideration, in which can be claimed, or there is sure or almost sure, or one can prove it or substantiate it - that the coefficients are known and justified for this medium. Which is especially good when the start is with the lowest scale possible. Then, there is need to know the properties of the higher level of material's organization. The problem as it can be written within the VAT and from this point it is the clear connection of structure, morphologies and properties. The problem that calculation and solution of integro-differential equations are not known for most in analytical and in numerical forms. Still, for simplest morphologies are solvable problems out there.

Among the important features of VAT are that it allows specific medium types and morphologies , lower-scale fluctuations of variables, cross-effects of different variable fluctuations, and interface variable fluctuations effects, etc. to be considered. We consider here mostly the influence of interface transport on bulk properties in layered morphologies.

Non-Local Electrodynamics and Heat Transport in Superstructures

Many microscale heterogeneous heat transport equations and some of the solutions provided elsewhere (Chen and Tien 94; Chen 97; Goodson and Flik, 1993) bare a substantial analysis and many advancements. Goodson (1996), for example, directly address the need to model the nonhomogeneous medium (diamond CVD layer) thermal transport with account to grains presence. The Peierls-Boltzmann equation for the phonon transport equation was used along with information on grains structure. Meanwhile, micro- and nanoscale thermal transport is indissolubly tight to electrodynamics in the same material. A full description of the derivation of the VAT non-local nanoscale electrodynamics governing equations is given by Travkin and Catton (2001). These equations and some of their variations as, for example, the electric field wave equation for the lower scale (in matrix)

$$\nabla^2\mathbf{E}_m-\mu_m\sigma_m\frac{\partial\mathbf{E}_m}{\partial t}-\mu_m\varepsilon_m\frac{\partial^2\mathbf{E}_m}{\partial t^2}=\boldsymbol{\nabla}\left(\frac{\rho_m}{\varepsilon_m}\right). \quad (1)$$

which becomes on the upper scale

$$\nabla^2\left(\langle s_m\rangle\widetilde{\mathbf{E}}_m\right)+\nabla\cdot\left[\frac{1}{\Delta\Omega}\int\limits_{\partial S_{ms}}\mathbf{E}_m d\vec{s}_m\right]+$$
$$+\frac{1}{\Delta\Omega}\int\limits_{\partial S_{ms}}\nabla\mathbf{E}_m\cdot d\vec{s}_m=\mu_m\sigma_m\frac{\partial\langle\mathbf{E}\rangle_m}{\partial t}+\mu_m\varepsilon_m\frac{\partial^2\langle\mathbf{E}\rangle_m}{\partial t^2}+$$
$$+\frac{1}{\varepsilon_m}\nabla\left(\langle s_m\rangle\widetilde{\rho}_m\right)+\frac{1}{\varepsilon_m\Delta\Omega}\int\limits_{\partial S_{ms}}\rho_m d\vec{s}_m, \quad (2)$$

form a basis for modeling of electric and magnetic fields at the microscale (upper scale) level in heterostructures. 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.

The most common way to treat heterogeneous problems has been to seek a solution of detailed microscale mathematical model by doing numerical experiments over more or less the exact morphology of interest - what can be called the Detailed Micro-Modeling (DMM) which often conducted using Direct Numerical Modeling (DNM). Consequently, the questions arise concerning the issues of difference between DMM-DNM and Heterogeneous Media Modeling (HMM) which is the modeling of overall averaged in some way medium properties.

Three driving forces can be mentioned while explaining the need for each sounding physical scale description and connection, transformation from and between the lower and upper levels.

I) The experimental abilities and comparison of measured field's variables with those which are considered as physically meaningful at the both scales. It is actually always an experiment is made on the only one scale - mostly on the upper scale of material or medium, because the practical needs mostly concern the upper scale properties.

II) Thus, modeling needs on the upper scale of hierarchy. Without proper theoretical model of upper scale (heterogeneous scale) phenomena neither measurements nor theoretical analysis is correct or complete.

III) Also, it is hard to pose a goal to improve characteristics or functionality in the problem without proper theoretical model and understanding of the phenomena in both scales.

The most sought after characteristics in heterogeneous media transport which are the effective transport coefficients can be correctly determined using conventional definition

$$-\langle\mathbf{j}\rangle=\sigma^*\nabla\langle\Phi\rangle=\sigma_2\nabla\langle\Phi\rangle+(\sigma_1-\sigma_2)\frac{1}{\Delta\Omega}\int\limits_{\Delta\Omega_1}\nabla\Phi\, d\omega,$$

while employing the DMM-DNM exact solution in only the fraction of problems. The issue is that in majority of problems, as for inhomogeneous, nonlinear coefficients, for example, and in many transient problems having the two-field DMM-DNM exact solution is not enough even to find effective coefficients.

