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Macroscopic modelling of multiperiodic composites

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Abstract By a multiperiodic composite we mean a composite solid in which all constituents are periodically distributed in a matrix but a representative element (unit cell) may not exist. The aim of this Note is to propose a nonasymptotic approach to the formation of averaged (macroscopic) models of multiperiodic composites. The approach is based on the concept of tolerance averaging, which in [2] was applied to the modelling of periodic composites. The derived model, in contrast to homogenization, describes the effect of microstructure size on the overall solid behaviour and yields necessary conditions for the physical correctness of solutions to special problems. ***To cite this article: C. Woźniak, C. R. Mecanique 330 (2002) 267–272.*** © 2002 Académie des sciences/Éditions scientifiques et médicales Elsevier SAS

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Modélisation macroscopique des composites multipériodiques

Résumé Nous définissons un composite multipériodique comme un solide composite dont tous les constituants sont distribués périodiquement dans l'espace et forment une matrice, mais dans lequel on peut constater l'absence d'un élément représentatif (c'est-à-dire, d'une cellule élémentaire). Le but de cette Note est de proposer une approche non-asymptotique à la formation des modèles moyennisés (macroscopiques) de tels composites multipériodiques. Notre méthode est basée sur le concept de moyennisation de tolérance, appliquée déjà dans [2] pour modélisation des composites périodiques. Le modèle que nous proposons décrit, contrairement à la méthode d'homogénéisation, l'effet de la taille des microstructures sur le comportement du solide dans son ensemble, et fournit les conditions nécessaires assurant la justesse de certaines solutions spécifiques du point de vue physique. ***Pour citer cet article : C. Woźniak, C. R. Mecanique 330 (2002) 267–272.*** © 2002 Académie des sciences/Éditions scientifiques et médicales Elsevier SAS

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1. Preliminaries

Let $\Lambda = (L_1, \ldots, L_n)$, where $L_\alpha = (l_\alpha^1, \ldots, l_\alpha^{m_\alpha})$, $\alpha = 1, \ldots, n$, are m_α-tuples of real numbers such that $l_\alpha^1 > l_\alpha^2 > \cdots > l_\alpha^{m_\alpha} > 0$. A function $\psi(x_1, \ldots, x_n)$ defined in R^n, will be called L_α-periodic if: (1) there exists function $\bar{\psi}_\alpha(x_1, \ldots, \bar{\boldsymbol{x}}_\alpha, \ldots, x_n)$, $\bar{\boldsymbol{x}}_\alpha = (\bar{x}_\alpha^1, \ldots, \bar{x}_\alpha^{m_\alpha})$; defined in $\mathbb{R}^{n+m_\alpha-1}$, which has periods l_α^a, with respect to $\bar{x}_\alpha^a$, $a = 1, \ldots, m_\alpha$; (2) The condition $\bar{\psi}_\alpha(x_1, \ldots, \bar{x}_\alpha, \ldots, x_n) = \psi(x_1, \ldots, x_n)$ holds for $\bar{x}_\alpha^1 = \bar{x}_\alpha^2 = \cdots = \bar{x}_\alpha^{m_\alpha} = x_\alpha$ in the whole domain of $\psi(\cdot)$. A function $\psi(\cdot)$ will be referred to as Λ-periodic if is L_α-periodic with respect to every argument $x_\alpha, \alpha = 1, \ldots, n$. If $m_\alpha = 1$ for $\alpha = 1, \ldots, n$ then the

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Λ-periodic function $\psi(x_1,\dots,x_n)$ becomes periodic (with periods l_α^1 related to x_α); otherwise it will be called multiperiodic.

For an arbitrary integrable multiperiodic function $\psi(x_1,\dots,x_n)$ we shall define function $\langle\psi\rangle_\alpha(\cdot)$, which is independent of x_α, by means of the formula

$$\langle\psi\rangle_\alpha = \frac{1}{l_\alpha^1\cdots l_\alpha^{m_\alpha}}\int_0^{l_\alpha^1}\cdots\int_0^{l_\alpha^{m_\alpha}} \bar{\psi}_\alpha(x_1,\dots,\bar{x}_\alpha,\dots,x_n)\,\mathrm{d}\bar{x}_\alpha^1\cdots\mathrm{d}\bar{x}_\alpha^{m_\alpha}$$

where $\bar{\boldsymbol{x}}_\alpha = (\bar{x}_\alpha^1,\dots,\bar{x}_\alpha^{m_\alpha})$. The real number $\langle\psi\rangle$, given by:

$$\langle\psi\rangle = \langle\cdots\langle\langle\psi\rangle_1\rangle_2\cdots\rangle_n \tag{1.1}$$

will be called the averaged value of $\psi(\cdot)$. For a periodic function ψ formula (1.1) represents the well known mean value of ψ.

