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ON THE MODELLING OF HYPERBOLIC HEAT CONDUCTION PROBLEMS IN PERIODIC LATTICE STRUCTURES*

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Abstract. A new modelling approach to the hyperbolic heat conduction problems in periodic lattice structures of an arbitrary form is discussed. Taking into account the results obtained in [5] we introduce a special description of the periodic lattice geometry which leads to the heat conduction model governed by the system of finite difference equations. The continuum models are derived from the finite difference equations by using the principle of stationary action.

1. Introduction

It is well known that the direct approach to the non-stationary heat conduction or dynamic problems for dense periodic lattice systems leads to the computational difficulties due to a large number of ordinary differential equations describing the problem under consideration. That is why the main attention in mathematical modelling of periodic structures is focused on the formulation of averaged continuum models. This approach is based either on certain heuristic assumptions and smoothness operations or on the asymptotic homogenisation procedures [2, 6]. The main drawback of homogenized models is that in the course of modelling the effect of the unit cell size on the global behaviour of lattice structure is neglected. More sophisticated modelling approach is based on the concept of the tolerance related to the accuracy of measured or calculated values of physical fields [10]. This method, referred to as the tolerance averaging technique, leads to a certain periodic cell problem which involves terms depending also on the period lengths. The application of the tolerance averaging method to the analysis of special engineering problems can be found in [10, 11]. Both the homogenisation and the tolerance averaging technique are restricted to the problems in which fluctuactions of basic fields (like temperature or displacement) are periodic-like functions [10]. More general modelling technique which does not contain this requirement was recently proposed in [3, 4, 8], where the continuum averaged models are derived from certain discrete models (by assuming that the typical macroscopic wavelength is sufficiently large when compared to the period lengths) of analysed periodic structures.

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The aim of this contribution is to outline a new modelling approach to the hyperbolic heat conduction problems in periodic lattice structures of an arbitrary form. To this end the Cattaneo constitutive heat conduction equation is taken as the physical basis of analysis.

Notations. Small and capital bold face characters stand for vectors and second order tensors in 3D-space, respectively. Indices a, b, run over 1,..., n while A,B and K over 0,1,..., M and 1,..., N, respectively. The summation convention holds for all the indices repeated twice (unless otherwise stated). Symbol t stands for a time coordinate.

2. Preliminaries

We begin this paper with some preliminary concepts which have been introduced in [5]. In order to describe geometry of an arbitrary periodic lattice structure we introduce the Bravais lattice Λ in the physical space E^3 with the base vectors $\mathbf{d}_1, \mathbf{d}_2, \mathbf{d}_3$. Hence

$$\Lambda = \left\{ \mathbf{z} \in E^3 : \mathbf{z} = \eta_1 \mathbf{d}_1 + \eta_2 \mathbf{d}_2 + \eta_3 \mathbf{d}_3, \ \eta_i = 0, \pm 1, \pm 2, ..., \ i = 1, 2, 3 \right\}$$

For every subset Ξ (point p) in E^3 and for every $\mathbf{z} \in \Lambda$ we define $\Xi(\mathbf{z}) \equiv \Xi + \mathbf{z}$ and $\mathbf{p}(\mathbf{z}) \equiv \mathbf{p} + \mathbf{z}$, respectively. Let Δ be the parallelepiped spanned on vectors $\mathbf{d}_1, \mathbf{d}_2, \mathbf{d}_3$, with a center at point **0** and \mathbf{p}^a , a = 1, ..., n, be the system of points in Δ . Hence $P := \{\mathbf{p}^a(\mathbf{z}): a = 1, ..., n, \mathbf{z} \in \Lambda\}$ represents the periodic system of points in E^3 . Define $\mathbf{d}_0 = \mathbf{0}$ and let $D = (\mathbf{d}_0, \mathbf{d}_1, ..., \mathbf{d}_M), \mathbf{d}_A \in \Lambda, A = 0, 1, ..., M, M \ge 3$, be the M+1-tuple of vectors such that $\mathbf{d}_A + \mathbf{d}_B = \mathbf{0}$ implies A = B = 0 for every $A, B \in \{0, 1, ..., M\}$. For an arbitrary real valued function $f(\mathbf{z}), \mathbf{z} \in \Lambda$ we introduce finite differences

$$\Delta_A f(\mathbf{z}) = f(\mathbf{z} + \mathbf{d}_A) - f(\mathbf{z}), \ \overline{\Delta}_A f(\mathbf{z}) = f(\mathbf{z}) - f(\mathbf{z} - \mathbf{d}_A), \ \mathbf{z} \in \Lambda$$