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 layered medium. As shown elsewhere (see, for example, Travkin and Catton, 1998) this mathematical statement is incorrect when the equation applied to the volume containing both phases, even when coefficient $k(\mathbf{r})$ 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 - $T = T(\mathbf{r})$, where at the point $\mathbf{r}$ there is the point value of potential T exists. Meanwhile, what is the point value on the upper scale then, due to nature of heterogeneous medium is a domain, volume of heterogeneous nature on the lower scale. Next, the microscale analysis shows that the coefficient $k = k(\mathbf{r})$, as long as in each separate lower scale point $\mathbf{r}$ there is exists the local k with the value either of phase 1 or phase 2, and in each of the phases the value of k_i is constant.

In the DMM-DNM approaches the mathematical statement usually deals with the local fields and as soon as the boundary conditions are taken in some way, the problem became formulated correctly and can be solved exactly as in work by Cheng and Torquato (1997), for example. Difficulties arise when the result of this solution needs to be interpreted - and this is in the majority of problem statements in heterogeneous media, in terms of non-local fields, but averaged in some way. The averaging procedure usually is proclaimed in one of the fashions - either doing stochastic or spacial, volumetric integration. Almost all of these averaging developments are done incorrectly due to disregard of averaging theorems for differential operators in heterogeneous medium on the upper scale of material.

Let us consider the conductivity problem in a two-phase medium. According to most accepted mathematical statements the standard definition of effective (macroscopic) conductivity tensor determines from the following equation

$$\langle \mathbf{j} \rangle = -k^*_{ij} \langle \nabla T \rangle , \tag{3}$$

in which assumed that

$$\langle \mathbf{j} \rangle = -k_1 \langle \nabla T \rangle_1 - k_2 \langle \nabla T \rangle_2 = -k^*_{ij} \langle \nabla T \rangle = -k^*_{ij} \nabla \langle T \rangle$$

$$= -k^*_{ij} \left[\langle \nabla T \rangle_1 + \langle \nabla T \rangle_2 \right] = -k^*_{ij} \langle \nabla T \rangle_1 - k^*_{ij} \langle \nabla T \rangle_2 , \tag{4}$$

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

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

$$\left. + (k_2 - k_1) \frac{1}{\Delta\Omega} \int_{\partial S_{12}} T_2 d\vec{s}_2 \right] \langle \nabla T \rangle^{-1} , \tag{5}$$

involving knowledge of three different functions $\widetilde{T}_1$, $\widetilde{T}_2$, $T_{1_{|\partial S_{12}}}$ in the volume Ω. This formula for the steady state effective conductivity can be shown is equal to the known expression

$$\begin{aligned} k^*_{ij} \langle \nabla T \rangle &= k_2 \nabla \langle T \rangle + (k_1 - k_2) \frac{1}{\Delta\Omega} \int_{\Delta\Omega_1} \nabla T \, d\omega = \\ &= k_2 \nabla \langle T \rangle + (k_1 - k_2) \langle \nabla T \rangle_1 . \end{aligned} \tag{6}$$

It is worth to note here that the known formulae for the effective heat conductivity (or dielectric permittivity) of the layered medium (Figs. 1-2)

$$k^*_e = \sum_{i=1} \langle m_i \rangle k_i , \; i = 1, 2, \tag{7}$$

for field applied in parallel to interface of layers, and

$$k_e^* = \left[\sum_{i=1} \frac{\langle m_i \rangle}{k_i} \right]^{-1}, \qquad (8)$$

when the heat flux is perpendicular to the interface, are easily derived from the general VAT expression using assumptions that intraphase fields are equal $\widetilde{T}_1 = \widetilde{T}_2$, that interface boundary conditions are valid for averaged fields, and that adjoining surface interface temperatures are close in magnitudes. The same assumptions are effectual when conventional analysis techniques are applied toward the derivation of formulae (7), (8).

The problem becomes not easier in the case when effective conductivity coefficient meant, for example, as for the transient heat conductivity problem in composite material. Combining both temperature equations (if only two of phases are present) for the simplest case of constant coefficients one can obtain the effective coefficient of conductivity equal to steady-state effective conductivity only when a local thermal equilibrium is assumed

$$\langle T \rangle = \langle s_1 \rangle \widetilde{T}_1 + \langle s_2 \rangle \widetilde{T}_2 = T^* = \widetilde{T}_1 = \widetilde{T}_2. \qquad (9)$$

As the number of layers in superlattice can be substantial then the actual response of superlattice and it's temperature and heat conductivity coefficient become a bulk (averaged) quantities. The volume of averaging can reach a proportion of a superlattice thickness in a cross-section Fig. 1-3. 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.

