Thermo-mechanical effects in perfect crystals

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Abstract Thermo-mechanical behavior of perfect crystals is investigated. The approach based on the averaging of equations of motion is considered. Long wave approximation is used to make link between the discrete system and equivalent continuum. Macroscopic thermo-mechanical values such as Piola and Cauchy stress tensors, thermal energy, heat flux are represented via microscopic parameters. Expansion of the expression for heat flux into series with respect to small thermal parameter is conducted. Connection between the heat flux and temperature is discussed. The influence of thermal motion on wave propagation is investigated. Nonlinear wave equation in adiabatic assumption is obtained. Linearization of this equation is considered. Equation of propagation of linear waves in uniformly deformed crystal which takes thermal motion into account is obtained.

1 Introduction

Determination of the connection between parameters of discrete and continual systems is one of the challenging problems for modern physics. In spite of the intensity and time period of investigations in this direction 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, 5] and discrete-continual [15, 14] methods of simulations of mechanical behavior of bodies under mechanical and thermal loadings. Various methods of tran-

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sition from discrete system to equivalent continual exist. Long wave assumption is used in [2]. The concept of quasicontinuum is proposed in [10]. Localization functions are used in [4, 16]. 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 is used for description of thermal properties. There are different approaches for decomposition. In papers [4, 16, 20] the decomposition of particles' velocities is conducted by the use of localization functions. As a result, the dependencies of stress tensor and heat flux on parameters of the discrete system were obtained and analyzed. Another approach was proposed in [19]. Fourier transformation was used for decomposition of displacements and velocities of particles. Different methods of decompositions 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 long wave assumption [2] was proposed in papers [7, 8]. It was used for the derivation of the expressions for stress tensors for ideal crystals 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 conduct analytical derivations. In particular, equation of state in Mie-Gruneisen form was obtained in papers [7, 8, 9].

In the present paper generalization of approaches proposed in [7, 8] for two and three-dimensional cases is conducted. The connection between macro and micro parameters is obtained. The expressions for Piola and Cauchy stress tensors, heat flux are derived. The symmetry of microscopical analog of Cauchy stress tensor is discussed. The nonlinear wave equation which takes thermal motion into account is derived in adiabatic approximation. The propagation of linear waves in deformed and heated crystal is considered.

2 Hypotheses

Let us consider discrete system consisted of the particles which form the infinite ideal crystal lattice in d-dimensional space ($d = 1, 2$ or 3). Only the crystals of simple structure will be investigated (i.e. crystals that do not change under translation on any vector connecting two lattice nodes). For the sake of simplicity let particles interact via pairwise potential of Lennard-Johns type.

Two main principles will be used for transition from discrete system to equivalent continual: decomposition of motions of particles into slow continual and fast thermal [19, 7] and long wave assumption [2]. First let us focus on decomposition. In literature it is conducted via different types of averaging such as spatial averaging, time averaging, averaging over phase space or over frequency spectrum, etc. It was noted in paper [19] that unique decomposition is impossible because rules of the choice of averaging parameters like period of averaging, representative volume, etc. do not exist. It is only clear that these parameters should be connected with time

and spatial scales of the problem being solved. Let us denote average and oscillating (thermal) components of physical value f as $\left\langle f \right\rangle$ and $\widetilde{f}$ respectively. Obviously,

$$f = \left\langle f \right\rangle + \widetilde{f}, \qquad \widetilde{f} \stackrel{\text{def}}{=} f - \left\langle f \right\rangle. \tag{1}$$

Different forms of averaging operator $\left\langle \right\rangle$ are proposed in literature. The following operator was used in paper [7] in one dimensional case

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

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 total number of particles. Obviously these limitations are too weak. Direct and inverse Fourier transformations were used for decomposition in paper [19]. The direct transformation gives

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

where

$$\left\langle F \right\rangle(\nu) = \begin{cases} F(\nu), \nu < \nu_{cutoff} \\ 0, \nu \geq \nu_{cutoff} \end{cases} \qquad \widetilde{F}(\nu) = \begin{cases} 0, \nu < \nu_{cutoff} \\ F(\nu), \nu \geq \nu_{cutoff} \end{cases} \tag{4}$$

Here F is Fourier transform of value f, i is imaginary unit, ν_{cutoff} is cut-off frequency which according to [2] should be taken in the range 0.5-50 THz. Inverse Fourier transformation was used for obtaining of $\left\langle f \right\rangle$ and $\widetilde{f}$

$$\left\langle f \right\rangle = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \left\langle F \right\rangle e^{-i\nu t} d\nu \qquad \widetilde{f} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \widetilde{F} e^{-i\nu t} d\nu. \tag{5}$$

In the framework of the given approach the choice of cut-off frequency is almost arbitrary. In papers [4, 20] the following relations were used for decomposition of velocities of particles

$$f_i = \left\langle f \right\rangle(\mathbf{x}, t) + \widetilde{f}_k(\mathbf{x}, t), \qquad \left\langle f \right\rangle(\mathbf{x}, t) = \frac{\sum_{k=1}^{M} m_k f_k \psi(\mathbf{x} - \mathbf{x}_k)}{\sum_{k=1}^{M} m_k \psi(\mathbf{x} - \mathbf{x}_k)}. \tag{6}$$

Here $f_k, m_k, \mathbf{x}_k$ are velocity, mass and radius-vector of particle number k; $\mathbf{x}$ is coordinate of the point in space where velocity is calculated; ψ is localization function; M is the total number of particles in the system. This decomposition can be considered as spatial averaging with weight determined by function ψ. Note that

according to this approach thermal component of the velocity $\widetilde{f}_k(\mathbf{x},t)$ is continual value (it is determined in points between particles). Though several thermal velocities $f_{k1}(\mathbf{x}_0,t), f_{k2}(\mathbf{x}_0,t),\ldots$ and one continual velocity $\left\langle f \right\rangle(\mathbf{x}_0,t)$ are simultaneously determined in one spatial point $\mathbf{x}_0$. However, formally it does no 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 functions. In particular, if localization area surrounds single atom, then thermal component of the velocity is equal to zero.

One can conclude that single-valued decomposition does not exist and evidently may not exist. Thus, according to the authors of the present paper, 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 this method. In most cases of the given paper the properties of particular methods of averaging will not be used. If they are, then it will be noted. Let us speak about averaged $\left\langle f \right\rangle$ and thermal $\widetilde{f}$ components of physical value f which are connected by formula (1).

