

Equivalent thermo-mechanical parameters for perfect crystals

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Abstract Thermo-elastic behavior of perfect single crystal is considered. The crystal is represented as a set of interacting particles (atoms). The approach for determination of equivalent continuum values for the discrete system is proposed. Averaging of equations of particles' motion and long wave approximation are used in order to make link between the discrete system and equivalent continuum. Basic balance equations for equivalent continuum are derived from microscopic equations. Macroscopic values such as Piola and Cauchy stress tensors and heat flux are represented via microscopic parameters. Connection between the heat flux and temperature is discussed. Equation of state in Mie-Gruneisen form connecting Cauchy stress tensor with deformation gradient and thermal energy is obtained from microscopic considerations.

1 Introduction

Determination of the relation between parameters of discrete and continuum systems is one of the challenging problems for modern physics. There were intensive investigations in this area for the last several decades. However the problem is far from its final solution. At the beginning the problem was only of a fundamental interest. However, practical interest is increasing now. The increase is caused by fast development of discrete [1] and discrete-continuum [17, 16] methods for simulation of mechanical behavior of bodies under mechanical and thermal loadings. Various methods for transition from discrete system to equivalent continuum are considered

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in literature. Long wave approximation is used in [2]. The concept of quasicontinuum is proposed in [10]. Localization functions are used in [4, 5, 18]. These approaches give the opportunity to spread mechanical parameters determined in lattice nodes on all volume of the body. Decomposition of motions on slow macroscopic and fast thermal ones is used for description of thermal properties. There are different approaches for decomposition. In papers [4, 5, 18, 22] the decomposition of particle velocities is carried out using localization functions. As a result, dependencies of stress tensor and heat flux on parameters of the discrete system were obtained and analyzed. Another approach was proposed in [21]. Fourier transformation was used for decomposition of displacements and particle velocities. Different methods for decomposition were discussed. It was noted that the result of the decomposition is not unique. It should depend on characteristic time and spatial scales of the problem.

The approach based on averaging of equations of motions and application of the long wave approximation [2] was proposed in papers [7, 8]. The derivation of expressions for stress tensors for ideal crystals was carried out in book [7]. Only pair potentials were considered. Thermal motion was neglected. The influence of thermal oscillations on mechanical properties was considered in [7, 8] for one-dimensional case. The proposed approach gives an opportunity to carry out analytical derivations. In particular, the equation of state in Mie-Gruneisen form was obtained in papers [7, 8, 9].

In the present paper a generalization of approaches proposed in [7, 8] for two and three-dimensional cases is carried out. The expressions connecting Piola and Cauchy stress tensors and heat flux with parameters of the discrete system are derived. The approach for derivation of constitutive relations for Cauchy stress tensor and heat flux is discussed.

2 Hypotheses

Let us consider discrete system consisted of particles, which form the infinite ideal crystal lattice in d -dimensional space ($d = 1, 2$ or 3). Crystals with simple structure are investigated only (i.e. crystals that are invariant to translation on any vector connecting lattice nodes). For the sake of simplicity let the particles interact via pairwise potential of Lennard-Jones type. Generalization of the approach discussed in the present paper for the case of multibody interatomic potentials is considered in papers [11, 12].

Two main principles are used for transition from discrete system to equivalent continuum: the long wave approximation [2] and decomposition of particles' motions into slow continuum and fast thermal one [8, 21]. First let us focus on decomposition. In literature it is carried out using different types of averaging such as spatial averaging, time averaging, averaging over phase space or over frequency spectrum, etc. It was noted in paper [21] that unique decomposition is impossible because rules for a choice of averaging parameters like averaging time, represen-

tative volume, etc. do not exist. The only possible rule for these parameters is that they should depend on time and spatial scales of the problem being solved. Let us denote average and oscillating (thermal) components of physical value f as $\langle f \rangle$ and \tilde{f} respectively. Obviously,

$$f = \langle f \rangle + \tilde{f}, \quad \tilde{f} \stackrel{\text{def}}{=} f - \langle f \rangle. \quad (1)$$

Different expressions for the averaging operator $\langle \rangle$ are proposed in literature. The following operator was used in paper [8] for one dimensional case

$$\langle f_n \rangle = \frac{1}{T\Lambda} \int_{t-T/2}^{t+T/2} \sum_{k=n-\Lambda/2}^{n+\Lambda/2} f_k(t) dt. \quad (2)$$

where f_k is magnitude of physical value f for particle number k . Parameters T and Λ should satisfy the following relations $1 \ll \Lambda \ll N$, $T_{min} \ll T \ll T_{max}$, where T_{min} and T_{max} are minimal and maximal periods of oscillations in the system, N is the total number of particles. Obviously these limitations are too weak. Direct and inverse Fourier transformations were used for decomposition in paper [21]. The direct transformation gives

$$F(\mathbf{v}) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f e^{i\mathbf{v}t} dt, \quad (3)$$

where

$$\langle F \rangle(\mathbf{v}) = \begin{cases} F(\mathbf{v}), \mathbf{v} < \mathbf{v}_{cutoff} \\ 0, \mathbf{v} \geq \mathbf{v}_{cutoff} \end{cases} \quad \tilde{F}(\mathbf{v}) = \begin{cases} 0, \mathbf{v} < \mathbf{v}_{cutoff} \\ F(\mathbf{v}), \mathbf{v} \geq \mathbf{v}_{cutoff} \end{cases} \quad (4)$$

Here F is Fourier transform of value f ; i is imaginary unit; \mathbf{v}_{cutoff} is cut-off frequency, which should be taken in the range 0.5-50 THz [2]. Inverse Fourier transformation was used in order to obtain $\langle f \rangle$ and \tilde{f}

$$\langle f \rangle = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \langle F \rangle e^{-i\mathbf{v}t} d\mathbf{v} \quad \tilde{f} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \tilde{F} e^{-i\mathbf{v}t} d\mathbf{v}. \quad (5)$$