The case of parallel layers (2 kinds) with d.c. electrical field applied parallel to the boundary surfaces: 2 alternating kind of plates the effective conductivity coefficient is

$$\sigma^*_{\shortparallel 2}(\mathbf{r}) = \left[\sigma_1 \langle \nabla \Phi(\mathbf{r}) \rangle_1 + \sigma_2 \langle \nabla \Phi(\mathbf{r}) \rangle_2 \right] / \langle \nabla \Phi(\mathbf{r}) \rangle =$$

$$= \Big[\sigma_1 \nabla \left(\langle m_1 \rangle \widetilde{\Phi}_1 \right) + \sigma_2 \nabla \left(\langle m_2 \rangle \widetilde{\Phi}_2 \right) +$$

$$(\sigma_2 - \sigma_1) \frac{1}{\Delta\Omega} \int\limits_{\partial S_{12}} \Phi_2 d\vec{s}_2 \Big] / \left[\langle \nabla \Phi \rangle_1 + \langle \nabla \Phi \rangle_2 \right] =$$

$$= \left(\sigma_1 \langle m_1 \rangle \nabla \widetilde{\Phi}_1(\mathbf{r}) + \sigma_2 \langle m_2 \rangle \nabla \widetilde{\Phi}_2(\mathbf{r}) \right) /$$

$$/ \left(\langle m_1 \rangle \nabla \widetilde{\Phi}_1(\mathbf{r}) + \langle m_2 \rangle \nabla \widetilde{\Phi}_2(\mathbf{r}) \right), \qquad (10)$$

in the interface surface flux one half surface integral eliminates the second surface because their values are equal and have opposite signs on the left L and right R interface surface bounding the plate 1, for example, so

$$(\sigma_2 - \sigma_1) \frac{1}{\Delta\Omega} \int\limits_{\partial S_{12}} \Phi_2 d\vec{s}_2 =$$

$$= (\sigma_2 - \sigma_1) \left(\frac{1}{\Delta\Omega} \int\limits_{\partial L} \Phi_2 ds_2 - \frac{1}{\Delta\Omega} \int\limits_{\partial R} \Phi_2 ds_2 \right) = 0.$$

It is obvious that because the averaged fields $\widetilde{\Phi}_1(\mathbf{r})$ and $\widetilde{\Phi}_2(\mathbf{r})$ are not equal generally, see Figs 3-4, then the problem of finding the solutions for both phases 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 electrical field for which coefficient (10) was found as

$$\begin{aligned} \nabla \cdot \left(\sigma^*_{\shortparallel 2}(\mathbf{r}) \nabla \langle \Phi(\mathbf{r}) \rangle \right) &= 0, \ \mathbf{r} \in \Omega, \\ \langle \Phi(\mathbf{r}) \rangle &= \langle m_1 \rangle \widetilde{\Phi}_1 + \langle m_2 \rangle \widetilde{\Phi}_2, \end{aligned}$$

with the boundary conditions (BC) which are not analogous to the homogeneous heat transfer BC - that is in the case when we want to analyze and simulate the problem from the bottom scale up - meaning, from nanoscale, for example, to microscale

The different is the situation when one needs to simulate from the upper scale down. Thus, one can see that the either of the two ways to solve this problem demands the solution for the fields $\widetilde{\Phi}_1$ and $\widetilde{\Phi}_2$:

1) In the case when one relies on effective conductivity coefficient - $\sigma^*_{\shortparallel 2}$, to solve the problem on the upper scale just from the beginning. For finding the $\sigma^*_{\shortparallel 2}$ one needs to know the fields $\widetilde{\Phi}_1$ and $\widetilde{\Phi}_2$. Then one needs to solve the equation

$$\nabla \cdot \left(\sigma^*_{\shortparallel 2} (\mathbf{r}) \nabla \langle \Phi (\mathbf{r}) \rangle \right) = 0, \;\; \mathbf{r} \in \Omega, \tag{11}$$

with the BC on the left hand side of the layer consisting of stack of parallel sublayers

$$\langle \Phi (\mathbf{r}) \rangle|_L = \left(\langle m_1 \rangle \widetilde{\Phi}_1 + \langle m_2 \rangle \widetilde{\Phi}_2 \right)\Big|_L = \Phi_L,$$

and on the right side the BC is

$$\langle \Phi (\mathbf{r}) \rangle|_R = \left(\langle m_1 \rangle \widetilde{\Phi}_1 + \langle m_2 \rangle \widetilde{\Phi}_2 \right)\Big|_R = \Phi_R. \tag{12}$$

Actually the second time solution for the field $\langle \Phi (\mathbf{r}) \rangle$ can be avoided if properly set up of the boundary conditions implemented in the solution governing equations for the $\widetilde{\Phi}_1$ and $\widetilde{\Phi}_2$, as we will see below.