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

3 Kinematics

Let us use Lagrangian (material) description of equivalent continuum. Two configurations of continual and discrete system will be considered: reference and actual. For the sake of simplicity let us take strain-less configuration of crystal lattice as the reference one. Radius-vectors of equivalent continuum in the reference and actual configurations will be denoted as $\mathbf{r}$ and $\mathbf{R}$ respectively. Two ways of identification of particles will be 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. Starting with one reference particle let us mark all its neighbors by index α. Let us denote the vector connecting the reference particle with its neighbor number α as $\mathbf{a}_\alpha$. The numbering will be conducted in such a manner that $\mathbf{a}_\alpha$ has the following property.

$$\mathbf{a}_\alpha = -\mathbf{a}_{-\alpha}. \tag{7}$$

The same vectors in actual configuration will be represented as a sum of averaged component $\mathbf{A}_\alpha$ and thermal component $\tilde{\mathbf{A}}_\alpha$. They are connected with vectors $\mathbf{a}_\alpha$ and displacements of particles by the following expressions

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

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

Introduced numbering system has some useful properties. In order to explain them let us use the following definitions. Let us call physical value which is determined by the state of one particle as single-particle value. For example, mass of the particle, radius-vector, velocity, displacement etc. If physical value depends on more then one particle let us call it many-particle. In the present paper the following two-particle values are used: vector connecting two particles and force acting between particles. Let us consider selected properties of one-particle and many-particle values. Let $f(\mathbf{r}_0)$ be one-particle value that corresponds to particle with radius-vector $\mathbf{r}_0$ in the reference configuration. Let us denote value f which corresponds to particle number α as $f_\alpha(\mathbf{r}_0)$. Then the following two designations are equivalent

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

In the framework of this approach the magnitude of physical value f in point $\mathbf{r}_0$ can be written down in three ways

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

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

$$[f_\alpha g](\mathbf{r}_0) = [f g_{-\alpha}](\mathbf{r}_0 + \mathbf{a}_\alpha) \qquad [f_{-\alpha} g](\mathbf{r}_0) = [f g_\alpha](\mathbf{r}_0 - \mathbf{a}_\alpha) \tag{10}$$

Hereinafter square brackets mean that all values in them are calculated in the same point. Two-particle values used in the present paper has the following properties

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

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

$$[f_\alpha h_\alpha](\mathbf{r}_0) = -[f h_{-\alpha}](\mathbf{r}_0 + \mathbf{a}_\alpha) \qquad [f h_{-\alpha}](\mathbf{r}_0) = -[f_\alpha h_\alpha](\mathbf{r}_0 - \mathbf{a}_\alpha) \tag{12}$$

Now let us consider kinematics of discrete system in a long wave approximation. Average values of radius-vectors of particles will be identified with positions of corresponding points of continual media. Thus if some particle had radius-vector $\mathbf{r}$ in the reference configuration then the average value of its radius-vector in the actual configuration will be equal to $\mathbf{R}(\mathbf{r})$. The average position of its neighbor number α will be determined by vector $\mathbf{R}(\mathbf{r} + \mathbf{a}_\alpha)$. Then one can show that $\mathbf{A}_\alpha$ and $\mathbf{a}_\alpha$ are connected by the following formula

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

where $\overset{\circ}{\nabla}$ is nabla-operator in the reference configuration. Here long wave assumption was used that allows to leave only the terms of the first order. One can see that this expression is similar to the formula used in continual mechanics which connects vectors $d\mathbf{r}$ and $d\mathbf{R}$. Using equation (13) one can derive the connection between vectors $\mathbf{A}_\alpha$, $\mathbf{a}_\alpha$ with the measures of deformations used in the nonlinear theory of elasticity [12]. For example, Cauchy-Green measure $\mathbf{G}$ has the following form

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

4 Equation of momentum balance

Let us obtain the equation of motion of equivalent continuum. Thereto let us write down the equation of motion of some particle which will be called "reference particle" and conduct the decomposition of motions

$$m\ddot{\mathbf{u}} = \sum_\alpha \Big\langle \mathbf{F}_\alpha(\mathbf{A}_\alpha + \tilde{\mathbf{A}}_\alpha)\Big\rangle \qquad m\ddot{\tilde{\mathbf{u}}} = \sum_\alpha \widetilde{\mathbf{F}}_\alpha(\mathbf{A}_\alpha + \tilde{\mathbf{A}}_\alpha) \tag{15}$$

where $\mathbf{F}_\alpha$ is the force acting on the reference particle from its neighbor α; m is mass of the particle. The first of equations (15) describes slow motions of the system which can be considered as motions of continual media. The second equation describes thermal oscillations. One can see that both equations are coupled via the argument of the force $\mathbf{F}_\alpha$. 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 [11].

Let us conduct the following transformations in the first of equations (15).

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

It was mentioned that $\mathbf{F}_\alpha$ is two-particle value then the identity (11) is satisfied.

$$\mathbf{F}_\alpha(\mathbf{r} - \mathbf{a}_\alpha) = -\mathbf{F}_{-\alpha}(\mathbf{r}) \tag{17}$$

Equation (17) reflects the third Newton's law. Averaging this equation and using long wave assumption one can obtain

$$\Big\langle \mathbf{F}_{-\alpha} \Big\rangle(\mathbf{r}) \approx -\Big\langle \mathbf{F}_\alpha \Big\rangle(\mathbf{r}) + \mathbf{a}_\alpha \cdot \overset{\circ}{\nabla} \Big\langle \mathbf{F}_\alpha \Big\rangle(\mathbf{r}) \tag{18}$$

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

$$\frac{m}{V_0}\ddot{\mathbf{u}} = \overset{\circ}{\nabla}\cdot\left(\frac{1}{2V_0}\sum_{\alpha}\mathbf{a}_\alpha\left\langle\mathbf{F}_\alpha\right\rangle\right) \tag{19}$$

Let us compare formula (19) with equation of motion of continuum in Piola's form [12]. In order to have discrete and continual systems equivalent the following identities should be satisfied

$$\mathbf{P} = \frac{1}{2V_0}\sum_{\alpha}\mathbf{a}_\alpha\left\langle\mathbf{F}_\alpha\right\rangle, \qquad \rho_0 = \frac{m}{V_0}, \tag{20}$$

where $\mathbf{P}$ is Piola stress tensor, ρ_0 is density in the reference configuration.

Now let us conduct the same derivations in arbitrary actual configuration. Equation of motion for the particle has form (16). Let us write down relations (17), (18) in the actual configuration

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

Substituting the given expression into equation (16) and dividing both parts by the volume of elementary cell in the actual configuration V one obtains

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

Let us conduct the following transformations in right side

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

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

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

The last expression is equal to zero in accordance to Piola's identity [12]

$$\nabla\cdot\left(\frac{V_0}{V}\left(\mathbf{R}\,\overset{\circ}{\nabla}\right)\right) \equiv 0.$$

Then equation of motion (22) has the following form

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

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

$$\tau = \frac{1}{2V}\sum_{\alpha}\mathbf{A}_{\alpha}\Big\langle\mathbf{F}_{\alpha}\Big\rangle, \qquad \rho = \frac{m}{V}. \tag{26}$$

If thermal motion is not taken into account this expression coincides with expressions derived in papers [7, 18].

It is known that Cauchy stress tensor is symmetrical in the systems without moment interactions. Let us show that tensor τ determined by formula (26) is not symmetrical in the general case. The force can be represented as

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

Substituting the given expression into expression (26) one obtains

$$\tau = -\frac{1}{2V}\sum_{\alpha}\Big\langle\Phi_{\alpha}\Big\rangle\mathbf{A}_{\alpha}\mathbf{A}_{\alpha} - \frac{1}{2V}\sum_{\alpha}\mathbf{A}_{\alpha}\Big\langle\widetilde{\Phi}_{\alpha}\tilde{\mathbf{A}}_{\alpha}\Big\rangle. \tag{28}$$

The first tensor in the right side of (28) is symmetrical. Therefore the second tensor also have to be symmetrical but in general it is not the case.