In the framework of the given approach the choice of cut-off frequency is almost arbitrary. In papers [4, 5, 22] the following relations were used for decomposition of particle velocities

$$f_k = \langle f \rangle(\mathbf{x}, t) + \tilde{f}_k(\mathbf{x}, t), \quad \langle f \rangle(\mathbf{x}, t) = \frac{\sum_{k=1}^M m_k f_k \psi(\mathbf{x} - \mathbf{x}_k)}{\sum_{k=1}^M m_k \psi(\mathbf{x} - \mathbf{x}_k)}. \quad (6)$$

Here f_k, m_k, \mathbf{x}_k are velocity, mass and radius-vector of particle number k ; \mathbf{x} is coordinate of the spatial point where velocity is calculated; ψ is localization function; M is

the total number of particles in the system. Decomposition (6) can be considered as spatial averaging with weight determined by function ψ . Note that according to this approach thermal component of the velocity $\tilde{f}_k(\mathbf{x}, t)$ is continuum value (it is determined at points between particles). Several thermal velocities $\tilde{f}_{k1}(\mathbf{x}_0, t), \tilde{f}_{k2}(\mathbf{x}_0, t), \dots$ and one continuum velocity $\langle f \rangle(\mathbf{x}_0, t)$ are simultaneously determined in one spatial point \mathbf{x}_0 . However, formally it does not lead to any contradictions. This type of decomposition as well as all mentioned above is not unique. It strongly depends on the choice of localization function. In particular, if localization area surrounds single atom, then thermal component of the velocity is equal to zero.

Since the unique decomposition does not exist, the theory should not be based on particular method of decomposition. In addition, the results of the theory should not qualitatively change with the change of the method. Properties of particular methods for averaging are not used in the present paper, unless otherwise stated. Let us speak about averaged $\langle f \rangle$ and thermal \tilde{f} components of physical value f , which are connected by formula (1).

The second important statement used in the present paper is the long wave approximation [2]. The idea of the approximation is the following: an average component of any physical value is assumed to be slowly changing in space on the distances of an order of the interatomic distance. Then the average component can be considered as a continuum function of a space variable and can be expanded into power series with respect to interatomic distance. The resulting series should converge rapidly. Exactly this assumption allows to make transition from a discrete system to an equivalent continuum.

3 Kinematics

Let us use material description of the equivalent continuum. Two configurations of continuum and discrete system are considered: reference and actual. For the sake of simplicity let us take undeformed configuration of the crystal lattice as the reference one. Radius-vectors of equivalent continuum in the reference and actual configurations are denoted as \mathbf{r} and \mathbf{R} respectively. Two ways of particles' identification are used. On the one hand, the position of the particle is determined by its radius-vector. On the other hand, let us use local numbering [7]. Starting with one reference particle let us mark all its neighbors by index α . Let us denote a vector connecting the reference particle with its neighbor number α as \mathbf{a}_α . By the definition vectors \mathbf{a}_α have the following property

$$\mathbf{a}_\alpha = -\mathbf{a}_{-\alpha}. \quad (7)$$

The same vectors in an actual configuration are represented as a sum of averaged component \mathbf{A}_α and thermal component $\tilde{\mathbf{A}}_\alpha$. They can be expressed in terms of vectors \mathbf{a}_α and displacements of particles as

$$\mathbf{A}_\alpha = \mathbf{a}_\alpha + \mathbf{u}_\alpha - \mathbf{u}, \quad \tilde{\mathbf{A}}_\alpha = \tilde{\mathbf{u}}_\alpha - \tilde{\mathbf{u}}.$$

Here \mathbf{u} , \mathbf{u}_α and $\tilde{\mathbf{u}}$, $\tilde{\mathbf{u}}_\alpha$ are average and thermal components of displacements respectively.

The introduced way of particle identification has several properties. Let us use the following definition. A physical value determined by the state of one particle is called a single-particle value. For example, particle's mass, radius-vector, velocity, displacement etc. Let $f(\mathbf{r}_0)$ be one-particle value that corresponds to the reference particle with radius-vector \mathbf{r}_0 in the reference configuration. Denote value f , which corresponds to particle number α , as $f_\alpha(\mathbf{r}_0)$. Then the following two designations are equivalent

$$f_\alpha(\mathbf{r}_0) \equiv f(\mathbf{r}_0 + \mathbf{a}_\alpha). \quad (8)$$

In the framework of this approach the magnitude of physical value f at the point \mathbf{r}_0 can be represented in the following equivalent forms

$$f(\mathbf{r}_0) = f_\alpha(\mathbf{r}_0 - \mathbf{a}_\alpha) = f_{-\alpha}(\mathbf{r}_0 + \mathbf{a}_\alpha). \quad (9)$$

One can show that for multiplication of two one-particle values f and g the following identities are satisfied

$$[f_\alpha g](\mathbf{r}_0) = [fg_{-\alpha}](\mathbf{r}_0 + \mathbf{a}_\alpha) \quad [f_{-\alpha} g](\mathbf{r}_0) = [fg_\alpha](\mathbf{r}_0 - \mathbf{a}_\alpha). \quad (10)$$

Hereinafter square brackets mean that all values in them are calculated at the same point. Let us also consider values that depend on the state the reference particle and its neighbor number α , notably vector connecting two particles and force acting between particles. These values have the following property

$$h_\alpha(\mathbf{r}_0) = -h_{-\alpha}(\mathbf{r}_0 + \mathbf{a}_\alpha). \quad (11)$$

If h is a force acting between particles, then equation (11) is a specific form of Newton's third law. The following identities are satisfied for one-particle value f and the value h

$$[f_\alpha h_\alpha](\mathbf{r}_0) = -[fh_{-\alpha}](\mathbf{r}_0 + \mathbf{a}_\alpha) \quad [fh_{-\alpha}](\mathbf{r}_0) = -[f_\alpha h_\alpha](\mathbf{r}_0 - \mathbf{a}_\alpha). \quad (12)$$