2) In the case when one wants to solve the problem starting from the lower scale simulation - he would consider the solution of the equation

$$\nabla^2 \left(\langle m_1 \rangle \widetilde{\Phi}_1 \right) + \nabla \cdot \left[\frac{1}{\Delta\Omega} \int\limits_{\partial S_{12}} \Phi_1 \vec{ds}_1 \right] + \\ + \frac{1}{\Delta\Omega} \int\limits_{\partial S_{12}} \nabla \Phi_1 \cdot \vec{ds}_1 = 0, \tag{13}$$

with account for the conservation of current $\mathbf{j}$ at the interface ∂S_{12}

$$\begin{aligned} \mathbf{n} \cdot \mathbf{j}_1|_{\partial S_{12}} &= \sigma_1 \mathbf{n} \cdot \nabla \Phi_1|_{\partial S_{12}} = && (14) \\ \sigma_2 \mathbf{n} \cdot \nabla \Phi_2|_{\partial S_{12}} &= \mathbf{n} \cdot \mathbf{j}_2|_{\partial S_{12}}, && (15) \end{aligned}$$

and equation

$$\nabla^2 \left(\langle m_2 \rangle \widetilde{\Phi}_2 \right) + \nabla \cdot \left[\frac{1}{\Delta\Omega} \int\limits_{\partial S_{12}} \Phi_2 \vec{ds}_2 \right] + \\ + \frac{1}{\Delta\Omega} \int\limits_{\partial S_{12}} \nabla \Phi_2 \cdot \vec{ds}_2 = 0, \tag{16}$$

with the same conservation law of current $\mathbf{j}$ at the interface ∂S_{12} plus the both equations need to have the BC at the both sides of the superlattice. Let 's assume that it would be the Ist kind of boundary conditions (going from upper scale - down)

$$\langle \Phi (\mathbf{r}) \rangle|_L = \langle m_1 \rangle \widetilde{\Phi}_1 + \langle m_2 \rangle \widetilde{\Phi}_2 \Big|_L = \Phi_L,$$

$$\langle m_1 \rangle \widetilde{\Phi}_1 \Big|_L = \Phi_L - \langle m_2 \rangle \widetilde{\Phi}_2 \Big|_L, \tag{17}$$

and on the right side BC

$$\langle m_1 \rangle \widetilde{\Phi}_1 \Big|_R = \Phi_R - \langle m_2 \rangle \widetilde{\Phi}_2 \Big|_R. \tag{18}$$

To find out the local fields $\Phi_1$and Φ_2 we can do the solution of the homogeneous local set of governing equations

$$\begin{aligned} \nabla \cdot (\sigma_1 \nabla \langle \Phi_1 (\mathbf{r}) \rangle) &= 0, \;\; \mathbf{r} \in \Omega_1, \\ \nabla \cdot (\sigma_2 \nabla \langle \Phi_2 (\mathbf{r}) \rangle) &= 0, \;\; \mathbf{r} \in \Omega_2, \end{aligned}$$

with

$$\begin{aligned} \Phi_1|_{\partial S_{12}} &= \Phi_2|_{\partial S_{12}}, && (19) \\ \mathbf{n} \cdot \mathbf{j}_1|_{\partial S_{12}} &= \sigma_1 \mathbf{n} \cdot \nabla \Phi_1|_{\partial S_{12}} = \end{aligned}$$

$$= \sigma_2 \mathbf{n} \cdot \nabla \Phi_2|_{\partial S_{12}} = \mathbf{n} \cdot \mathbf{j}_2|_{\partial S_{12}}, \tag{20}$$

$$\begin{aligned} \Phi_1|_L &= \Phi_L, \;\; \Phi_1 (\mathbf{r})|_R = \\ \Phi_R, \;\; \Phi_2|_L &= \Phi_L, \;\; \Phi_2 (\mathbf{r})|_R = \Phi_R. \end{aligned}$$

This set of equations has singularity points where their interface surfaces are laying on the left or right boundary surfaces. For example at the point

$$\Phi_1|_{\partial S_{12}} \cap \Phi_1|_L \equiv \Phi_2|_{\partial S_{12}} \cap \Phi_2|_L \,. \qquad (21)$$

These singularities should be resolved in the manner just adopted in other approaches used as, for example, we can use the generalized BC as

$$\begin{aligned} \langle m_1\rangle \, \Phi_1|_L \;&\simeq\; \langle m_1\rangle \, \widetilde{\Phi}_1\Big|_L = \Phi_L - \langle m_2\rangle \, \widetilde{\Phi}_2\Big|_L, \qquad (22)\\ \lim_{\xi\in\Pi_s}\left(\Phi_{1\xi}|_L\right) \;&=\; \frac{\left(\Phi_L - \langle m_2\rangle \, \widetilde{\Phi}_2\Big|_L\right)}{\langle m_1\rangle}, \;\; \xi\in\Pi_s, \qquad (23)\end{aligned}$$