5 Equation of balance of moment of momentum

It is known from continual mechanics [13] that the symmetry of Cauchy stress tensor follows from equation of balance of moment of momentum for elementary volume. In discrete case elementary cell plays the role of elementary volume. Let us write down the averaged equation of balance of moment of momentum for elementary cell. Moments will be calculated with respect to the center of the cell determined by vector $\mathbf{R}$.

$$m\Big\langle\widetilde{\mathbf{u}}\times\dot{\widetilde{\mathbf{u}}}\Big\rangle^{\cdot} = \Big\langle\widetilde{\mathbf{u}}\times\sum_{\alpha}\widetilde{\mathbf{F}}_{\alpha}\Big\rangle = \frac{1}{2}\Big\langle\widetilde{\mathbf{u}}\times\sum_{\alpha}\Big(\widetilde{\mathbf{F}}_{\alpha}+\widetilde{\mathbf{F}}_{-\alpha}\Big)\Big\rangle. \tag{29}$$

Transforming the right side of the given equation with the use of identity (12) one obtains

$$\begin{aligned}\Big[\widetilde{\mathbf{u}}\times\widetilde{\mathbf{F}}_{\alpha}\Big](\mathbf{r}) &= -\Big[\tilde{\mathbf{A}}_{\alpha}\times\widetilde{\mathbf{F}}_{\alpha}\Big](\mathbf{r}) + \Big[\widetilde{\mathbf{u}}_{\alpha}\times\widetilde{\mathbf{F}}_{\alpha}\Big](\mathbf{r}) = \\ &= -\Big[\tilde{\mathbf{A}}_{\alpha}\times\widetilde{\mathbf{F}}_{\alpha}\Big](\mathbf{r}) - \Big[\widetilde{\mathbf{u}}\times\widetilde{\mathbf{F}}_{-\alpha}\Big](\mathbf{r}+\mathbf{a}_{\alpha})\end{aligned} \tag{30}$$

Averaging this expression and applying long wave assumption one obtains

$$\Big\langle\widetilde{\mathbf{u}}\times\Big(\widetilde{\mathbf{F}}_{\alpha}+\widetilde{\mathbf{F}}_{-\alpha}\Big)\Big\rangle \approx -\Big\langle\tilde{\mathbf{A}}_{\alpha}\times\widetilde{\mathbf{F}}_{\alpha}\Big\rangle - \mathbf{a}_{\alpha}\cdot\overset{\circ}{\nabla}\Big\langle\widetilde{\mathbf{u}}\times\widetilde{\mathbf{F}}_{-\alpha}\Big\rangle \tag{31}$$

Substituting the result into equation (29) and solving it with respect to $\Big\langle\tilde{\mathbf{A}}_{\alpha}\times\widetilde{\mathbf{F}}_{\alpha}\Big\rangle$ one can obtain

$$\frac{1}{2}\sum_{\alpha}\left\langle \tilde{\mathbf{A}}_{\alpha}\times\widetilde{\mathbf{F}}_{\alpha}\right\rangle = \frac{1}{2}\sum_{\alpha}\mathbf{a}_{\alpha}\cdot\overset{\circ}{\nabla}\left\langle \widetilde{\mathbf{u}}\times\widetilde{\mathbf{F}}_{\alpha}\right\rangle - m\left\langle \widetilde{\mathbf{u}}\times\dot{\widetilde{\mathbf{u}}}\right\rangle^{\cdot} \tag{32}$$

Using formula (27) one can show that

$$\sum_{\alpha}\left\langle \tilde{\mathbf{A}}_{\alpha}\times\widetilde{\mathbf{F}}_{\alpha}\right\rangle = -\sum_{\alpha}\mathbf{A}_{\alpha}\times\left\langle \widetilde{\Phi}_{\alpha}\tilde{\mathbf{A}}_{\alpha}\right\rangle. \tag{33}$$

As a result one obtains

$$-\frac{1}{2}\sum_{\alpha}\mathbf{A}_{\alpha}\times\left\langle \widetilde{\Phi}_{\alpha}\tilde{\mathbf{A}}_{\alpha}\right\rangle = m\left\langle \widetilde{\mathbf{u}}\times\dot{\widetilde{\mathbf{u}}}\right\rangle^{\cdot} - \frac{1}{2}\sum_{\alpha}\mathbf{a}_{\alpha}\cdot\overset{\circ}{\nabla}\left\langle \widetilde{\mathbf{u}}\times\widetilde{\mathbf{F}}_{\alpha}\right\rangle. \tag{34}$$

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

$$\tau\cdot\times\mathbf{E} = -\frac{1}{2V}\sum_{\alpha}\mathbf{a}_{\alpha}\cdot\overset{\circ}{\nabla}\left\langle \widetilde{\mathbf{u}}\times\widetilde{\mathbf{F}}_{\alpha}\right\rangle + \rho\left\langle \widetilde{\mathbf{u}}\times\dot{\widetilde{\mathbf{u}}}\right\rangle^{\cdot}, \tag{35}$$

where $\mathbf{E}$ is unit tensor. Multiplying both parts by $\mathbf{E}$ one obtains

$$\tau^{A} = -\frac{1}{2V}\sum_{\alpha}\mathbf{a}_{\alpha}\cdot\overset{\circ}{\nabla}\left\langle \widetilde{\mathbf{u}}\widetilde{\mathbf{F}}_{\alpha}\right\rangle^{A} + \rho\left\langle \widetilde{\mathbf{u}}\ddot{\widetilde{\mathbf{u}}}\right\rangle^{A}. \tag{36}$$

Here A denotes an 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 can be neglected because of long wave assumption. The second term is small only on the average over the space. In order to show this let us conduct the following reasoning. Obviously, the following identity is satisfied

$$\rho\left\langle \widetilde{\mathbf{u}}\times\dot{\widetilde{\mathbf{u}}}\right\rangle^{\cdot} = \rho\left\langle (\mathbf{R}+\widetilde{\mathbf{u}})\times\dot{\widetilde{\mathbf{u}}}\right\rangle^{\cdot}. \tag{37}$$

Right side of this equation is derivative of the part of moment of momentum which corresponds to thermal motion. Moment of momentum is calculated with respect to origin of coordinates. Let the averaging operator incudes spatial averaging over significantly big volume and let us assume that thermal motion does not lead to macroscopic rotation of the volume. Then expressions (37) are equal to zero. As a result τ^{A} has the same order as terms which were neglected in long wave approximation. Consequently, $||\tau^{A}|| \ll ||\tau^{S}||$ and tensor (26) can be considered as approximately symmetrical.

Thus averaging operator proposed above can not be arbitrary. It should include spatial averaging. Otherwise tensor τ will not be symmetrical and the usage of formula (26) in calculations can leads to incorrect results.

6 Equation of energy balance

For the sake of simplicity let us consider the case when volumetrical forces and volumetrical heat sources are equal to zero. Derivations will be conducted in the reference configuration. In this case averaged specific total energy per volume V_0 has the following form

$$\rho_0 \mathscr{E} = \frac{1}{2}\rho_0 \Big\langle (\dot{\mathbf{u}} + \dot{\tilde{\mathbf{u}}})^2 \Big\rangle + \frac{1}{2V_0}\sum_{\alpha} \Big\langle \Pi(\mathbf{A}_\alpha + \tilde{\mathbf{A}}_\alpha) \Big\rangle, \tag{38}$$

where $\mathscr{E}$ is the total energy of the particle divided by its mass, i.e. discrete analog of mass density of the energy. Let us average this expression and introduce the following designations

$$\begin{aligned} &\rho_0 \mathscr{E} = \rho_0 \left(\mathscr{K} + \mathscr{U} \right), \\ &\rho_0 \mathscr{K} = \frac{1}{2}\rho_0 \dot{\mathbf{u}}^2, \qquad \rho_0 \mathscr{U} = \frac{1}{2}\rho_0 \Big\langle \dot{\tilde{\mathbf{u}}}^2 \Big\rangle + \frac{1}{2V_0}\sum_{\alpha} \Big\langle \Pi(\mathbf{A}_\alpha + \tilde{\mathbf{A}}_\alpha) \Big\rangle. \end{aligned} \tag{39}$$