Let us consider kinematics of the discrete system in the long wave approximation. It is assumed that average values of particle radius-vectors are identical to positions of corresponding points of continuum media. Thus if some particle has radius-vector \mathbf{r} in the reference configuration, then the average value of the radius-vector in actual configuration is equal to $\mathbf{R}(\mathbf{r})$. The average position of its neighbor number α is determined by vector $\mathbf{R}(\mathbf{r} + \mathbf{a}_\alpha)$. Then one can show that vectors \mathbf{A}_α and \mathbf{a}_α , connecting the particles, are related by the following formula

$$\mathbf{A}_\alpha = \mathbf{R}(\mathbf{r} + \mathbf{a}_\alpha) - \mathbf{R}(\mathbf{r}) \approx \mathbf{a}_\alpha \cdot \overset{\circ}{\nabla} \mathbf{R}, \quad (13)$$

where $\overset{\circ}{\nabla}$ is nabla-operator in the reference configuration. Here the long wave approximation was used, which allows to leave the first order terms only. One can

see that expression (13) is similar to the formula used in continuum mechanics that connects vectors $d\mathbf{r}$ and $d\mathbf{R}$. Using equation (13) one can derive relations between vectors \mathbf{A}_α , \mathbf{a}_α and measures of deformation used in nonlinear theory of elasticity [14]. For example, the following identity fulfills for Cauchy-Green measure \mathbf{G}

$$\mathbf{A}_\alpha^2 = \mathbf{a}_\alpha \mathbf{a}_\alpha \cdot \mathbf{G}, \quad \mathbf{G} \stackrel{\text{def}}{=} (\overset{\circ}{\nabla} \mathbf{R}) \cdot (\mathbf{R} \overset{\circ}{\nabla}). \quad (14)$$

4 Equation of momentum balance

Let us obtain the equation of motion for the equivalent continuum. Thereto let us write down the equation of motion for the reference particle and use the decomposition of motions

$$m\ddot{\mathbf{u}} = \sum_{\alpha} \langle \mathbf{F}_\alpha(\mathbf{A}_\alpha + \tilde{\mathbf{A}}_\alpha) \rangle, \quad m\tilde{\ddot{\mathbf{u}}} = \sum_{\alpha} \tilde{\mathbf{F}}_\alpha(\mathbf{A}_\alpha + \tilde{\mathbf{A}}_\alpha), \quad (15)$$

where \mathbf{F}_α is a force acting on the reference particle from its neighbor α ; m is particle's mass. The first equation from (15) describes slow motion of the system. The motion can be considered as motion of continuum media. The second equation describes thermal oscillations. One can see that both equations are coupled via the argument of the force \mathbf{F}_α . However, if the dependence of the force on the distance between particles is linear, then equations become independent. It reflects the well-known fact that harmonic models can not describe coupled thermo-mechanical effects such as thermal expansion [13]. Let us conduct the following transformations in the first equation from (15).

$$m\ddot{\mathbf{u}} = \sum_{\alpha} \langle \mathbf{F}_\alpha \rangle = \sum_{\alpha} \langle \mathbf{F}_{-\alpha} \rangle = \frac{1}{2} \sum_{\alpha} \langle \mathbf{F}_\alpha + \mathbf{F}_{-\alpha} \rangle. \quad (16)$$

Force \mathbf{F}_α satisfies Newton's third law, i.e. $\mathbf{F}_\alpha(\mathbf{r} - \mathbf{a}_\alpha) = -\mathbf{F}_{-\alpha}(\mathbf{r})$ (see formula (11)). Averaging this expression and using long wave approximation one obtains

$$\langle \mathbf{F}_{-\alpha} \rangle(\mathbf{r}) \approx -\langle \mathbf{F}_\alpha \rangle(\mathbf{r}) + \mathbf{a}_\alpha \cdot \overset{\circ}{\nabla} \langle \mathbf{F}_\alpha \rangle(\mathbf{r}) \quad (17)$$

Substituting formula (17) into equation (16) and dividing both parts by volume of elementary cell in the reference configuration V_0 one obtains

$$\frac{m}{V_0} \ddot{\mathbf{u}} = \overset{\circ}{\nabla} \cdot \left(\frac{1}{2V_0} \sum_{\alpha} \mathbf{a}_\alpha \langle \mathbf{F}_\alpha \rangle \right) \quad (18)$$

Let us compare formula (18) with equation of motion for continuum in Piola's form [14].

$$\rho_0 \ddot{\mathbf{u}} = \overset{\circ}{\nabla} \cdot \mathbf{P}. \quad (19)$$

where \mathbf{P} is Piola stress tensor, ρ_0 is a density in the reference configuration. Comparing equations (18) and (19) one can deduce that

$$\mathbf{P} = \frac{1}{2V_0} \sum_{\alpha} \mathbf{a}_{\alpha} \langle \mathbf{F}_{\alpha} \rangle, \quad \rho_0 = \frac{m}{V_0}, \quad (20)$$

Strictly speaking the first formula from (20) is satisfied only with accuracy of tensor with zero divergency. This tensor corresponds to some equilibrium stress field in the crystal.