where the sequence ξ belongs to the field $\Pi_s$in which the iterations are produced. And

$$\langle m_2\rangle \, \Phi_2|_L \simeq \langle m_2\rangle \, \widetilde{\Phi}_2\Big|_L = \Phi_L - \langle m_1\rangle \, \widetilde{\Phi}_1\Big|_L, \qquad (24)$$

also on the right hand side boundary R the same approach is used

$$\langle m_1\rangle \, \Phi_1|_R \simeq \langle m_1\rangle \, \widetilde{\Phi}_1\Big|_R = \Phi_R - \langle m_2\rangle \, \widetilde{\Phi}_2\Big|_R, \qquad (25)$$

and

$$\langle m_2\rangle \, \Phi_2|_R \simeq \langle m_2\rangle \, \widetilde{\Phi}_2\Big|_R = \Phi_R - \langle m_1\rangle \, \widetilde{\Phi}_1\Big|_R. \qquad (26)$$

In all of the above only after acceptance of the idea of **potential equilibrium** $\widetilde{\Phi}_1 = \widetilde{\Phi}_2$, the known conventional formula for the effective conductivity will work

$$\sigma^*_{\shortparallel 2} = \sum_{i=1} \langle m_i\rangle \, \sigma_i, \;\; i = 1, 2. \qquad (27)$$

This assumption of potential equilibrium is too obviously inappropriate, then this widely used formula is incorrect and must be replaced by (10). When three or more alternating kind of parallel plates (layers) stacked altogether with electrical field applied parallel to the boundary surfaces, then this problem is still qualified as a symmetrical problem - because transposition of two middle layers (say 1 and 2) in the REV does not change the situation with the fluxes to adjacent layers - let's $(1-2-3)$ to be rearranged as $(2-1-3)$, then will be no difference for the REV averaging: $\left[^{(t2)}\langle\Phi\rangle\right] = \langle m_2\rangle \, \widetilde{\Phi}_2 + \langle m_1\rangle \, \widetilde{\Phi}_1 + \langle m_3\rangle \, \widetilde{\Phi}_3 = \left[^{(t1)}\langle\Phi\rangle\right] = \langle m_1\rangle \, \widetilde{\Phi}_1 + \langle m_2\rangle \, \widetilde{\Phi}_2 + \langle m_3\rangle \, \widetilde{\Phi}_3$. Meanwhile, if one to imagine more complicated situation as with the period: $(2-3-1-2-3)$ when the same three different kinds of layers are organized in the 5 layer stack periodic medium. It is still the 3 kind plates composite, but the REV averaged variable will not be equal to the $(1-2-3)$ morphology $\left[^{(t2)}\langle\Phi\rangle\right] = \langle m_2\rangle \, \widetilde{\Phi}_2 + \langle m_3\rangle \, \widetilde{\Phi}_3 + \langle m_1\rangle \, \widetilde{\Phi}_1 + \langle m_2\rangle \, \widetilde{\Phi}_2 + \langle m_3\rangle \, \widetilde{\Phi}_3 \neq \left[^{(t1)}\langle\Phi\rangle\right] =$
$= \langle m_1\rangle \, \widetilde{\Phi}_1 + \langle m_2\rangle \, \widetilde{\Phi}_2 + \langle m_3\rangle \, \widetilde{\Phi}_3$.

Still, let's just start with the morphology $(1-2-3)$

$$\sigma^*_{\shortparallel 3(123)} = \left[\sigma_1 \langle\nabla\Phi\rangle_1 + \sigma_2 \langle\nabla\Phi\rangle_2 + \sigma_3 \langle\nabla\Phi\rangle_3\right] / \langle\nabla\Phi\rangle =$$

$$= \Bigg(\sigma_1 \langle m_1\rangle \nabla\widetilde{\Phi}_1 + \sigma_2 \langle m_2\rangle \nabla\widetilde{\Phi}_2 + \sigma_3 \langle m_3\rangle \nabla\widetilde{\Phi}_3 +$$

$$+ (\sigma_1-\sigma_2)\frac{1}{\Delta\Omega}\int\limits_{\partial S_{12}} \Phi_1 d\vec{s}_1 + (\sigma_1-\sigma_3)\frac{1}{\Delta\Omega}\int\limits_{\partial S_{13}} \Phi_1 d\vec{s}_1 +$$

$$+ (\sigma_2-\sigma_3)\frac{1}{\Delta\Omega}\int\limits_{\partial S_{23}} \Phi_2 d\vec{s}_2\Bigg)$$

$$/ \left(\langle m_1\rangle \nabla\widetilde{\Phi}_1 + \langle m_2\rangle \nabla\widetilde{\Phi}_2 + \langle m_3\rangle \nabla\widetilde{\Phi}_3\right), \qquad (28)$$