Values $\mathscr{K}$ and $\mathscr{U}$ corresponds to mass densities of macroscopic kinetic and internal energies. Let us calculate the derivative of the energy with respect to time. The derivation is shown in details in appendix A. Here only final result is shown.

$$\rho_0 \dot{\mathscr{E}} = \overset{\circ}{\nabla} \cdot (\mathbf{P} \cdot \dot{\mathbf{u}}) + \frac{1}{2V_0}\sum_{\alpha} \Big\langle \widetilde{\mathbf{F}}_\alpha \cdot (\dot{\tilde{\mathbf{u}}}_\alpha + \dot{\tilde{\mathbf{u}}}) \Big\rangle. \tag{40}$$

Using equation of balance of momentum one can show that $\rho_0 \dot{\mathscr{K}} = \left(\overset{\circ}{\nabla} \cdot \mathbf{P} \right) \cdot \dot{\mathbf{u}}$. Substituting this expression into equation (40) one obtains

$$\rho_0 \dot{\mathscr{U}} = \mathbf{P} \cdot\cdot \left(\dot{\mathbf{u}} \overset{\circ}{\nabla} \right) + \frac{1}{2V_0}\sum_{\alpha} \Big\langle \widetilde{\mathbf{F}}_\alpha \cdot (\dot{\tilde{\mathbf{u}}}_\alpha + \dot{\tilde{\mathbf{u}}}) \Big\rangle. \tag{41}$$

Comparing the last expression with equation of balance of energy of continual media [13] one can conclude that expression for divergency of heat flux in the reference configuration $\mathbf{h}$ has form

$$\overset{\circ}{\nabla} \cdot \mathbf{h} = -\frac{1}{2V_0}\sum_{\alpha} \Big\langle \widetilde{\mathbf{F}}_\alpha \cdot (\dot{\tilde{\mathbf{u}}}_\alpha + \dot{\tilde{\mathbf{u}}}) \Big\rangle. \tag{42}$$

Let us represent the right side of this expression in the form of divergency of some value. For this purpose let us conduct the following transformations

$$\sum_{\alpha} \Big\langle \widetilde{\mathbf{F}}_\alpha \cdot (\dot{\tilde{\mathbf{u}}}_\alpha + \dot{\tilde{\mathbf{u}}}) \Big\rangle = \sum_{\alpha} \Big\langle \widetilde{\mathbf{F}}_\alpha \cdot \dot{\tilde{\mathbf{u}}}_\alpha \Big\rangle + \sum_{\alpha} \Big\langle \widetilde{\mathbf{F}}_{-\alpha} \cdot \dot{\tilde{\mathbf{u}}} \Big\rangle \tag{43}$$

Using the first of identities (12) in right side one obtains

$$\begin{aligned}\left\langle \widetilde{\mathbf{F}}_\alpha \cdot \dot{\widetilde{\mathbf{u}}}_\alpha \right\rangle(\mathbf{r}) &= -\left\langle \widetilde{\mathbf{F}}_{-\alpha} \cdot \dot{\widetilde{\mathbf{u}}} \right\rangle(\mathbf{r}+\mathbf{a}_\alpha),\\ \left\langle \widetilde{\mathbf{F}}_{-\alpha} \cdot \dot{\widetilde{\mathbf{u}}} \right\rangle(\mathbf{r}) &= -\left\langle \widetilde{\mathbf{F}}_{\alpha} \cdot \dot{\widetilde{\mathbf{u}}}_\alpha \right\rangle(\mathbf{r}-\mathbf{a}_\alpha).\end{aligned} \tag{44}$$

Then substituting results of formulae (44) and (43) into equation (42) and applying long wave assumption one can obtain

$$\overset{\circ}{\nabla} \cdot \mathbf{h} = \overset{\circ}{\nabla} \cdot \left(-\frac{1}{2V_0} \sum_\alpha \mathbf{a}_\alpha \left\langle \widetilde{\mathbf{F}}_\alpha \cdot \dot{\widetilde{\mathbf{u}}}_\alpha \right\rangle \right) = \overset{\circ}{\nabla} \cdot \left(-\frac{1}{2V_0} \sum_\alpha \mathbf{a}_\alpha \left\langle \widetilde{\mathbf{F}}_\alpha \cdot \dot{\widetilde{\mathbf{u}}} \right\rangle \right). \tag{45}$$

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

$$\mathbf{h} = -\frac{1}{4V_0} \sum_\alpha \mathbf{a}_\alpha \left\langle \widetilde{\mathbf{F}}_\alpha \cdot (\dot{\widetilde{\mathbf{u}}}_\alpha + \dot{\widetilde{\mathbf{u}}}) \right\rangle = -\frac{1}{2V_0} \sum_\alpha \mathbf{a}_\alpha \left\langle \widetilde{\mathbf{F}}_\alpha \cdot \dot{\widetilde{\mathbf{u}}}_\alpha \right\rangle = -\frac{1}{2V_0} \sum_\alpha \mathbf{a}_\alpha \left\langle \widetilde{\mathbf{F}}_\alpha \cdot \dot{\widetilde{\mathbf{u}}} \right\rangle \tag{46}$$

These formulae will have the following form for heat flux in the actual configuration $\mathbf{H}$

$$\mathbf{H} = -\frac{1}{4V} \sum_\alpha \mathbf{A}_\alpha \left\langle \widetilde{\mathbf{F}}_\alpha \cdot (\dot{\widetilde{\mathbf{u}}}_\alpha + \dot{\widetilde{\mathbf{u}}}) \right\rangle = -\frac{1}{2V} \sum_\alpha \mathbf{A}_\alpha \left\langle \widetilde{\mathbf{F}}_\alpha \cdot \dot{\widetilde{\mathbf{u}}}_\alpha \right\rangle = -\frac{1}{2V} \sum_\alpha \mathbf{A}_\alpha \left\langle \widetilde{\mathbf{F}}_\alpha \cdot \dot{\widetilde{\mathbf{u}}} \right\rangle \tag{47}$$

Here the following connection of heat fluxes in different configurations were used [6]

$$\mathbf{H} = \frac{V_0}{V} \left(\mathbf{R} \overset{\circ}{\nabla} \right) \cdot \mathbf{h}. \tag{48}$$

Note that different expressions for $\mathbf{h}$ and $\mathbf{H}$ in formulae (46), (47) are equal with accuracy of order of terms which were neglected in long wave assumption (42). Thus any of these formulae may be used in practice.