Let us conduct the same derivations in an actual configuration. Equation of motion for the particle has form (16). Let us rewrite formula (17) in an actual configuration.

$$\mathbf{F}_{\alpha}(\mathbf{R} - \mathbf{A}_{\alpha}) = -\mathbf{F}_{-\alpha}(\mathbf{R}) \Rightarrow \langle \mathbf{F}_{-\alpha} \rangle(\mathbf{R}) \approx -\langle \mathbf{F}_{\alpha} \rangle(\mathbf{R}) + \mathbf{A}_{\alpha} \cdot \nabla \langle \mathbf{F}_{\alpha} \rangle(\mathbf{R}). \quad (21)$$

Here it was used that in the long wave approximation $\mathbf{A}_{-\alpha} \approx -\mathbf{A}_{\alpha}$. Substituting expression (21) into equation (16) and dividing both parts by the volume of elementary cell in the actual configuration V one obtains

$$\frac{m}{V} \ddot{\mathbf{u}} = \frac{1}{2V} \sum_{\alpha} \mathbf{A}_{\alpha} \cdot \nabla \langle \mathbf{F}_{\alpha} \rangle. \quad (22)$$

Let us conduct the following transformations in the right side of formula (22)

$$\frac{1}{2V} \sum_{\alpha} \mathbf{A}_{\alpha} \cdot \nabla \langle \mathbf{F}_{\alpha} \rangle = \nabla \cdot \left(\frac{1}{2V} \sum_{\alpha} \mathbf{A}_{\alpha} \langle \mathbf{F}_{\alpha} \rangle \right) - \sum_{\alpha} \nabla \cdot \left(\frac{1}{2V} \mathbf{A}_{\alpha} \right) \langle \mathbf{F}_{\alpha} \rangle \quad (23)$$

The second term in the right side of the given equation can be written down in the following form using equation (13)

$$\sum_{\alpha} \nabla \cdot \left(\frac{1}{2V} \mathbf{A}_{\alpha} \right) \langle \mathbf{F}_{\alpha} \rangle = \frac{V_0}{2} \sum_{\alpha} \nabla \cdot \left(\frac{V_0}{V} (\mathbf{R} \overset{\circ}{\nabla}) \right) \cdot \mathbf{a}_{\alpha} \langle \mathbf{F}_{\alpha} \rangle = 0, \quad (24)$$

where Piola's identity $\nabla \cdot \left(\frac{V_0}{V} (\mathbf{R} \overset{\circ}{\nabla}) \right) \equiv 0$ was used (see, for example, [14]). Then equation of motion (22) has the following form

$$\frac{m}{V} \ddot{\mathbf{u}} = \nabla \cdot \left(\frac{1}{2V} \sum_{\alpha} \mathbf{A}_{\alpha} \langle \mathbf{F}_{\alpha} \rangle \right). \quad (25)$$

The requirement of equivalence of discrete and continuum systems leads to the following expressions for Cauchy stress tensor and density in the actual configuration

$$\boldsymbol{\tau} = \frac{1}{2V} \sum_{\alpha} \mathbf{A}_{\alpha} \langle \mathbf{F}_{\alpha} \rangle, \quad \rho = \frac{m}{V}. \quad (26)$$

If thermal motion is not taken into account, then expression (26) coincides with expressions derived in papers [7, 20].

It is known that Cauchy stress tensor is symmetrical in systems without moment interactions. Let us consider tensor τ determined by formula (26). Force \mathbf{F}_α can be represented as

$$\mathbf{F}_\alpha = -\Phi_\alpha((\mathbf{A}_\alpha + \tilde{\mathbf{A}}_\alpha)^2)(\mathbf{A}_\alpha + \tilde{\mathbf{A}}_\alpha), \quad \Phi(A^2) \stackrel{\text{def}}{=} -\frac{\Pi'(A)}{A} \quad (27)$$

Substituting the given expression into formula (26) one obtains

$$\tau = -\frac{1}{2V} \sum_\alpha \langle \Phi_\alpha \rangle \mathbf{A}_\alpha \mathbf{A}_\alpha - \frac{1}{2V} \sum_\alpha \mathbf{A}_\alpha \langle \tilde{\Phi}_\alpha \tilde{\mathbf{A}}_\alpha \rangle. \quad (28)$$

The first tensor in the right side of formula (28) is symmetrical indeed. However the symmetry of the second tensor is not evident. Further it will be shown that antisymmetrical part of this tensor is small with respect to symmetrical part.

5 Equation of angular momentum balance

It is known from continuum mechanics [15] that the symmetry of Cauchy stress tensor follows from equation of angular momentum balance for elementary volume. In the discrete case elementary cell plays the role of elementary volume. Let us write down the averaged equation of angular momentum balance for elementary cell (moments are calculated with respect to the center of the cell determined by vector \mathbf{R}).

$$m \langle \tilde{\mathbf{u}} \times \dot{\tilde{\mathbf{u}}} \rangle = \langle \tilde{\mathbf{u}} \times \sum_\alpha \tilde{\mathbf{F}}_\alpha \rangle = -\sum_\alpha \langle \tilde{\mathbf{A}}_\alpha \times \tilde{\mathbf{F}}_\alpha \rangle + \sum_\alpha \langle \tilde{\mathbf{u}}_\alpha \times \tilde{\mathbf{F}}_\alpha \rangle. \quad (29)$$

Transforming the second term in the right side of the given equation using the long wave approximation one obtains

$$\langle \tilde{\mathbf{u}}_\alpha \times \tilde{\mathbf{F}}_\alpha \rangle(\mathbf{R}) = -\langle \tilde{\mathbf{u}} \times \tilde{\mathbf{F}}_{-\alpha} \rangle(\mathbf{R} + \mathbf{A}_\alpha) \approx -\langle \tilde{\mathbf{u}} \times \tilde{\mathbf{F}}_{-\alpha} \rangle - \mathbf{A}_\alpha \cdot \nabla \langle \tilde{\mathbf{u}} \times \tilde{\mathbf{F}}_{-\alpha} \rangle. \quad (30)$$

Let us substitute the result into equation (29) and resolve it with respect to $\langle \tilde{\mathbf{A}}_\alpha \times \tilde{\mathbf{F}}_\alpha \rangle$.