because in the denominator

$$\frac{1}{\Delta\Omega}\int\limits_{\partial S_{12}} \Phi_1 d\vec{s}_1 + \frac{1}{\Delta\Omega}\int\limits_{\partial S_{13}} \Phi_1 d\vec{s}_1 + \frac{1}{\Delta\Omega}\int\limits_{\partial S_{12}} \Phi_2 d\vec{s}_2 +$$

$$+ \frac{1}{\Delta\Omega}\int\limits_{\partial S_{23}} \Phi_2 d\vec{s}_2 + \frac{1}{\Delta\Omega}\int\limits_{\partial S_{13}} \Phi_3 d\vec{s}_3 + \frac{1}{\Delta\Omega}\int\limits_{\partial S_{23}} \Phi_3 d\vec{s}_3\Bigg) = 0.$$

The sum of these integrals should be equal to zero. Thus, for 3 layers even the potential equilibrium constrain won't help to eliminate the interface surface potential integrals indicating that the charge traversing the medium via the surface is the part of the effective conductivity. And only when conductivities $\sigma_2 \cong \sigma_3$ then the approximation

$$\sigma^*_{\shortparallel 3} \cong \sum_{i=1} \langle m_i \rangle \sigma_i, \ i = 1, 2, 3, \tag{29}$$

can be used along with the potential equilibrium constrain. When more than 3 phases are participating in the charge transfer then the general approach outlined above should apply. The 4 phase effective coefficient would be calculated using the formula (when homogeneous morphology conditions are in force, meaning that medium is periodic with the only one period of sublayers arrangement)

$$\sigma^*_{\shortparallel 4} = \Big(\sigma_1 \langle m_1 \rangle \nabla\widetilde{\Phi}_1 + \sigma_2 \langle m_2 \rangle \nabla\widetilde{\Phi}_2 + \sigma_3 \langle \nabla\Phi \rangle_3 + \sigma_4 \langle \nabla\Phi \rangle_4$$

$$+ (\sigma_1 - \sigma_2) \frac{1}{\Delta\Omega} \int\limits_{\partial S_{12}} \Phi_1 \vec{ds}_1 + (\sigma_1 - \sigma_3) \frac{1}{\Delta\Omega} \int\limits_{\partial S_{13}} \Phi_1 \vec{ds}_1 +$$

$$+ (\sigma_1 - \sigma_4) \frac{1}{\Delta\Omega} \int\limits_{\partial S_{14}} \Phi_1 \vec{ds}_1 + (\sigma_2 - \sigma_3) \frac{1}{\Delta\Omega} \int\limits_{\partial S_{23}} \Phi_2 \vec{ds}_2 +$$

$$+ (\sigma_2 - \sigma_4) \frac{1}{\Delta\Omega} \int\limits_{\partial S_{24}} \Phi_2 \vec{ds}_2 + (\sigma_3 - \sigma_4) \frac{1}{\Delta\Omega} \int\limits_{\partial S_{34}} \Phi_3 \vec{ds}_3 \Big)$$

$$/ \Big(\langle m_1 \rangle \nabla\widetilde{\Phi}_1 + \langle m_2 \rangle \nabla\widetilde{\Phi}_2 + \langle m_3 \rangle \nabla\widetilde{\Phi}_3 + \langle m_4 \rangle \nabla\widetilde{\Phi}_4 \Big). \tag{30}$$

When electrical field applied perpendicular to the boundary surfaces of stack of parallel sublayers, and when two alternating kind of plates present the medium, then the effective (bulk) electric conductivity is (Figs. 3-4)

$$\sigma^*_{\perp 2} = \left[\sigma_1 \langle \nabla\Phi(x) \rangle_1 + \sigma_2 \langle \nabla\Phi(x) \rangle_2\right] / \langle \nabla\Phi(x) \rangle =$$

$$= \Big[\sigma_1 \nabla \Big(\langle m_1 \rangle \widetilde{\Phi}_1\Big) + \sigma_2 \nabla \Big(\langle m_2 \rangle \widetilde{\Phi}_2\Big) +$$

$$+ (\sigma_2 - \sigma_1) \frac{1}{\Delta\Omega} \int\limits_{\partial S_{12}} \Phi_2 \vec{ds}_2 \Big] /$$

$$/ \Big(\langle m_1 \rangle \nabla\widetilde{\Phi}_1(x) + \langle m_2 \rangle \nabla\widetilde{\Phi}_2(x) \Big). \tag{31}$$