7 Constitutive relations for heat flux in undeformed crystal

Let us consider propagation of small thermal disturbances. Let us assume that the amplitude of thermal oscillations is small in comparison with the distance between particles. Then one can expand all expressions with respect to $\tilde{\mathbf{A}}_\alpha$ and leave only terms of order of $\tilde{\mathbf{A}}_\alpha^2$. Let us conduct this expansion in expression (27).

$$\mathbf{F}_\alpha = -\Phi(\mathbf{A}_\alpha^2)\mathbf{A}_\alpha - \left(\Phi(\mathbf{A}_\alpha^2)\mathbf{E} + 2\Phi'(\mathbf{A}_\alpha^2)\mathbf{A}_\alpha\mathbf{A}_\alpha \right) \cdot \tilde{\mathbf{A}}_\alpha + o(\tilde{\mathbf{A}}_\alpha^2), \tag{49}$$

where $\Phi' \overset{\text{def}}{=} \dfrac{d\Phi}{dA_\alpha^2}$. Calculating $\widetilde{\mathbf{F}}_\alpha$ and substituting the result into the second of formulae (47) one obtains

$$\mathbf{H} = \frac{1}{2V} \sum_\alpha \left(\Phi(\mathbf{A}_\alpha^2)\mathbf{A}_\alpha\mathbf{E} + 2\Phi'(\mathbf{A}_\alpha^2)\mathbf{A}_\alpha\mathbf{A}_\alpha\mathbf{A}_\alpha \right) \cdot\cdot \left\langle \tilde{\mathbf{A}}_\alpha \dot{\tilde{\mathbf{u}}}_\alpha \right\rangle. \tag{50}$$

The last expression is satisfied for arbitrary deformations. Now let us consider the case when discrete system is free from internal mechanical loads and constraints. In this case deformations are caused only by thermal expansion. In the case of small thermal oscillations vectors $\mathbf{A}_\alpha$ are almost equal to corresponding vectors $\mathbf{a}_\alpha$[1]. Therefore one can assume that $\mathbf{A}_\alpha \approx \mathbf{a}_\alpha$. Also the reference and actual configurations almost coincide, so $\mathbf{H} = \mathbf{h}$. Then linearized expression for heat flux has form

$$\mathbf{h} = \sum_\alpha {}^3\mathbf{C}_\alpha \cdot\cdot \left\langle \tilde{\mathbf{A}}_\alpha \dot{\tilde{\mathbf{u}}}_\alpha \right\rangle = \sum_\alpha {}^3\mathbf{C}_\alpha \cdot\cdot \left\langle \tilde{\mathbf{A}}_\alpha \dot{\tilde{\mathbf{u}}} \right\rangle, \tag{51}$$

where ${}^3\mathbf{C}_\alpha \stackrel{\text{def}}{=} \frac{1}{2V_0}\left(\Phi(a_\alpha^2)\mathbf{a}_\alpha\mathbf{E} + 2\Phi'(a_\alpha^2)\mathbf{a}_\alpha\mathbf{a}_\alpha\mathbf{a}_\alpha\right)$. One can show that tensor ${}^3\mathbf{C}_\alpha$ has the following properties

$${}^3\mathbf{C}_\alpha = -{}^3\mathbf{C}_{-\alpha}, \qquad {}^3\mathbf{C}_\alpha \cdot\cdot \mathbf{B} = {}^3\mathbf{C}_\alpha \cdot\cdot \mathbf{B}^S, \qquad \textstyle\sum_\alpha {}^3\mathbf{C}_\alpha = 0, \tag{52}$$

where $\mathbf{B}$ is arbitrary second-rank tensor. Using the first of properties (52) one can obtain

$$\mathbf{h} = \sum_\alpha {}^3\mathbf{C}_\alpha \cdot\cdot \left\langle \tilde{\mathbf{A}}_\alpha \dot{\tilde{\mathbf{u}}}_\alpha \right\rangle. \tag{53}$$

Let us represent the expression for heat flux in the form of divergency.

$$\begin{aligned} \mathbf{h} &= \sum_\alpha {}^3\mathbf{C}_\alpha \cdot\cdot \left\langle \tilde{\mathbf{A}}_\alpha \dot{\tilde{\mathbf{u}}}_\alpha \right\rangle = \sum_\alpha {}^3\mathbf{C}_\alpha \cdot\cdot \left\langle \tilde{\mathbf{u}}_\alpha \dot{\tilde{\mathbf{u}}}_\alpha - \tilde{\mathbf{u}}\dot{\tilde{\mathbf{u}}} \right\rangle - \sum_\alpha {}^3\mathbf{C}_\alpha \cdot\cdot \left\langle \tilde{\mathbf{u}}\dot{\tilde{\mathbf{u}}}_\alpha \right\rangle \approx \\ &\approx \nabla\cdot\left(\sum_\alpha \mathbf{a}_\alpha {}^3\mathbf{C}_\alpha \cdot\cdot \left\langle \tilde{\mathbf{u}}\dot{\tilde{\mathbf{u}}} \right\rangle\right) - \sum_\alpha {}^3\mathbf{C}_\alpha \cdot\cdot \left\langle \tilde{\mathbf{u}}\dot{\tilde{\mathbf{u}}}_\alpha \right\rangle \end{aligned} \tag{54}$$

Here the following identity was used $\sum_\alpha {}^3\mathbf{C}_\alpha \cdot\cdot \left\langle \tilde{\mathbf{u}}\tilde{\mathbf{u}} \right\rangle = 0$. Transforming equation (54) using the second of properties (52) one obtains

$$\mathbf{h} = \nabla\cdot\left(\frac{1}{2}\sum_\alpha \mathbf{a}_\alpha {}^3\mathbf{C}_\alpha \cdot\cdot \left\langle \tilde{\mathbf{u}}\tilde{\mathbf{u}} \right\rangle^{\cdot}\right) - \sum_\alpha {}^3\mathbf{C}_\alpha \cdot\cdot \left\langle \tilde{\mathbf{u}}\dot{\tilde{\mathbf{u}}}_\alpha \right\rangle^S. \tag{55}$$

From equation (55) it follows that heat flux depends on two symmetrical tensors $\left\langle \tilde{\mathbf{u}}\tilde{\mathbf{u}} \right\rangle$ and $\left\langle \tilde{\mathbf{u}}\dot{\tilde{\mathbf{u}}}_\alpha \right\rangle^S$ in contrast to classical Fourier law, where it depends on one scalar parameter (temperature).

Let us try to connect heat flux with temperature. Let us use classical definition of temperature

$$dkT = m\left\langle \dot{\tilde{\mathbf{u}}}^2 \right\rangle, \tag{56}$$

where k is Boltsman constant. Equation (56) can be transformed using the following identity

$$\left\langle \dot{\tilde{\mathbf{u}}}^2 \right\rangle = \left\langle \tilde{\mathbf{u}}\cdot\dot{\tilde{\mathbf{u}}} \right\rangle^{\cdot} - \left\langle \tilde{\mathbf{u}}\cdot\ddot{\tilde{\mathbf{u}}} \right\rangle. \tag{57}$$

[1] Coefficient of thermal expansion for metals has an order of $10^{-6}K^{-1}$

Then taking into account the equation of motion (15) one obtains

$$dkT = m\left\langle \widetilde{\mathbf{u}} \cdot \dot{\widetilde{\mathbf{u}}} \right\rangle^{\cdot} - \left\langle \sum_{\alpha} \widetilde{\mathbf{F}}_{\alpha} \cdot \widetilde{\mathbf{u}} \right\rangle. \tag{58}$$

Let us expand this expression into series with respect to $\tilde{\mathbf{A}}_{\alpha}$.

$$dkT = m\left\langle \widetilde{\mathbf{u}} \cdot \dot{\widetilde{\mathbf{u}}} \right\rangle^{\cdot} - \frac{1}{2}\sum_{\alpha} \left(\Phi \mathbf{E} + 2\Phi' \mathbf{a}_{\alpha}\mathbf{a}_{\alpha} \right) \cdot\cdot \left\langle \widetilde{\mathbf{u}}\tilde{\mathbf{A}}_{\alpha} \right\rangle \tag{59}$$