In the subsequent considerations $n=3$ (hence $\Lambda=(L_1,L_2,L_3)$) and x_1,x_2,x_3 stand for the orthogonal Cartesian coordinates of points $\boldsymbol{x}$ in the physical space E^3. By Ω we denote a region in E^3 occupied by the composite solid under consideration. We assume that: (1) all material properties of a solid are described by multiperiodic functions related to a certain Λ; (2) the maximum period $l=\max\{l_1^1,l_2^1,l_3^1\}$ is very small when compared with the smallest characteristic length dimension L_Ω of Ω. Under these conditions a composite solid will be referred to as multiperiodic. Plane fragments of two multiperiodic solids are shown in Fig. 1, where $L_1=(l_1^1,l_1^2)$, $L_2=l_2$.

If for every period l_α^a, $\alpha=1,2,3$ (related to a certain Λ) there exists a positive integer k_α^a such that $k_\alpha^a l_\alpha^a = l_\alpha$ for some $l_\alpha>0$ (no summation) then the parellelepided $(-l_1/2,l_1/2)\times(-l_2/2,l_2/2)\times(-l_3/2,l_3/2)$ can be taken as a unit (representative) cell of the periodic structure of the solid. However, for some multiperiodic solids the length dimensions l_α of a unit cell may be not small when compared with L_Ω. This is the motivation for modelling the multiperiodic solids without using the concept of the unit cell.

Throughout the note symbols $\cdot$ and ∇ stand for the scalar product and the gradient, respectively. Superscripts A, B run over $1,\dots,N$, summation convention holds. We also denote $\Delta=(-l_1^1/2,l_1^1/2)\times$

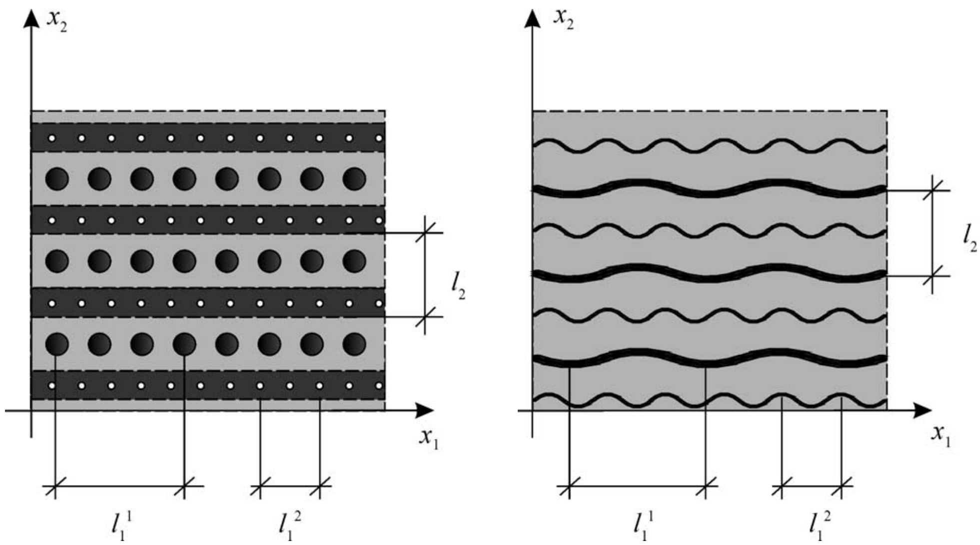

Figure 1. Cross sections of composite materials with a double period along x_1-axis.

$(-l_2^1/2, l_2^1/2) \times (-l_3^1/2, l_3^1/2)$ (in general Δ is not a unit cell!), $\Delta(\boldsymbol{x}) = \boldsymbol{x} + \Delta$, $\Omega_\Delta = \{\boldsymbol{x} \in \Omega : \Delta(\boldsymbol{x}) \subset \Omega\}$ and $l_\Delta = \sqrt{(l_1^1)^2 + (l_2^1)^2 + (l_3^1)^2}$, where l_Δ is referred to as the microstructure length, $l_\Delta \ll L_\Omega$.