where for A = 0 we have $\Delta_0 f = \overline{\Delta}_0 f = 0$. We shall also introduce function

$$\varphi: \{1, \dots, N\} \ni K \to \varphi(K) \equiv (b, a, A) \in \{1, \dots, n\}^2 \times \{0, 1, \dots, M\}$$

where $\varphi(K) = (b, a, 0), a > b$, and under extra denotation $\mathbf{p}_A^a = \mathbf{p}^a + \mathbf{d}_A, a = 1,..., n$, A = 1,..., M, we define $B^K = (\mathbf{p}^b, \mathbf{p}_A^a)$ provided that $\varphi(K) = (b, a, A)$. It follows that

$$B \coloneqq \left\{ B^{K} \left(\mathbf{z} \right) \colon K = 1, ..., N, \ \mathbf{z} \in \Lambda \right\}$$

represents the periodic system of pairs of points $(\mathbf{p}^{b}(\mathbf{z}), \mathbf{p}_{A}^{a}(\mathbf{z})), \mathbf{z} \in \Lambda$, in E^{3} .

Throughout this contribution the space E^3 will be interpreted as the physical space, set P as the system of nodes of the lattice structure under consideration, whereas set B will represent the system of pairs of nodes which are assumed to be interconnected by means of certain thin prismatic rods. Hence the pair S = (P, B) describes the geometry of the periodic lattice structure and the pair $E = \{\{\mathbf{p}_1, ..., \mathbf{p}_n\}, \{B_1, ..., B_N\}\}$ represents the representative element of this structure. For the sake of simplicity every $B^{\mathcal{K}}(\mathbf{z}), \mathbf{z} \in \Lambda$, will be referred to as a rod of the lattice structure. Subsequently, we restrict ourselves to unbounded lattice structures.

Following [8], we shall outline now some basic physical concepts related to the hyperbolic heat conduction. Let θ be the temperature field, **q** the heat flux field and k the coefficient of thermal conductivity. It can be shown, [8], that using Cattaneo heat conduction equation [1]

$$\mathbf{q} + \tau \dot{\mathbf{q}} = -k\nabla \theta$$

and introducing a modified temperature defined by

$$\vartheta \coloneqq \theta \exp \frac{t}{2\tau} \tag{1}$$

we obtain the hyperbolic heat conduction equation of the form

$$-\nabla (k\nabla \vartheta) - \frac{c}{4\tau} \vartheta + \tau c \ddot{\vartheta} = (f + \tau \dot{f}) \exp \frac{t}{2\tau}$$

where f represents the heat sources. This equation can be derived from the principle of stationary action by adopting the lagrangian function L in the form

$$L = \frac{1}{8} \frac{c_w}{\tau} \left(\vartheta\right)^2 + \frac{1}{2} \tau c_w \left(\dot{\vartheta}\right)^2 - \frac{1}{2} k \nabla \cdot \nabla \vartheta + \left(f + \tau \dot{f}\right) \vartheta \exp \frac{t}{2\tau}$$
(2)

and using the Euler-Lagrange equations

$$\frac{\partial L}{\partial \vartheta} - \frac{\partial}{\partial t} \left(\frac{\partial L}{\partial \dot{\vartheta}} \right) - \nabla \cdot \frac{\partial L}{\partial \nabla \vartheta} = 0$$

Using the above concepts we shall formulate in the subsequent section a finite difference model of the heat conduction in the periodic lattice under considerations.