$$\frac{1}{2} \sum_\alpha \langle \tilde{\mathbf{A}}_\alpha \times \tilde{\mathbf{F}}_\alpha \rangle = \frac{1}{2} \sum_\alpha \mathbf{A}_\alpha \times \langle \tilde{\Phi}_\alpha \tilde{\mathbf{A}}_\alpha \rangle = -\frac{1}{2} \sum_\alpha \mathbf{A}_\alpha \cdot \nabla \langle \tilde{\mathbf{u}} \times \tilde{\mathbf{F}}_{-\alpha} \rangle - m \langle \tilde{\mathbf{u}} \times \dot{\tilde{\mathbf{u}}} \rangle. \quad (31)$$

Using expression (28) for the stress tensor one can transform formula (31) to the following form

$$\mathbf{E} \cdot \times \tau^A = \frac{1}{2V} \sum_{\alpha} \mathbf{A}_{\alpha} \cdot \nabla \langle \tilde{\mathbf{u}} \times \tilde{\mathbf{F}}_{-\alpha} \rangle + \rho \langle \tilde{\mathbf{u}} \times \ddot{\tilde{\mathbf{u}}} \rangle. \quad (32)$$

Here A denotes antisymmetrical part of the tensor. One can see that if there is no thermal motion, then $\tau^A \equiv 0$. Let us show that in general case τ^A is small in comparison with τ^S . The first term in formula (32) is small in the long wave approximation. Let us show that if operator $\langle \rangle$ contains spatial averaging, then the second term is also small. Consider the following identity

$$\rho \langle \tilde{\mathbf{u}} \times \dot{\tilde{\mathbf{u}}} \rangle = \rho \langle (\mathbf{R} + \tilde{\mathbf{u}}) \times \dot{\tilde{\mathbf{u}}} \rangle. \quad (33)$$

The right side of formula (33) is a derivative of angular momentum, which corresponds to thermal motion. Angular momentum is calculated with respect to the origin of coordinates. Let the averaging operator include spatial averaging over significantly large volume and let us assume that thermal motion does not lead to macroscopic rotation of the volume. Then expressions (33) are equal to zero. As a result τ^A has the same order as terms that were neglected in long wave assumption. Consequently, tensor (26) can be considered as approximately symmetrical.

Thus averaging operator proposed above can not be arbitrary. It should include spatial averaging. Otherwise one can not prove the symmetry of tensor τ determined by formula (26).

6 Equation of energy balance

For the sake of simplicity let us assume that volumetrical forces and volumetrical heat sources are equal to zero. Derivations are carried out in the reference configuration. In this case averaged specific total energy per volume V_0 has the following form

$$\rho_0 \mathcal{E} = \frac{1}{2} \rho_0 \langle (\dot{\tilde{\mathbf{u}}} + \dot{\tilde{\mathbf{u}}})^2 \rangle + \frac{1}{2V_0} \sum_{\alpha} \langle \Pi(\mathbf{A}_{\alpha} + \tilde{\mathbf{A}}_{\alpha}) \rangle, \quad (34)$$

where \mathcal{E} is particle's total energy divided by the mass, i.e. discrete analog for mass density of the energy. Let us introduce the following designations

$$\begin{aligned} \rho_0 \mathcal{E} &= \rho_0 (\mathcal{K} + \mathcal{U}), \\ \rho_0 \mathcal{K} &= \frac{1}{2} \rho_0 \dot{\tilde{\mathbf{u}}}^2, \quad \rho_0 \mathcal{U} = \frac{1}{2} \rho_0 \langle \dot{\tilde{\mathbf{u}}}^2 \rangle + \frac{1}{2V_0} \sum_{\alpha} \langle \Pi(\mathbf{A}_{\alpha} + \tilde{\mathbf{A}}_{\alpha}) \rangle. \end{aligned} \quad (35)$$

Values \mathcal{K} and \mathcal{U} correspond to mass densities of macroscopic kinetic and internal energies. Calculating derivatives of kinetic and potential energies taking into account formulas (15), (20) one can obtain

$$\begin{aligned} \frac{1}{2}\rho_0 \frac{d}{dt} \left(\dot{\mathbf{u}}^2 + \langle \dot{\tilde{\mathbf{u}}} \rangle^2 \right) &= \rho_0 \left(\dot{\mathbf{u}} \cdot \dot{\mathbf{u}} + \langle \dot{\tilde{\mathbf{u}}} \cdot \dot{\tilde{\mathbf{u}}} \rangle \right) = \left(\overset{\circ}{\nabla} \cdot \mathbf{P} \right) \cdot \dot{\mathbf{u}} + \frac{1}{V_0} \sum_{\alpha} \langle \dot{\tilde{\mathbf{u}}} \cdot \tilde{\mathbf{F}}_{\alpha} \rangle, \\ \frac{1}{2V_0} \frac{d}{dt} \sum_{\alpha} \langle \Pi(\mathbf{A}_{\alpha} + \tilde{\mathbf{A}}_{\alpha}) \rangle &= \frac{1}{2V_0} \sum_{\alpha} \langle \mathbf{F}_{\alpha} \cdot (\dot{\mathbf{A}}_{\alpha} + \dot{\tilde{\mathbf{A}}}_{\alpha}) \rangle \end{aligned} \quad (36)$$

where formula $\mathbf{F}_{\alpha} = \frac{d\Pi}{d\mathbf{A}_{\alpha}}$ was used. Let us conduct the following transformations

$$\sum_{\alpha} \langle \mathbf{F}_{\alpha} \rangle \cdot \dot{\mathbf{A}}_{\alpha} = \sum_{\alpha} \langle \mathbf{F}_{\alpha} \rangle \cdot (\dot{\mathbf{u}}(\mathbf{r} + \mathbf{a}_{\alpha}) - \dot{\mathbf{u}}(r)) \approx \sum_{\alpha} \mathbf{a}_{\alpha} \langle \mathbf{F}_{\alpha} \rangle \cdot \dot{\mathbf{u}} \overset{\circ}{\nabla} \quad (37)$$