2. Formulation of the problem

The behaviour of multiperiodic composites is described by differential equations with functional coefficients which are multiperiodic and non-continuous. The problem we are going to solve is *how to derive an approximate mathematical model of multiperiodic composites which is represented by differential equation with constant coefficients* (a macroscopic model). For the reasons explained in Section 1, in the course of modelling, we shall not use the concept of the unit cell.

Macroscopic models of multiperiodic composites can be formulated by the reiterated homogenization, cf. [1], p. 96, under the assumption that the periods l_α^a, $a = 1, \ldots, m_\alpha$ can be treated as quantities of the different orders. In this Note we derive a macroscopic model of a multiperiodic composite without the above assumption. To this end we shall adapt the tolerance averaging method which in [2] was used for periodic composites. This nonasymptotic method, in contrast to homogenization, leads to equations which describe the effect of microstructure size on a macroscopic behaviour of a composite and yields some *a posteriori* conditions necessary for the physical correctness of solutions to special problems.

3. Foundations

To make this note self-consistent, following [2], we outline in this section some mathematical concepts, lemmas and corollaries which constitute the mathematical background of the modelling procedure applied in Section 4.

We begin with the concept of the tolerance space [3]. The simplest example of this space is a pair $(R, \approx)$ where $\approx$ is a tolerance on R, i.e., a symmetric and reflexive binary relation in R which is not transitive. Subsequently, every tolerance will be determined by what is called a tolerance parameter $\varepsilon > 0$ such that $(\forall a, b \in R)\ [a \approx^\varepsilon b \Leftrightarrow |a - b| \leqslant \varepsilon]$. We shall assume that every $\approx^\varepsilon$ can be interpreted as an indiscernibility relation; it means that R is endowed with a certain unit measure and if $a \approx^\varepsilon b$ then the values a and b of a pertinent physical quantity cannot be discerned in the problem under consideration. Roughly speaking, a tolerance parameter ε is some positive constant, which depends either on the degree of refinement of the instruments which have been used for performing the measurements, [4], or on the accuracy of performed calculations. By a tolerance system we understand a pair $(F(\overline{\Omega}), \varepsilon(\cdot))$, where $F(\overline{\Omega})$ is a set of functions and their derivatives in the problem under consideration (including also time derivatives for the time dependent functions) and $\varepsilon : F(\overline{\Omega}) \ni f \to \varepsilon(f)$ is a mapping which assignes to every f a certain tolerance parameter $\varepsilon(f)$. Subsequently we shall assume that a certain tolerance system $(F(\overline{\Omega}), \varepsilon(\cdot))$ and the microstructure length l_Δ are known and we denote $T = ((F(\overline{\Omega}), \varepsilon(\cdot)), l_\Delta)$.

Let Df stand for a function $f \in F(\overline{\Omega})$ as well as for any partial derivative of f which belong to $F(\overline{\Omega})$. Function $\psi \in F(\overline{\Omega})$ will be called *slowly varying* (with respect to T), $\psi \in \mathrm{SV}(T)$, if for every $D\psi$ and every $\boldsymbol{x}_1, \boldsymbol{x}_2 \in \Omega$ condition $\|\boldsymbol{x}_1 - \boldsymbol{x}_2\| \leqslant l_\Delta$ implies $D\psi(\boldsymbol{x}_1) \approx^\varepsilon D\psi(\boldsymbol{x}_2)$ where $\varepsilon = \varepsilon(D\psi)$. Function $\varphi \in F(\overline{\Omega})$ will be termed *periodic-like* (with respect to T), $\varphi \in \mathrm{PL}(T)$, if for every $D\varphi$ and every $\boldsymbol{x} \in \Omega_\Delta$ there exists a Λ-periodic function $(D\varphi)_{\boldsymbol{x}}$ such that for every $\boldsymbol{y}$ from the domain of φ condition $\|\boldsymbol{x} - \boldsymbol{y}\| \leqslant l_\Delta$ implies $(D\varphi)_{\boldsymbol{x}}(\boldsymbol{y}) \approx^\varepsilon D\varphi(\boldsymbol{y})$ where $\varepsilon = \varepsilon(D\varphi)$; function $(D\varphi)_{\boldsymbol{x}}(\cdot)$ will be referred to as *a Λ-periodic approximation* of $D\varphi(\cdot)$ in $\overline{\Delta}(\boldsymbol{x})$. A periodic-like function φ will be called *oscillating* (with the weight ρ where ρ is a positive Λ-periodic function), $\varphi \in \mathrm{PL}^\rho(T)$, if $\langle \rho \varphi_{\boldsymbol{x}} \rangle = 0$ for every $\boldsymbol{x} \in \Omega_\Delta$.