Using the definition of tensor ${}^{3}\mathbf{C}_{\alpha}$ let us write down the resulting system for connection between heat flux and temperature.

$$\begin{aligned} \mathbf{h} &= \nabla \cdot \left(\frac{1}{2}\sum_{\alpha} \mathbf{a}_{\alpha}\, {}^{3}\mathbf{C}_{\alpha} \cdot\cdot \left\langle \widetilde{\mathbf{u}}\widetilde{\mathbf{u}} \right\rangle^{\cdot} \right) - \sum_{\alpha} {}^{3}\mathbf{C}_{\alpha} \cdot\cdot \left\langle \widetilde{\mathbf{u}}\dot{\widetilde{\mathbf{u}}}_{\alpha} \right\rangle^{S} \\ dkT &= \frac{1}{2} m\mathbf{E} \cdot\cdot \left\langle \widetilde{\mathbf{u}}\widetilde{\mathbf{u}} \right\rangle^{\cdot\cdot} + V_0 \sum_{\alpha} \frac{1}{a_{\alpha}^2} \mathbf{a}_{\alpha} \cdot {}^{3}\mathbf{C}_{\alpha} \cdot\cdot \left\langle \widetilde{\mathbf{u}}\tilde{\mathbf{A}}_{\alpha} \right\rangle. \end{aligned} \tag{60}$$

According to system (60) the thermal state in the given point is determined by symmetrical tensors $\left\langle \widetilde{\mathbf{u}}\widetilde{\mathbf{u}} \right\rangle, \left\langle \widetilde{\mathbf{u}}\widetilde{\mathbf{u}}_{\alpha} \right\rangle^{S}, \left\langle \widetilde{\mathbf{u}}\dot{\widetilde{\mathbf{u}}}_{\alpha} \right\rangle^{S}$. In general, these tensors are independent therefore the system (60) is not closed.

8 Adiabatic approximation

In practice [3] the so called adiabatic assumption is used for modelling of the high speed processes such as impacts, shock wave propagation, etc. The idea is that for small characteristic times of the problem one can neglect the thermal conduction and consider the deformation process as adiabatic. In this case the equation of balance of energy (41) has form

$$\rho_0 \dot{\mathscr{U}} = \mathbf{P} \cdot\cdot \left(\mathbf{R} \overset{\circ}{\nabla} \right)^{\cdot} \tag{61}$$

Let us consider only thermo-elastic behavior of the system. Then one can write down the following constitutive relations

$$\mathscr{U} = \mathscr{U}_0(\overset{\circ}{\nabla}\mathbf{R}) + \mathscr{U}_T, \qquad \mathbf{P} = \mathbf{P}_0(\overset{\circ}{\nabla}\mathbf{R}) + \mathbf{P}_T(\overset{\circ}{\nabla}\mathbf{R}, \mathscr{U}_T), \qquad \mathbf{P}_T(\overset{\circ}{\nabla}\mathbf{R}, 0) = 0. \tag{62}$$

Here tensor Piola and internal energy $\mathscr{U}$ are divided into two components. This division is usual for high pressure physics [17]. Components with subscript 0 corresponds to values calculated at zero level of thermal motion. They will be called "cold". Components with subscript T will be called "thermal". There are two constitutive parameters in the system (61): $\overset{\circ}{\nabla}\mathbf{R}$ and $\mathscr{U}_T$. At first glance they are independent but it is not the case indeed. Expressions (62) allow two write down equation (61) for cold and thermal components separately. For cold components one has

$$\frac{d}{dt}\left(\rho_0 \mathscr{U}_0(\overset{\circ}{\nabla}\mathbf{R})\right) = \mathbf{P}_0 \cdot\cdot (\mathbf{R}\overset{\circ}{\nabla})^{\cdot} \quad \longrightarrow \quad (\rho_0 \mathscr{U}_0^* - \mathbf{P}_0)\cdot\cdot(\mathbf{R}\overset{\circ}{\nabla})^{\cdot} = 0. \tag{63}$$

Here "$*$" denotes full derivative with respect to $\overset{\circ}{\nabla}\mathbf{R}$. The following definition for derivative with respect to tensor argument was taken [12]. The derivative of n-rank tensor ${}^n\mathbf{A}$ with respect to the second rank tensor $\mathbf{Q}$ is $(n+2)$-rank tensor ${}^{n+2}\mathbf{B}$, where

$$\delta\, {}^n\mathbf{A} = {}^{n+2}\mathbf{B}\cdot\cdot\delta\mathbf{Q}^T. \tag{64}$$

Here δ means variation. In general case $(\mathbf{R}\overset{\circ}{\nabla})^{\cdot}$ is not equal to zero, therefore

$$\mathbf{P}_0 = \rho_0 \mathscr{U}_0^*. \tag{65}$$

Let us assume that $\mathscr{U}_T = \mathscr{U}_T(\overset{\circ}{\nabla}\mathbf{R})$. Then equation of balance of energy for thermal components has form

$$\rho_0 \dot{\mathscr{U}}_T = \mathbf{P}_T \cdot\cdot (\mathbf{R}\overset{\circ}{\nabla})^{\cdot} \quad \longrightarrow \quad \mathbf{P}_T(\overset{\circ}{\nabla}\mathbf{R}, \mathscr{U}_T) = \rho_0 \mathscr{U}_T^*. \tag{66}$$

Expression (66) is partial differential equation with respect to $\mathscr{U}_T(\overset{\circ}{\nabla}\mathbf{R})$. It can be solved if the dependence $\mathbf{P}_T(\overset{\circ}{\nabla}\mathbf{R}, \mathscr{U}_T)$ is known.

Let us derive nonlinear wave equation using formulae (65), (66). Substituting these expressions into equation of motion in Piola's form one obtains

$$\ddot{\mathbf{u}} = \overset{\circ}{\nabla}\cdot(\mathscr{U}_0^* + \mathscr{U}_T^*). \tag{67}$$

Let us conduct the following transformations

$$\overset{\circ}{\nabla}\cdot\mathscr{U}^* = \mathscr{U}^{*T}\cdot\overset{\circ}{\nabla} = \frac{d}{dx_k}\mathscr{U}^{*T}\cdot\mathbf{e}_k = \left(\left(\mathscr{U}^{*T}\right)^* \cdot\cdot \frac{d\mathbf{R}\overset{\circ}{\nabla}}{dx_k}\right)\cdot\mathbf{e}_k = \left(\mathscr{U}^{*T}\right)^*\cdots\mathbf{R}\overset{\circ}{\nabla}\overset{\circ}{\nabla}, \tag{68}$$

where x_k are material coordinates in the reference configuration. Then taking into account that $\mathbf{R}\,\overset{\circ}{\nabla}\overset{\circ}{\nabla} = \mathbf{u}\,\overset{\circ}{\nabla}\overset{\circ}{\nabla}$ one obtains the following wave equation

$$\ddot{\mathbf{u}} = \left(\mathscr{U}_0^{*T} + \mathscr{U}_T^{*T}\right)^*\cdots\mathbf{u}\,\overset{\circ}{\nabla}\overset{\circ}{\nabla}. \tag{69}$$

Thus if the dependence of internal energy on $\overset{\circ}{\nabla}\mathbf{R}$ is known, then equation (69) can be solved. If constitutive relation is given in the form $\mathbf{P} = \mathbf{P}(\overset{\circ}{\nabla}\mathbf{R}, \mathscr{U}_T)$, then it is more convenient to use the following equation

$$\rho_0\ddot{\mathbf{u}} = \mathbf{P}_0^{T*}\cdots\mathbf{u}\,\overset{\circ}{\nabla}\overset{\circ}{\nabla} + \left(\frac{\partial\mathbf{P}_T^T}{\partial\,\overset{\circ}{\nabla}\mathbf{R}} + \frac{1}{\rho_0}\frac{\partial\mathbf{P}_T^T}{\partial\mathscr{U}_T}\mathbf{P}_T\right)\cdots\mathbf{u}\,\overset{\circ}{\nabla}\overset{\circ}{\nabla}. \tag{70}$$

The last expression can be obtained substituting formulae (65), (66) into (69). The second term in the right side of equation (70) reflects the influence of thermal motion on the process of wave propagation. Note that equation (70) is not closed as it contains unknown function $\mathscr{U}_T(\overset{\circ}{\nabla}\mathbf{R})$. This function should be found from the solution of equation (66).