3. Finite difference model

Let us assume that every rod $B^{K}(\mathbf{z})$ interconnecting nodes $\mathbf{p}^{b}(\mathbf{z})$, $\mathbf{p}_{A}^{a}(\mathbf{z})$, where $\varphi(K) = (b, a, A)$, is a heat conductor between these nodes. Let c^{K} , λ^{K} , τ , F^{K} stand for the specific heat, thermal conductivity, relaxation time, cross-sectional area of rod $B^{K}(\mathbf{z})$, $\mathbf{z} \in \Lambda$, K = 1, ..., N, respectively. We also assume that the heat flow in every rod is one dimensional and heat sources can depend only on time. Denote by $\theta^{a} = \theta^{a}(\mathbf{z}, t)$, $\mathbf{z} \in \Lambda$, a = 1, ..., n, the temperature of the node $\mathbf{p}^{a}(\mathbf{z})$, $\mathbf{z} \in \Lambda$, at time t; hence the temperature of the node $\mathbf{p}_{A}^{a}(\mathbf{z})$, $\mathbf{z} \in \Lambda$, will be given by $\theta_{A}^{a}(\mathbf{z}, t) = \theta^{a}(\mathbf{z}, t) + \Delta_{A}\theta^{a}(\mathbf{z}, t)$; similar denotations also hold for the modified temperature \mathcal{G} . Let l^{K} be the length of a rod B^{K} and $|\Delta|$ stand for the volume of Δ . Bearing in mind (1) and (2) we shall introduce Lagrangian L_{K} for the rod $B^{K} = (\mathbf{p}^{b}, \mathbf{p}_{A}^{a})$, K = 1, ..., N, $(b, a, A) = \varphi(K)$, in the form

$$L_{K} = \frac{1}{4\tau} W \left(\vartheta^{b}, \Delta_{A} \vartheta^{a} \right) + \tau W \left(\dot{\vartheta}^{b}, \Delta_{A} \dot{\vartheta}^{a} \right) - V \left(\vartheta^{a} - \vartheta^{b}, \Delta_{A} \vartheta^{a} \right) + \left(f + \tau \dot{f} \right) \exp \frac{t}{2\tau} E \left(\vartheta^{b}, \Delta_{A} \vartheta^{a} \right)$$
(3)

where:

$$W\left(\vartheta^{b}, \Delta_{A}\vartheta^{a}\right) = \frac{c^{K}l^{K}F^{K}}{6|\Delta|} \left(\left(\vartheta^{b}\right)^{2} + \left(\vartheta^{b} + \vartheta^{a} + \Delta_{A}\vartheta^{a}\right)\left(\vartheta^{a} + \Delta_{A}\vartheta^{a}\right)\right)$$
$$E\left(\vartheta^{b}, \Delta_{A}\vartheta^{a}\right) = \frac{l^{K}F^{K}}{2|\Delta|}\left(\vartheta^{b} + \vartheta^{a} + \Delta_{A}\vartheta^{a}\right)$$
$$V\left(\vartheta^{b}, \Delta_{A}\vartheta^{a}\right) = \frac{F^{K}}{2l^{K}|\Delta|}\left(\vartheta^{b} - \vartheta^{a} - \Delta_{A}\vartheta^{a}\right)^{2}, \quad \varphi(K) = (b, a, A)$$

Hence, the Lagrangian L for the representative element E is

$$L = \sum_{K=1}^{N} L_K \tag{4}$$

Using the results obtained in [9] for dynamic problems, it can be proved that functions $\vartheta^a(\mathbf{z}, \cdot)$, $a = 1, ..., n, \mathbf{z} \in \Lambda$ satisfy the following system of finite-difference equations

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$$\frac{\partial L}{\partial \vartheta^{a}} - \overline{\Delta}_{A} \frac{\partial L}{\partial \Delta_{A} \vartheta^{a}} = \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{\vartheta}^{a}} - \overline{\Delta}_{A} \frac{\partial L}{\partial \Delta_{A} \dot{\vartheta}^{a}} \right), \quad A = 1, \dots, M$$
(5)

Thus, we have arrived at the infinite system of finite difference equations (with respect to argument $\mathbf{z} \in \Lambda$) for the modified temperature $\mathcal{P}^a(\mathbf{z}, t)$, a = 1, ..., n, $\mathbf{z} \in \Lambda$. Equations (5) have to hold for an arbitrary instant *t* and every $\mathbf{z} \in \Lambda$ and represent the finite difference model of the hyperbolic heat conduction of the periodic unbounded lattice under consideration.

4. Continuum models

Let $\vartheta^a(\cdot, t)$, a = 1, ..., n be sufficiently smooth functions defined on E^3 for every time *t*, such that for every $z \in \Lambda$ their values can be physically interpreted as close approximation of values $\vartheta^a(\mathbf{z}, t), \mathbf{z} \in \Lambda$ of fields occurring in the finite difference model. The continuum models of the hyperbolic heat conduction problem in a periodic lattice structure will be derived on the basis of the assumption that for every $\mathbf{x} \in E^3$ and for every vector \mathbf{d}_A , increments $\Delta_A \vartheta^a(\mathbf{x}, t)$ and $\Delta_A \dot{\vartheta}^a(\mathbf{x}, t)$ can be approximated by using expansions of the form (no summation over A!)