As one can see that in this morphology the only one coordinate argument is used. The key element to obtain the simplified formula used in textbooks, is the recognition that the traversing charge flux at steady state conditions is the same for both phases $\sigma_1 \nabla\Phi_1 = \sigma_2 \nabla\Phi_2$. That formula may be used for substitution as $\nabla\Phi_2 = (\sigma_1/\sigma_2) \nabla\Phi_1$, and **the specific assumption for this morphology** is that the averaged variables can be used in this equality (meaning that $\sigma_1 \nabla\widetilde{\Phi}_1 = \sigma_2 \nabla\widetilde{\Phi}_2$), then following the above precaution remarks one can get for this morphology

$$\sigma^*_{\perp 2} = \Big[(\langle m_1 \rangle + \langle m_2 \rangle) \sigma_1 \nabla\widetilde{\Phi}_1\Big] /$$

$$\Big[(\langle m_1 \rangle + (\sigma_1/\sigma_2) \langle m_2 \rangle) \nabla\widetilde{\Phi}_1\Big] =$$

$$= \left[(\langle m_1 \rangle + \langle m_2 \rangle) \sigma_1\right] / \left[\left(\frac{\langle m_1 \rangle}{\sigma_1} + \frac{\langle m_2 \rangle}{\sigma_2}\right) \sigma_1\right] =$$

$$= \left[\sum_{i=1} \frac{\langle m_i \rangle}{\sigma_i}\right]^{-1}, i = 1, 2, \tag{32}$$

because if the values $\Phi_2(\partial S_{12})$ on both surfaces can be very close then the term

$$(\sigma_2 - \sigma_1) \frac{1}{\Delta\Omega} \int\limits_{\partial S_{12}} \Phi_2 \vec{ds}_2 \ \cong 0. \tag{33}$$

The integral term (33) is never shown up in the homogeneous heat transfer treatment of this problem. It is instrumental to note here that the assumption $\sigma_1 \nabla\widetilde{\Phi}_1 = \sigma_2 \nabla\widetilde{\Phi}_2$ **is generally not correct -** some of the reasons are evident when we recognize the lower scales phenomena see, for example, some of them in Figs. 3-4, but

$$\sigma_1 \langle \nabla \Phi (x) \rangle_1 = \sigma_2 \langle \nabla \Phi (x) \rangle_2 ,$$

is correct. More complicated cases when number of phases are more than 2 and interface transport includes the longitudinal component should be the subject of similar study.

CONCLUSIONS

This work presents a new approach for the modeling of layered superstructures and possibilities for design. The theoretical proof of direct dependencies between the morphology of the medium and the transport equations on two scales have been presented. They were strictly derived and compared for macroscale transport for canonical morphologies. 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.

Effective coefficient VAT models as for conductivities, dielectric permittivity, magnetic permeability, and reflection coefficient are done at present time on the basis of homogeneous medium governing equations. The models for coefficients constructed on the basis of homogeneous medium provisions do not reflect the most influencial and dominant physical phenomena in the heterogeneous media, as - polarizations, microscale heterogeneities, interface demagnitization microfields, domain walls collective as well as individual behavior, interplay of different effects etc.

Those described features are the part of the VAT physical and mathematical formulations of problem. Different methods of calculating complex effective coefficients as conductivity or permittivity of heterogeneous media are used right now, as: composite approximation, Bergman-Milton theory, Grain Consolidation Model, local porosity theory, etc. The VAT present the possibility to form the basics of methodology for thermal transport, fluid mechanics, and electrodynamics experimental data reduction for porous and heterogeneous media. Few heterogeneous media experimental approaches in thermal physics, fluid mechanics and electrodynamics, started analysis based on the VAT tools are just having few initial steps (Ponomarenko et al., 1999a,b; Ryvkina et al., 1998,1999; Travkin et al., 2001a,b).

Accurate evaluation of various kinds of medium morphology irregularities results from the modeling methodology once a heterogeneous medium morphology is chosen. An attempt was made to address classical morphologies with irregularities associated with different specific kinds of scale morphology and to quantify the impact of morphology on the mathematical forms of the electrostatic and transient effective coefficients in VAT governing equations in addition to the impact on the modeling results.

As it appears due to application of VAT models the issue of effective coefficients in heterogeneous media is multivariant. Unlike in homogeneous medium, there are few coefficients can be derived for heterogeneous medium transport coefficients which have effective characteristics. This should find a way to the design and modeling of experiments in heterogeneous media.

Acknowledgment

This work was sponsored by the Department of Energy, Office of Basic Energy Sciences through the grant DE-FG03-89ER14033 A002.