9 First approximation

In order to solve equation (70) one have to define the constitutive relation. Expressions connecting micro- and macro parameters obtained above allow to derive nonlinear constitutive relations for thermo-elastic behavior of the crystal. This problem is considered in works [7, 9]. Only the main ideas and results will be shown here. The connection between stresses and strains in the absence of thermal motion was obtained in the book [7] using relations (13), (26), (27).

$$\tau_0 = \frac{1}{2V_0|\mathbf{G}|}(\mathbf{R}\overset{\circ}{\nabla})\cdot\left(\sum_\alpha \Phi(\mathbf{a}_\alpha\mathbf{a}_\alpha\cdot\cdot\mathbf{G})\mathbf{a}_\alpha\mathbf{a}_\alpha\right)\cdot(\overset{\circ}{\nabla}\mathbf{R}). \tag{71}$$

In paper [9] the expansion of thermal components of Cauchy stress and internal energy with respect to $\tilde{\mathbf{A}}_\alpha$ was conducted. As a result, in the first approximation the following system was obtained

$$\begin{gathered}\tau_T = -\frac{1}{2V}\sum_\alpha\left[2\Phi'_\alpha\mathbf{A}_\alpha\mathbf{E}\mathbf{A}_\alpha+\Phi'_\alpha\mathbf{A}_\alpha\mathbf{A}_\alpha\mathbf{E}+2\Phi''_\alpha\mathbf{A}_\alpha\mathbf{A}_\alpha\mathbf{A}_\alpha\mathbf{A}_\alpha\right]\cdot\cdot\left\langle\tilde{\mathbf{A}}_\alpha\tilde{\mathbf{A}}_\alpha\right\rangle,\\ U_T = -\frac{1}{2}\sum_\alpha\left[\Phi_\alpha\mathbf{E}+2\Phi'_\alpha\mathbf{A}_\alpha\mathbf{A}_\alpha\right]\cdot\cdot\left\langle\tilde{\mathbf{A}}_\alpha\tilde{\mathbf{A}}_\alpha\right\rangle;\qquad \Phi_\alpha^{(n)}\overset{\text{def}}{=}\Phi^{(n)}(A_\alpha^2)\end{gathered} \tag{72}$$

Here $U_T = m\mathscr{U}_T$ is thermal energy. The following assumption was used for closure of the system (72)

$$\left\langle\tilde{\mathbf{A}}_\alpha\tilde{\mathbf{A}}_\alpha\right\rangle = \frac{1}{d}\kappa^2\mathbf{E},\qquad \kappa^2\overset{\text{def}}{=}\left\langle\tilde{\mathbf{A}}_\alpha^2\right\rangle \tag{73}$$

Using this assumption the system (72) can be rewritten in form

$$\tau_T = \frac{1}{V}\Gamma U_T,\qquad \Gamma\overset{\text{def}}{=}\frac{\sum_\alpha\left((d+2)\Phi'_\alpha+2\Phi''_\alpha A_\alpha^2\right)\mathbf{A}_\alpha\mathbf{A}_\alpha}{\sum_\alpha\left(d\,\Phi_\alpha+2\Phi'_\alpha A_\alpha^2\right)}. \tag{74}$$

The expression (74) is generalized Mie-Gruneisen equation, where Γ is tensor Gruneisen coefficient. Using the connection between Cauchy and Piola stress tensors one can write down the same expression for $\mathbf{P}_T$

$$\mathbf{P}_T = \frac{1}{V_0}\Gamma_0 U_T,\qquad \Gamma_0\overset{\text{def}}{=}\left(\mathbf{R}\overset{\circ}{\nabla}\right)^{-1}\cdot\Gamma. \tag{75}$$

Let us consider wave propagation in the material with such constitutive equation. Calculating derivatives in formula (70) one obtains

$$\frac{\partial \mathbf{P}_T^T}{\partial \overset{\circ}{\nabla} \mathbf{R}} = \frac{U_T}{V_0} \Gamma_0^{T*}, \quad \frac{\partial \mathbf{P}_T^T}{\partial \mathscr{U}_T} = \rho_0 \Gamma_0^T. \tag{76}$$

Substituting results into equation (70) one has

$$\rho_0 \ddot{\mathbf{u}} = \mathbf{P}_0^{T*} \cdots \mathbf{u} \overset{\circ}{\nabla} \overset{\circ}{\nabla} + \frac{U_T}{V_0} \left(\Gamma_0^{T*} + \Gamma_0^T \Gamma_0 \right) \cdots \mathbf{u} \overset{\circ}{\nabla} \overset{\circ}{\nabla}. \tag{77}$$

The given equation should be solved together with equation (66) which can be represented in the following

$$\mathscr{U}_T^* = \Gamma_0 \mathscr{U}_T. \tag{78}$$

Thus equations (71), (74), (75), (77), (78) give the closed system describing propagation of nonlinear waves in the crystal.

Now let us consider the propagation of linear waves in crystal under finite uniform deformation. It can be shown that for this purpose one can only linearize equation (77) in the vicinity of the reference configuration. The matter is that the only requirement for vectors of the reference configuration $\mathbf{a}_\alpha$ was that they have to satisfy the identity (7). In addition they should be independent on $\mathbf{r}$. Any uniform deformation of the lattice satisfies these requirements. Therefore any uniformly deformed configuration can be chosen as the reference one. It will not change results obtained above. The linearization of (77) is shown in appendix B. The result is as follows

$$\rho_0 \ddot{\mathbf{u}} = \left[\tau_0^* + \frac{U_T}{V_0} \left(\left(\frac{V_0}{V} \Gamma \right)^* + \Gamma \Gamma \right) \right] \cdots \mathbf{u} \nabla \nabla. \tag{79}$$

Here all values in brackets are calculated in the reference configuration. Formula (79) represents the influence of thermal motion on linear wave propagation.

10 Concluding remarks

The generalization of approach proposed in [7], which allows to conduct transformation from discrete system to equivalent continual was conducted. Two main principles were used for transformation: the decomposition of motions of particles into continual and thermal parts, and long wave assumption [2]. The review of different methods of decomposition is given. It is shown that all of them contains uncertain parameters. Therefore, the result of decomposition is principally nonunique. Thus, one can conclude that derivations should not be based on any specific type of decomposition. It was proposed to conduct decomposition with the use of averaging operator of general type. Kinematics of discrete system was considered. The relation between vectors connecting neighboring particles in reference and actual configurations and Cauchy-Green's measure of deformations is obtained. It was shown that

this relation is similar to equation for vectors $d\mathbf{r}$ and $d\mathbf{R}$ used in continual mechanics. The equation of motion of some particle is considered. The transition to equation of motion of continual media was conducted. Expressions which connect Cauchy and Piola stress tensors with parameters of 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 contains spatial averaging. The equation of balance of energy of discrete system was considered. The equation was transformed to the form similar to equation of balance of energy of continual 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 considered. It was shown that heat flux is determined by several independent symmetrical tensors. This fact does not allow to connect heat flux with temperature. Propagation of waves in the heated crystal was considered in adiabatic approximation. Nonlinear wave equation was derived. Linearization of this equation in the case of small disturbances of uniformly deformed crystal was conducted. Linear wave equation which takes thermal motion into account was obtained.