$$\Delta_A w(\mathbf{x}, t) \cong \mathbf{d}_A \cdot \nabla w(\mathbf{x}, t) + \frac{1}{2} \mathbf{d}_A \otimes \mathbf{d}_A : (\nabla \otimes \nabla) w(\mathbf{x}, t)$$
(6)

where w stands for ϑ^a and $\dot{\vartheta}^a$. Denoting

$$\mathbf{D}_A \coloneqq \frac{1}{2} \mathbf{d}_A \otimes \mathbf{d}_A$$

and substituting (6) into (3) we obtain the new Lagrangian L_2 defined by

$$L_{2}\left(\boldsymbol{\vartheta}^{b}, \nabla\boldsymbol{\vartheta}^{a}, \nabla\otimes\nabla\boldsymbol{\vartheta}^{a}, \dot{\boldsymbol{\vartheta}}^{b}, \nabla\dot{\boldsymbol{\vartheta}}^{a}, \nabla\otimes\nabla\dot{\boldsymbol{\vartheta}}^{a}\right) \coloneqq L\left(\boldsymbol{\vartheta}^{b}, \mathbf{d}_{A}\cdot\nabla\boldsymbol{\vartheta}^{a} + \mathbf{D}_{A}: (\nabla\otimes\nabla)\boldsymbol{\vartheta}^{a}, \dot{\boldsymbol{\vartheta}}^{b}, \mathbf{d}_{A}\cdot\nabla\dot{\boldsymbol{\vartheta}}^{a} + \mathbf{D}_{A}: (\nabla\otimes\nabla)\dot{\boldsymbol{\vartheta}}^{a}\right)$$
(7)

which implies the following Euler-Lagrange equations for functions \mathcal{G}^a , a = 1, ..., n

$$(\nabla \otimes \nabla) : \frac{\partial L_2}{\partial (\nabla \otimes \nabla) \vartheta^a} - \nabla \cdot \frac{\partial L_2}{\partial \nabla \vartheta^a} + \frac{\partial L_2}{\partial \vartheta^a} =$$

$$= \frac{\partial}{\partial t} \left((\nabla \otimes \nabla) : \frac{\partial L_2}{\partial (\nabla \otimes \nabla) \dot{\vartheta}^a} - \nabla \cdot \frac{\partial L_2}{\partial \nabla \dot{\vartheta}^a} + \frac{\partial L_2}{\partial \dot{\vartheta}^a} \right), \quad a = 1, ..., n$$

$$(8)$$

The above equations are assumed to hold for every $\mathbf{x} \in E^3$ and every time *t* and represent the system of *n* partial differential equations for the fields $\mathcal{P}^a(\cdot, t)$ defined in E^3 for every *t*. Equations (8) represent what will be called the second order continuum model of the hyperbolic heat conduction problem in the periodic lattice under consideration. Bearing in mind only the first gradients in expansions (6) we obtain the Lagrangian L_1 defined by

$$L_1\left(\boldsymbol{\vartheta}^b, \, \nabla\boldsymbol{\vartheta}^a, \, \dot{\boldsymbol{\vartheta}}^b, \, \nabla\dot{\boldsymbol{\vartheta}}^a\right) \coloneqq L\left(\boldsymbol{\vartheta}^b, \, \mathbf{d}_A \cdot \nabla\boldsymbol{\vartheta}^a, \, \dot{\boldsymbol{\vartheta}}^b, \, \mathbf{d}_A \cdot \nabla\dot{\boldsymbol{\vartheta}}^a\right) \tag{9}$$

In this case the corresponding Euler-Lagrange equations are

$$\frac{\partial L_1}{\partial \vartheta^a} - \nabla \cdot \frac{\partial L_1}{\partial (\nabla \vartheta^a)} - \frac{\partial}{\partial t} \left(\frac{\partial L_1}{\partial \dot{\vartheta}^a} - \nabla \cdot \frac{\partial L_1}{\partial (\nabla \dot{\vartheta}^a)} \right) = 0, \ a = 1, ..., n$$
(10)

and represent what will be called the first order continuum model of the heat conduction in the periodic lattice under consideration. It can be shown that equations (8) and (10) can be obtained directly from equations (5) by using (6), i.e. without the principle of stationary action. This procedure will be shown in the prepared for print publication.

The detailed discussion of the modelling approach outlined in this contribution as well as examples of its application will be given in the forthcoming paper.

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