The following lemmas are used in the subsequent considerations.

(L1) If $\varphi = \mathrm{PL}^\rho(T)$ then for every Λ-periodic positive function ρ there exists a decomposition $\varphi = \varphi^0 + \varphi^*$ where $\varphi^0 \in \mathrm{SV}(T)$ and $\varphi^* = \mathrm{PL}^\rho(T)$.

(L2) If $\psi^A \in \mathrm{SV}(T)$ and h^A are Λ-periodic functions then $\psi^A h^A \in \mathrm{PL}(T)$.

(L3) If $\psi \in \mathrm{SV}(T) \cap C^1(\overline{\Omega})$ then $l_\Delta|\partial\psi| \leqslant \varepsilon(\psi) + l_\Delta\varepsilon(\partial\psi)$ where $\partial\psi$ stand for an arbitrary partial derivative of ψ.

We close this section with the following corollaries:

(C1) If $\psi \in \mathrm{SV}_\Delta(T)$ and every $D\psi \in F(\overline{\Omega})$ is a continuous function then

$$D\psi(\boldsymbol{y}) \approx^{\varepsilon} D\psi(\boldsymbol{x}) \quad \text{for } \varepsilon = \varepsilon(D\psi) \tag{3.1}$$

holds for every $\boldsymbol{x} \in \Omega_\Delta$ and $\boldsymbol{y} \in \Delta(\boldsymbol{x})$.

(C2) If $\varphi \in \mathrm{PL}(T)$ and every $D\varphi \in F(\overline{\Omega})$ is a piecewise continuous function then

$$D\varphi(\boldsymbol{y}) \approx^{\varepsilon} (D\varphi)_{\boldsymbol{x}}(\boldsymbol{y}) \quad \text{for } \varepsilon = \varepsilon(D\varphi) \tag{3.2}$$

holds for every $\boldsymbol{x} \in \Omega_\Delta$ and $\boldsymbol{y} \in \Delta(\boldsymbol{x}) \cap \mathrm{Dom}\, D\varphi$.

(C3) If $\psi \in \mathrm{SV}(T) \cap C^1(\overline{\Omega})$ and ϑ is Λ-periodic smooth function then

$$\nabla(\vartheta\psi)(\boldsymbol{y}) \approx^{\varepsilon} \nabla\vartheta(\boldsymbol{y})\psi(\boldsymbol{y}) \quad \text{for} \quad \varepsilon = \big(\varepsilon(\psi) + l_\Delta\varepsilon(\nabla\psi)\big)\big|\vartheta(\boldsymbol{y})\big|l_\Delta^{-1} \tag{3.3}$$

holds for every $\boldsymbol{y} \in \Omega$.

For the proofs of lemmas (L1)–(L3) and a discussion of corollaries, see [2].

4. Tolerance modelling

The macroscopic (tolerance) modelling of multiperiodic composites, which was applied in [2] to periodic composites, will be based on two assumptions.

CONFORMABILITY ASSUMPTION (CA). – Every unknown field $\varphi(\cdot)$ in equations describing the behaviour of a multiperiodic composite has to conform to the Λ-periodic structure of this composite; it means that the relation

$$\varphi(\cdot, t) \in \mathrm{PL}(T) \tag{4.1}$$

has to hold for every time t and for some tolerance system.

TOLERANCE APPROXIMATION ASSUMPTION (TAA). – In the course of macroscopic modelling the left-hand sides of formulae (3.1)–(3.3) will be approximated by their right-hand sides.