Summarizing expressions (36) and taking into account formulas (20), (37) one obtains the expression for derivative of the total energy with respect to time

$$\rho_0 \dot{\mathcal{E}} = \overset{\circ}{\nabla} \cdot (\mathbf{P} \cdot \dot{\mathbf{u}}) + \frac{1}{2V_0} \sum_{\alpha} \langle \tilde{\mathbf{F}}_{\alpha} \cdot (\dot{\tilde{\mathbf{u}}}_{\alpha} + \dot{\tilde{\mathbf{u}}}) \rangle. \quad (38)$$

Using equation of momentum balance one can show that $\rho_0 \dot{\mathcal{K}} = \left(\overset{\circ}{\nabla} \cdot \mathbf{P} \right) \cdot \dot{\mathbf{u}}$. Substituting this expression into equation (38) one obtains

$$\rho_0 \dot{\mathcal{K}} = \mathbf{P} \cdot \left(\dot{\mathbf{u}} \overset{\circ}{\nabla} \right) + \frac{1}{2V_0} \sum_{\alpha} \langle \tilde{\mathbf{F}}_{\alpha} \cdot (\dot{\tilde{\mathbf{u}}}_{\alpha} + \dot{\tilde{\mathbf{u}}}) \rangle. \quad (39)$$

Comparing the last expression with energy balance equation for a continuum media [15] one can conclude that expression for divergency of heat flux in the reference configuration \mathbf{h} has form

$$\overset{\circ}{\nabla} \cdot \mathbf{h} = -\frac{1}{2V_0} \sum_{\alpha} \langle \tilde{\mathbf{F}}_{\alpha} \cdot (\dot{\tilde{\mathbf{u}}}_{\alpha} + \dot{\tilde{\mathbf{u}}}) \rangle = -\frac{1}{2V_0} \sum_{\alpha} \langle \tilde{\mathbf{F}}_{\alpha} \cdot \dot{\tilde{\mathbf{u}}}_{\alpha} \rangle - \frac{1}{2V_0} \sum_{\alpha} \langle \tilde{\mathbf{F}}_{-\alpha} \cdot \dot{\tilde{\mathbf{u}}} \rangle. \quad (40)$$

Let us represent the right side of this expression in the form of divergency. Using the first identity form (12) in the right side of formula (40) one obtains

$$\langle \tilde{\mathbf{F}}_{\alpha} \cdot \dot{\tilde{\mathbf{u}}}_{\alpha} \rangle(\mathbf{r}) = -\langle \tilde{\mathbf{F}}_{-\alpha} \cdot \dot{\tilde{\mathbf{u}}} \rangle(\mathbf{r} + \mathbf{a}_{\alpha}), \quad \langle \tilde{\mathbf{F}}_{-\alpha} \cdot \dot{\tilde{\mathbf{u}}} \rangle(\mathbf{r}) = -\langle \tilde{\mathbf{F}}_{\alpha} \cdot \dot{\tilde{\mathbf{u}}}_{\alpha} \rangle(\mathbf{r} - \mathbf{a}_{\alpha}). \quad (41)$$

Substituting formulas (41) into formula (40) and applying the long wave approximation one can obtain

$$\overset{\circ}{\nabla} \cdot \mathbf{h} = \overset{\circ}{\nabla} \cdot \left(-\frac{1}{2V_0} \sum_{\alpha} \mathbf{a}_{\alpha} \langle \tilde{\mathbf{F}}_{\alpha} \cdot \dot{\tilde{\mathbf{u}}}_{\alpha} \rangle \right) = \overset{\circ}{\nabla} \cdot \left(-\frac{1}{2V_0} \sum_{\alpha} \mathbf{a}_{\alpha} \langle \tilde{\mathbf{F}}_{\alpha} \cdot \dot{\tilde{\mathbf{u}}} \rangle \right). \quad (42)$$

Using this expression one can write down three representations for heat flux in the reference configuration¹

¹ Note that heat flux is determined with the accuracy of vector with zero divergency.

$$\mathbf{h} = -\frac{1}{4V_0} \sum_{\alpha} \mathbf{a}_{\alpha} \langle \tilde{\mathbf{F}}_{\alpha} \cdot (\dot{\tilde{\mathbf{u}}}_{\alpha} + \dot{\tilde{\mathbf{u}}}) \rangle = -\frac{1}{2V_0} \sum_{\alpha} \mathbf{a}_{\alpha} \langle \tilde{\mathbf{F}}_{\alpha} \cdot \dot{\tilde{\mathbf{u}}}_{\alpha} \rangle = -\frac{1}{2V_0} \sum_{\alpha} \mathbf{a}_{\alpha} \langle \tilde{\mathbf{F}}_{\alpha} \cdot \dot{\tilde{\mathbf{u}}} \rangle \quad (43)$$

Analogous formulas can be obtained for heat flux in the actual configuration \mathbf{H}

$$\mathbf{H} = -\frac{1}{4V} \sum_{\alpha} \mathbf{A}_{\alpha} \langle \tilde{\mathbf{F}}_{\alpha} \cdot (\dot{\tilde{\mathbf{u}}}_{\alpha} + \dot{\tilde{\mathbf{u}}}) \rangle = -\frac{1}{2V} \sum_{\alpha} \mathbf{A}_{\alpha} \langle \tilde{\mathbf{F}}_{\alpha} \cdot \dot{\tilde{\mathbf{u}}}_{\alpha} \rangle = -\frac{1}{2V} \sum_{\alpha} \mathbf{A}_{\alpha} \langle \tilde{\mathbf{F}}_{\alpha} \cdot \dot{\tilde{\mathbf{u}}} \rangle \quad (44)$$

Here formula $\mathbf{H} = \frac{V_0}{V} (\mathbf{R} \overset{\circ}{\nabla}) \cdot \mathbf{h}$ relating heat fluxes in different configurations was used [6]. Note that different expressions for \mathbf{h} and \mathbf{H} in formulas (43), (44) are equal with accuracy of terms, which were neglected in the long wave approximation.