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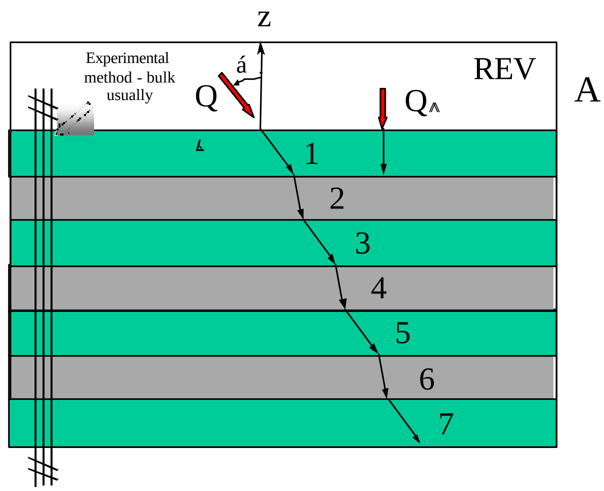

Fig. 1 Layered regular 1D medium (2 different component layers) lower

scale flux flow with perfect interface conductance

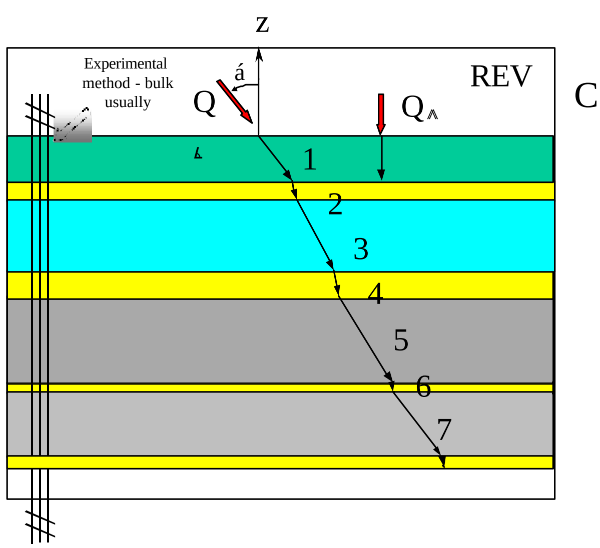

Fig. 2 Layered irregular 1D medium (n different component layers) lower scale flux flow with perfect interface conductance

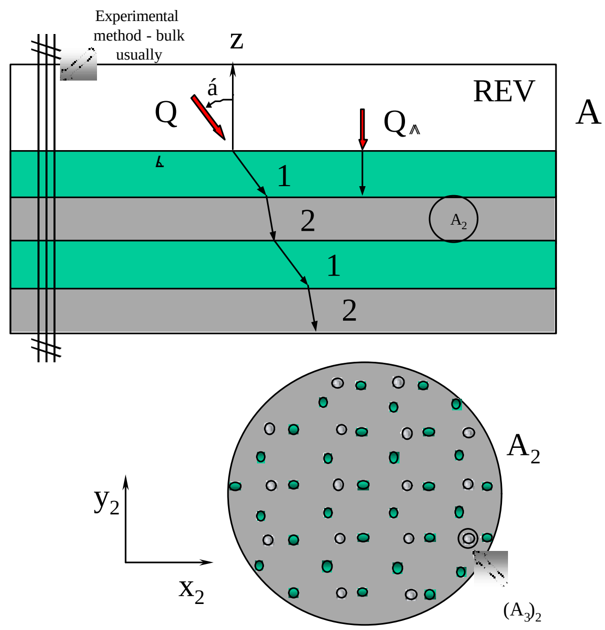

Fig. 3 Layered regular 1D medium (2 different component layers) lower scale flux flow with the second layer globulars of 3 kinds of amorphous substances (2 gradient and 1 isotropic phases)

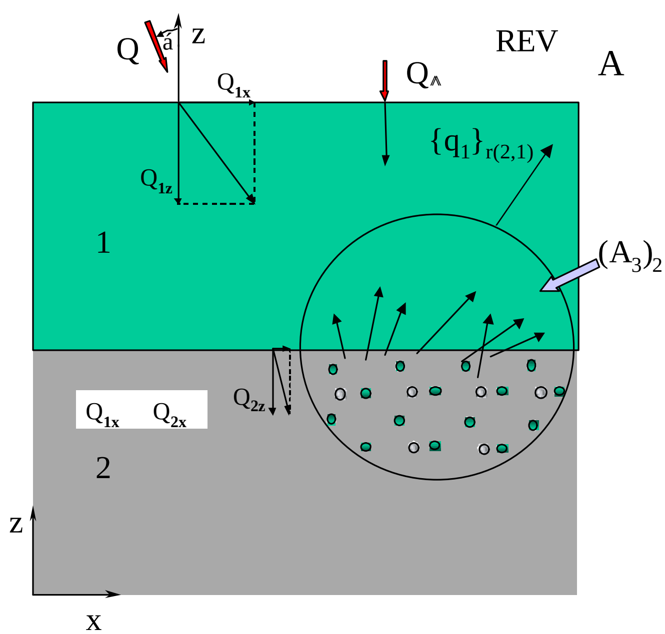

Fig. 4 The 3rd lower scale averaged EM field $\{q_1\}_{r21}$ reflected from the interface between the second and first layer