In the subsequent part of this section we shall illustrate the tolerance modelling on the example of the heat conduction equation

$$\nabla \cdot (\boldsymbol{A} \cdot \nabla\theta) - c\dot{\theta} = g \tag{4.2}$$

which has to hold in Ω for every time t. Here $\theta(\cdot)$ is a temperature field, $\boldsymbol{A} = \boldsymbol{A}(\cdot)$ is the second order heat conduction tensor field, $c = c(\cdot)$ is the specific heat field and g is the heat source field. For multiperiodic composites $\boldsymbol{A}(\cdot), c(\cdot)$ are the known Λ-periodic functions. To simplify the analysis we assume that all aforementioned fields satisfy smoothness conditions required in the subsequent considerations. From CA we obtain $\theta(\cdot, t) \in \mathrm{PL}(T)$ and by means of (L1) the decomposition $\theta = \theta^0 + \theta^*$ takes place, where $\theta^0(\cdot, t) \in \mathrm{SV}(T)$ and $\theta^*(\cdot, t) \in \mathrm{PL}^c(T)$ are referred to as the macroscopic and fluctuating parts of $\theta(\cdot, t)$, respectively. We also assume that $g(\cdot, t) \in \mathrm{PL}(T)$ and hence $g = g^0 + g^*$ where $g^0 \in \mathrm{SV}(T)$, $g^* \in \mathrm{PL}^c(T)$. Subsequently we shall restrict the domain of functions in (4.2) to $\overline{\Delta}(\boldsymbol{x})$ for some $\boldsymbol{x} \in \Omega_\Delta$.

Tolerance modelling can be divided into four steps.

1. We formulate the variational equation for $\theta^*_{\boldsymbol{x}}$. To this end we substitute $\theta = \theta^0(\boldsymbol{y}, t) + \theta^*_{\boldsymbol{x}}(\boldsymbol{y}, t)$, $\boldsymbol{y} \in \overline{\Delta}(x)$, into (4.2) and multiply both sides of (4.2) by a Λ-periodic test function $\vartheta \in C^1(\overline{\Omega})$ satisfying conditions $\langle c\vartheta\rangle = 0$, $\vartheta(\boldsymbol{x}) \in \mathcal{O}(l_\Delta), l_\Delta\nabla\vartheta(\boldsymbol{x}) \in \mathcal{O}(l_\Delta)$. Using (3.1), (3.3) and applying TAA, after

averaging the resulting equation by means of (1.1) and some manipulations, we obtain the following variational equation for $\theta^*_{\boldsymbol{x}}$:

$$\langle \nabla\vartheta \cdot \boldsymbol{A} \cdot \nabla\theta^*_{\boldsymbol{x}} \rangle + \langle c\vartheta\dot{\theta}^*_{\boldsymbol{x}} \rangle = -\langle \nabla\vartheta \cdot \boldsymbol{A} \rangle \cdot \nabla\theta^0(\boldsymbol{x}, t) - \langle \vartheta \rangle g^0(\boldsymbol{x}, t) - \langle \vartheta g^*_{\boldsymbol{x}} \rangle \tag{4.3}$$

where $\langle c\theta^*_{\boldsymbol{x}} \rangle = 0$. The boundary conditions related to (4.3) reduce to the periodic conditions and are identically satisfied. Variational equation (4.3) has to hold for every test function ϑ; let us observe that $\boldsymbol{x} \in \Omega_\Delta$ can be treated as a parameter in (4.3).

2. We look for the approximate solution to (4.3) in the form:

$$\theta^*_{\boldsymbol{x}}(\boldsymbol{y}, t) = h^A(\boldsymbol{y})V^A(\boldsymbol{x}, t), \quad \boldsymbol{y} \in \Delta(\boldsymbol{x}),\ \boldsymbol{x} \in \Omega_\Delta \tag{4.4}$$

where $V^A(\boldsymbol{x}, t)$ are unknowns and $h^A(\cdot)$ are postulated *a priori* Λ-periodic shape functions satisfying conditions: $\langle h^A c \rangle = 0$, $h^A(\boldsymbol{x}) \in \mathcal{O}(l_\Delta)$, $l_\Delta \nabla h^A(\boldsymbol{x}) \in \mathcal{O}(l_\Delta)$. We also assume that $N \times N$ matrices of elements $\langle ch^A h^B \rangle$, $\langle \nabla h^B \cdot \boldsymbol{A} \cdot \nabla h^A \rangle$ are positive definite. Substituting the right-hand sides of (4.4) into (4.3) and setting $\vartheta = h^B$, $B = 1, \ldots, N$, we arrive at the system of N ordinary differential equations for V^A:

$$\begin{aligned} &\langle ch^A h^B \rangle \dot{V}^A(\boldsymbol{x}, t) + \langle \nabla h^B \cdot \boldsymbol{A} \cdot \nabla h^A \rangle V^A(\boldsymbol{x}, t) + \langle \nabla h^B \cdot \boldsymbol{A} \rangle \cdot \nabla\theta^0(\boldsymbol{x}, t) \\ &\quad + \langle h^B \rangle g^0(\boldsymbol{x}, t) + \langle h^B g^*_{\boldsymbol{x}} \rangle = 0,\ B = 1, \ldots, N \end{aligned} \tag{4.5}$$

3. From the decomposition $\theta = \theta^0 + \theta^*$ and (L2), taking into account the approximation (4.4), we conclude that $V^A(\cdot, t) \in \mathrm{SV}(T)$. By means of (3.1) and TAA we arrive at the following formula for the temperature field

$$\theta(\boldsymbol{y}, t) = \theta^0(\boldsymbol{y}, t) + h^A(\boldsymbol{y})V^A(\boldsymbol{y}, t), \quad \boldsymbol{y} \in \Omega \tag{4.6}$$

4. We substitute the right-hand side of (4.6) into (4.2). Restricting the domain of functions in (4.2) to $\overline{\Delta}(\boldsymbol{x})$, using (3.1) and TAA, after averaging the resulting equation by means of (2.2), we obtain the partial differential equation for θ^0:

$$\nabla \cdot \left(\langle \boldsymbol{A} \rangle \cdot \nabla\theta^0 + \left\langle \boldsymbol{A} \cdot \nabla h^A \right\rangle V^A \right) - \langle c \rangle \dot{\theta}^0 = g^0 \tag{4.7}$$

Eqs. (4.5), (4.7) for unknowns $\theta^0(\boldsymbol{x}, t)$, $V^A(\boldsymbol{x}, t)$, $A = 1, \ldots, N$, have constant coefficients and hold for every $\boldsymbol{x} \in \Omega_\Delta$ and every time t. These equations together with formula (4.6) and conditions

$$\theta^0(\cdot, t) \in \mathrm{SV}(T), \qquad V^A(\cdot, t) \in \mathrm{SV}(T) \tag{4.8}$$

represent *a macroscopic model for the heat conduction in a multiperiodic composite.* Thus, the problem formulated in Section 2 has been solved for the linear heat conduction. However, the above tolerance modelling can be also applied to any other problem described by equations of mathematical physics with Λ-periodic coefficients.

5. Conclusions

We close this Note with a summary of some new results and information on the macroscopic modelling of composite materials.

1° The derived model describes the heat conduction in a multiperiodic composite and takes into account the effect of microstructure size on the overall composite behaviour. This effect is described by coefficients $\langle ch^A h^B \rangle \in \varnothing(l^2_\Delta)$ in Eqs. (4.5).

2° Neglecting in (4.5) terms with coefficients $\langle ch^A h^B \rangle$, $\langle h^B \rangle$ and $\langle h^B g^*_{\boldsymbol{x}} \rangle$ of an order $\mathcal{O}(l_\Delta)$ we can eliminate unknowns V^A from (4.7) and hence derive equation $\nabla \cdot (\tilde{A} \cdot \nabla\theta^0) - \langle c \rangle \dot{\theta} = g^0$ where $\tilde{A}$ can be treated as an approximate value (due to the approximation (4.4)) of the effective heat conduction tensor for a multiperiodic composite.

3° The proposed model includes conditions (4.8) which are necessary for the physical correctness of solutions θ^0, V^A to the BVP for Eqs. (4.5), (4.7) and can be used as *a posteriori* estimates of accuracy of these solutions [2].

4° In contrast to the reiterated homogenization the obtained model equations make it possible to analyze problems of multiperiodic composites without any restrictions imposed on the length of periods.

5° The main drawback of the proposed approach lies in a proper choice of approximate solutions (4.4) to the Λ-periodic variational problem (4.3) which can lead to a large number N of unknowns V^A.

For periodic composites the obtained results reduce to those given in [2]. An example of the application of the proposed modelling approach to some special problems will be given in a subsequent note.

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