7 Constitutive relations for stress tensor and heat flux

Expressions (26), (35) connecting micro- and macro-parameters allow to derive nonlinear constitutive relations (equations of state) for thermo-elastic behavior of the crystal. This problem is considered in detail in works [7, 9]. Only main ideas and results are shown below. The relation between “cold” component of Cauchy stress² τ_0 and Cauchy-Green measure of deformation can be obtained substituting formulas (13), (27) into formula (26) (see [7] for details).

$$\tau_0 = -\frac{1}{2V_0 \sqrt{|\mathbf{G}|}} (\mathbf{R} \overset{\circ}{\nabla}) \cdot \left(\sum_{\alpha} \Phi(\mathbf{a}_{\alpha} \mathbf{a}_{\alpha} \cdot \cdot \mathbf{G}) \mathbf{a}_{\alpha} \mathbf{a}_{\alpha} \right) \cdot (\overset{\circ}{\nabla} \mathbf{R}), \quad (45)$$

where $|\mathbf{G}|$ is a determinant of tensor \mathbf{G} . Equations of state connecting thermal component of Cauchy stress $\tau_T \stackrel{\text{def}}{=} \tau - \tau_0$ with thermal energy were obtained in paper [9]. The expansion of Cauchy stress and internal energy with respect to $\tilde{\mathbf{A}}_{\alpha}$ was conducted. In particular, in the first approximation the following system was obtained

$$\begin{aligned} \tau_T &= -\frac{1}{2V} \sum_{\alpha} [2\Phi'_{\alpha} \mathbf{A}_{\alpha} \mathbf{E} \mathbf{A} + \Phi'_{\alpha} \mathbf{A}_{\alpha} \mathbf{A}_{\alpha} \mathbf{E} + 2\Phi''_{\alpha} \mathbf{A}_{\alpha} \mathbf{A}_{\alpha} \mathbf{A}_{\alpha} \mathbf{A}_{\alpha}] \cdot \cdot \langle \tilde{\mathbf{A}}_{\alpha} \tilde{\mathbf{A}}_{\alpha} \rangle, \\ U_T &= -\frac{1}{2} \sum_{\alpha} [\Phi_{\alpha} \mathbf{E} + 2\Phi'_{\alpha} \mathbf{A}_{\alpha} \mathbf{A}_{\alpha}] \cdot \cdot \langle \tilde{\mathbf{A}}_{\alpha} \tilde{\mathbf{A}}_{\alpha} \rangle, \quad \Phi_{\alpha}^{(n)} \stackrel{\text{def}}{=} \frac{d^n \Phi}{d(A_{\alpha}^2)^n} \end{aligned} \quad (46)$$

Here U_T is a thermal energy per unit volume. It was assumed that $\langle \tilde{\mathbf{A}}_{\alpha} \tilde{\mathbf{A}}_{\alpha} \rangle = \frac{1}{d} \kappa^2 \mathbf{E}$, $\kappa^2 \stackrel{\text{def}}{=} \langle \tilde{\mathbf{A}}_{\alpha}^2 \rangle$ in order to close system (46). In the framework of the assumption system (46) takes form

$$\tau_T = \frac{1}{V} \Gamma U_T, \quad \Gamma \stackrel{\text{def}}{=} \frac{\sum_{\alpha} ((d+2)\Phi'_{\alpha} + 2\Phi''_{\alpha} A_{\alpha}^2) \mathbf{A}_{\alpha} \mathbf{A}_{\alpha}}{\sum_{\alpha} (d\Phi_{\alpha} + 2\Phi'_{\alpha} A_{\alpha}^2)}. \quad (47)$$

² Stress in the crystal in the absence of thermal motion.

Expression (47) is generalized Mie-Gruneisen equation, where Γ is tensor Gruneisen coefficient. Note that more accurate equations of state can be obtained leaving higher order terms in expansions (46). For further details about the approach for derivation of equations of state see paper [9].

Let us consider propagation of small thermal disturbances. Assume that the amplitude of thermal oscillations is small in comparison with interatomic distance. Expanding expression for heat flux (44) with respect to $\tilde{\mathbf{A}}_\alpha$ and leaving terms of order of $\tilde{\mathbf{A}}_\alpha^2$ only one obtains

$$\mathbf{H} = \frac{1}{2V} \sum_{\alpha} (\Phi(\mathbf{A}_\alpha^2) \mathbf{A}_\alpha \mathbf{E} + 2\Phi'(\mathbf{A}_\alpha^2) \mathbf{A}_\alpha \mathbf{A}_\alpha \mathbf{A}_\alpha) \cdot \langle \tilde{\mathbf{A}}_\alpha \dot{\tilde{\mathbf{u}}}_\alpha \rangle, \quad \Phi' \stackrel{\text{def}}{=} \frac{d\Phi}{dA_\alpha^2}. \quad (48)$$

Expression (48) is satisfied for arbitrary nonlinear elastic deformations. Let us consider the case when discrete system is free from internal mechanical loads and constraints. In this case deformations are caused by thermal expansion only. Then the reference and actual configurations approximately coincide. Linearizing expression (48) assuming that $\mathbf{A}_\alpha \approx \mathbf{a}_\alpha$ one obtains

$$\mathbf{H} = \sum_{\alpha} {}^3\mathbf{C}_\alpha \cdot \langle \tilde{\mathbf{A}}_\alpha \dot{\tilde{\mathbf{u}}}_\alpha \rangle = \sum_{\alpha} {}^3\mathbf{C}_\alpha \cdot \langle \tilde{\mathbf{A}}_\alpha \dot{\tilde{\mathbf{u}}} \rangle, \quad (49)$$

where ${}^3\mathbf{C}_\alpha \stackrel{\text{def}}{=} \frac{1}{2V_0} (\Phi(a_\alpha^2) \mathbf{a}_\alpha \mathbf{E} + 2\Phi'(a_\alpha^2) \mathbf{a}_\alpha \mathbf{a}_\alpha \mathbf{a}_\alpha)$. Let us represent the expression for heat flux in the form of divergency.