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Appendix A

Let us write down averaged specific total energy per volume V_0

$$\rho_0 \mathscr{E} = \frac{1}{2}\rho_0 \dot{\mathbf{u}}^2 + \frac{1}{2}\rho_0 \left\langle \dot{\tilde{\mathbf{u}}} \right\rangle^2 + \frac{1}{2V_0}\sum_\alpha \left\langle \Pi(\mathbf{A}_\alpha + \tilde{\mathbf{A}}_\alpha) \right\rangle \tag{80}$$

Let us derive total energy with respect to time and consider derivatives of kinetic and potential energy separately. For kinetic energy one has the following expression

$$\frac{1}{2}\rho_0 \frac{d}{dt}\left(\dot{\mathbf{u}}^2 + \left\langle \dot{\tilde{\mathbf{u}}} \right\rangle^2\right) = \rho_0 \left(\dot{\mathbf{u}}\cdot\ddot{\mathbf{u}} + \left\langle \dot{\tilde{\mathbf{u}}}\cdot\ddot{\tilde{\mathbf{u}}} \right\rangle\right) = \left(\overset{\circ}{\nabla}\cdot\mathbf{P}\right)\cdot\dot{\mathbf{u}} + \frac{1}{V_0}\sum_\alpha \left\langle \dot{\tilde{\mathbf{u}}}\cdot\widetilde{\mathbf{F}}_\alpha \right\rangle. \tag{81}$$

Deriving the potential energy one obtains

$$\frac{1}{2V_0}\frac{d}{dt}\sum_\alpha \left\langle \Pi(\mathbf{A}_\alpha + \tilde{\mathbf{A}}_\alpha) \right\rangle = \frac{1}{2V_0}\sum_\alpha \left\langle \mathbf{F}_\alpha \cdot (\dot{\mathbf{A}}_\alpha + \dot{\tilde{\mathbf{A}}}_\alpha) \right\rangle \tag{82}$$

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

$$\begin{aligned}&\sum_\alpha \left\langle \mathbf{F}_\alpha \right\rangle \cdot \dot{\mathbf{A}}_\alpha = \sum_\alpha \left\langle \mathbf{F}_\alpha \right\rangle \cdot (\dot{\mathbf{u}}_\alpha - \dot{\mathbf{u}}) = \\ &= \sum_\alpha \left\langle \mathbf{F}_\alpha \right\rangle \cdot (\dot{\mathbf{u}}(\mathbf{r}+\mathbf{a}_\alpha) - \dot{\mathbf{u}}(r)) \approx \sum_\alpha \mathbf{a}_\alpha \left\langle \mathbf{F}_\alpha \right\rangle \cdot\cdot \dot{\mathbf{u}} \overset{\circ}{\nabla}\end{aligned} \tag{83}$$

Substituting the result in formula (82) and taking into account the expression for Piola stress tensor (20) one obtains

$$\frac{1}{2V_0}\frac{d}{dt}\sum_\alpha \left\langle \Pi(\mathbf{A}_\alpha + \tilde{\mathbf{A}}_\alpha) \right\rangle = \mathbf{P} \cdot\cdot \dot{\mathbf{u}} \overset{\circ}{\nabla} + \frac{1}{2V_0}\sum_\alpha \left\langle \widetilde{\mathbf{F}}_\alpha \cdot \dot{\tilde{\mathbf{A}}}_\alpha \right\rangle \tag{84}$$

Thus summarizing expression (81) and (84) one obtains the expression for derivative of the total energy with respect to time

$$\rho_0 \dot{\mathscr{E}} = \overset{\circ}{\nabla} \cdot (\mathbf{P} \cdot \dot{\mathbf{u}}) + \frac{1}{2V_0}\sum_\alpha \left\langle \widetilde{\mathbf{F}}_\alpha \cdot \left(\dot{\tilde{\mathbf{u}}}_\alpha + \dot{\tilde{\mathbf{u}}} \right) \right\rangle. \tag{85}$$

Appendix B

In order to linearize equation (77) let us rewrite it in actual configuration. For this purpose let us consider expressions in equation (77) separately.

$$\mathbf{P}_0^{T*} \cdots \mathbf{u} \overset{\circ}{\nabla}\overset{\circ}{\nabla} = \overset{\circ}{\nabla} \cdot \mathbf{P} = \overset{\circ}{\nabla} \cdot \left(\frac{V}{V_0} \left(\mathbf{R} \overset{\circ}{\nabla} \right)^{-1} \right) \cdot \tau_0 + \frac{V}{V_0} \nabla \cdot \tau_0 = \frac{V}{V_0} \nabla \cdot \tau_0. \tag{86}$$

Here the analog of Piola's identity $\overset{\circ}{\nabla} \cdot (\frac{V}{V_0}(\mathbf{R}\overset{\circ}{\nabla})^{-1}) = 0$ was used. Similarly one can show that

$$\Gamma_0^{T*} \cdots \mathbf{u} \overset{\circ}{\nabla}\overset{\circ}{\nabla} = V \nabla \cdot \left(\frac{1}{V} \Gamma \right). \tag{87}$$

Also let us conduct the following derivations

$$\begin{aligned}&\Gamma_0^T \Gamma_0 \cdots \mathbf{u} \overset{\circ}{\nabla}\overset{\circ}{\nabla} = \Gamma_0^T \cdot \overset{\circ}{\nabla} \Gamma_0 \cdot\cdot \mathbf{u} \overset{\circ}{\nabla} = \Gamma \cdot \nabla \Gamma_0 \cdot\cdot \mathbf{u} \overset{\circ}{\nabla} = \\ &= \Gamma \Gamma_0 \cdots \left(\mathbf{u} \overset{\circ}{\nabla} \right) \nabla = \Gamma \left(\mathbf{R} \overset{\circ}{\nabla} \right)^{-1} \cdot \Gamma \cdots \left(\mathbf{u} \nabla \cdot \mathbf{R} \overset{\circ}{\nabla} \right) \nabla.\end{aligned} \tag{88}$$

Substitution of equations (86)—(88) into equation (77) gives nonlinear wave equation in actual configuration.

$$\rho \ddot{\mathbf{u}} = \nabla \cdot \tau_0 + \frac{U_T}{V} \left[V \nabla \cdot \left(\frac{1}{V} \Gamma \right) + \Gamma (\Gamma - (\mathbf{u}\nabla) \cdot \Gamma) \cdots \left(\mathbf{u} \nabla \cdot (\mathbf{E} - \mathbf{u}\nabla)^{-1} \right) \nabla \right]. \tag{89}$$

Here the expression $\overset{\circ}{\nabla}\mathbf{R} = (\mathbf{E} - \nabla\mathbf{u})^{-1}$ was used. Linearizing equation (89) in the case of small deformations one obtains equation (79).

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