$$\mathbf{H} = \sum_{\alpha} {}^3\mathbf{C}_\alpha \cdot \langle \tilde{\mathbf{A}}_\alpha \dot{\tilde{\mathbf{u}}}_\alpha \rangle \approx \nabla \cdot \left(\frac{1}{2} \sum_{\alpha} \mathbf{a}_\alpha {}^3\mathbf{C}_\alpha \cdot \langle \widetilde{\mathbf{u}\mathbf{u}} \rangle \right) - \sum_{\alpha} {}^3\mathbf{C}_\alpha \cdot \langle \widetilde{\mathbf{u}\dot{\mathbf{u}}}_\alpha \rangle^S. \quad (50)$$

Here the following identity was used $\sum_{\alpha} {}^3\mathbf{C}_\alpha = 0$. From formula (50) it follows that, in contrast to classical Fourier law, the heat flux depends on the set of symmetrical tensors $\langle \widetilde{\mathbf{u}\mathbf{u}} \rangle, \langle \widetilde{\mathbf{u}\dot{\mathbf{u}}}_\alpha \rangle^S$. Let us try to connect heat flux with temperature. Classical ideal gas definition of temperature is used

$$dkT = m \langle \widetilde{\mathbf{u}}^2 \rangle, \quad (51)$$

where k is Boltzman constant. Equation (51) can be transformed taking into account equation of motion (15)

$$dkT = m \langle \widetilde{\mathbf{u}} \cdot \dot{\tilde{\mathbf{u}}} \rangle - \left\langle \sum_{\alpha} \tilde{\mathbf{F}}_\alpha \cdot \tilde{\mathbf{u}} \right\rangle \approx m \langle \widetilde{\mathbf{u}} \cdot \dot{\tilde{\mathbf{u}}} \rangle + \sum_{\alpha} (\Phi \mathbf{E} + 2\Phi' \mathbf{a}_\alpha \mathbf{a}_\alpha) \cdot \langle \tilde{\mathbf{u}} \tilde{\mathbf{A}}_\alpha \rangle. \quad (52)$$

Here the expansion into series with respect to $\tilde{\mathbf{A}}_\alpha$ is carried out. The second order terms are leaved only. Using the definition of tensor ${}^3\mathbf{C}_\alpha$ let us write down the resulting system for connection between heat flux and temperature.

$$\begin{aligned}
\mathbf{H} &= \nabla \cdot \left(\frac{1}{2} \sum_{\alpha} \mathbf{a}_{\alpha} {}^3\mathbf{C}_{\alpha} \cdot \langle \widetilde{\mathbf{u}\mathbf{u}} \rangle \right) - \sum_{\alpha} {}^3\mathbf{C}_{\alpha} \cdot \langle \widetilde{\mathbf{u}\mathbf{u}}_{\alpha} \rangle^S \\
dkT &= \frac{m}{2} \mathbf{E} \cdot \langle \widetilde{\mathbf{u}\mathbf{u}} \rangle + \sum_{\alpha} \frac{2V_0}{a_{\alpha}^2} \mathbf{a}_{\alpha} \cdot {}^3\mathbf{C}_{\alpha} \cdot \langle \widetilde{\mathbf{u}\mathbf{u}}_{\alpha} - \widetilde{\mathbf{u}\mathbf{u}} \rangle^S.
\end{aligned} \tag{53}$$

According to system (53) the thermal state at the given point is determined by symmetrical tensors³ $\langle \widetilde{\mathbf{u}\mathbf{u}} \rangle, \langle \widetilde{\mathbf{u}\mathbf{u}}_{\alpha} \rangle^S$. In general, these tensors are independent. Therefore system (53) is not closed.

8 Concluding remarks

The generalization of the approach proposed in [7] that allows to carry out the transformation from discrete system to equivalent continuum was presented. Two main principles were used for the transformation: the decomposition of particles' motions into continuum and thermal parts, and the long wave assumption [2]. The review of different methods for decomposition was given. It was shown that all of them contain uncertain parameters. Therefore, the result of decomposition is principally nonunique. Thus, one can conclude that derivations should not be based on any specific decomposition type. The connection between kinematics of discrete system and kinematics equivalent continuum was analyzed. Equivalent Cauchy-Green measure of deformation for discrete system was introduced. The transition from single particle's equation of motion to equation of motion for equivalent continuum was carried out. Expressions connecting Cauchy and Piola stress tensors with parameters of the discrete system were derived. It was shown that discrete analog of Cauchy stress tensor can be non-symmetrical. Spatial averaging is necessary for the symmetry of this tensor. Thus, averaging operator cannot be arbitrary and should contain spatial averaging. The energy balance equation for discrete system was considered. The equation was transformed to the form similar to energy balance equation for a continuum system. As a result, the expression connecting heat flux with parameters of discrete system was obtained. Propagation of small thermal disturbances in undeformed crystal was analyzed. It was shown that thermal state at the point is determined by the set of independent symmetrical tensors $\langle \widetilde{\mathbf{u}\mathbf{u}} \rangle, \langle \widetilde{\mathbf{u}\mathbf{u}}_{\alpha} \rangle^S$. This fact does not allow to connect heat flux with temperature. Equation of state in generalized Mie-Gruneisen form connecting Cauchy stress tensor with deformation gradient and thermal energy is obtained from microscopic considerations.

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³ Tensors $\langle \widetilde{\mathbf{u}\mathbf{u}}_{\alpha} \rangle^S$ can be represented via time derivatives of tensors $\langle \widetilde{\mathbf{u}\mathbf{u}}_{\alpha} \rangle^S$ using long wave approximation.

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