Equivalent thermo-mechanical parameters for perfect crystals with arbitrary multibody potential

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Abstract

Derivation of equivalent thermo-mechanical parameters for perfect crystals in the case of arbitrary interatomic potential is conducted. 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 parameters such as Piola and Cauchy stress tensors, heat flux are represented via microscopic parameters.

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, 2] and discrete-continual [3, 4] methods of simulation of mechanical behavior of bodies under mechanical and thermal loadings. Various methods of transition from discrete system to equivalent continual exist. Long wave assumption is used in [5]. The concept of quasicontinuum is proposed in [6]. Localization functions are used in [7, 8, 9]. 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 [7, 8, 9] 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 [10]. 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 [5] was proposed in papers [11, 12]. It was used for derivation of expressions for stress tensors for ideal crystals in book [11]. Only pair potentials were considered. Thermal motion was neglected. The influence of thermal oscillations on mechanical properties was considered in [11, 12] for one dimensional case. Proposed approach gives opportunity to conduct analytical derivations. In particular, equation of state in Mie-Gruneisen form was obtained in papers [11, 12, 13].

Different assumptions about interatomic potentials were used in all papers mentioned above. This fact decreases the range of applications of results of these papers. In the present paper derivations are conducted for arbitrary many-body potential. It is assumed that the energy per one particle depends on all vectors connecting this particle with its neighbors. The approach proposed in works [11, 12] is used for transition from discrete system to equivalent continual. Equations of motion of particles are derived. The connection of Cauchy and Piola stress tensors and heat flux with parameters of discrete systems is determined. The symmetry of obtained Cauchy stress tensor is proved. Comparison with known expressions for Cauchy stress tensor is discussed.

2 Hypotheses

Let us consider discrete system of interacting particles which form perfect simple crystal lattice in $\mathsf{d} = 1, 2$ or 3 dimensions. Two main principles are used for transition from discrete system to equivalent continual: decomposition of motions of particles on slow macroscopic and fast thermal [10, 11], and long wave assumption [5]. First let us focus on decomposition. In practice different types of averaging such as time averaging, spatial averaging are used for decomposition. In paper [10] it was noted that unique decomposition is impossible because there are no rules for the choice of the period of averaging, size of representative volume, etc. These parameters should depend somehow on time and spatial scales of the considered problem. According to the opinion of the author of the present paper derivations should not be based on the particular method of decomposition. In addition results should not change qualitatively with replacement of the method of averaging. Therefore let us consider average component $\left\langle \mathsf{f} \right\rangle$ and thermal component $\widetilde{\mathsf{f}}$ of physical value f that are connected by the following expression

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

Also long wave assumption will be used [5]. The idea of the assumption is as follows: average component of any physical value is assumed to be slowly changing in space on distances of 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 allows to make transition from discrete system to continuum.

3 Kinematics

Let us use Lagrangian (material) description of equivalent continuum and consider the reference and actual configurations of discrete and continual systems. Let us take an unstrained configuration of crystal lattice as the reference one for discrete system. Let us denote radius-vectors of equivalent continuum in reference and actual configurations as $\underline{\mathrm{r}}$ and $\underline{\mathrm{R}}$ respectively. Two ways for identification of the 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 vector connecting the reference particle with its neighbor number α as $\underline{\mathrm{a}}_\alpha$. The numbering will be conducted in such a manner that $\underline{\mathrm{a}}_\alpha$ has the following property

$$\underline{\mathrm{a}}_\alpha = -\underline{\mathrm{a}}_{-\alpha}. \tag{2}$$

The same vectors in actual configuration $\underline{\mathcal{A}}_\alpha$ will be represented as a sum of averaged component $\underline{\mathrm{A}}_\alpha$ and thermal component $\underset{\sim}{\mathrm{A}}_\alpha$. The connection between vectors $\underline{\mathrm{a}}_\alpha$ and $\underline{\mathrm{A}}_\alpha$ in long wave approximation is as follows

$$\underline{\mathrm{A}}_\alpha = \underline{\mathrm{R}}(\underline{\mathrm{r}} + \underline{\mathrm{a}}_\alpha) - \underline{\mathrm{R}}(\underline{\mathrm{r}}) \approx \underline{\mathrm{a}}_\alpha \cdot \overset{\circ}{\nabla}\, \underline{\mathrm{R}}, \tag{3}$$

where $\overset{\circ}{\nabla}$ is nabla-operator in the reference configuration. Note that equation (3) is similar to equation for connection between vectors $\mathrm{d}\underline{\mathrm{R}}$ and $\mathrm{d}\underline{\mathrm{r}}$ in continual mechanics [18].

Let us consider properties of introduced numbering system. If $\mathrm{f}(\underline{\mathrm{r}})$ is a physical value which corresponds to the particle with radius-vector $\underline{\mathrm{r}}$ in the reference configuration. Then $\mathrm{f}_\alpha(\underline{\mathrm{r}})$ is the same physical value for particle α. Thus the following two expressions are equivalent

$$\mathrm{f}_\alpha(\underline{\mathrm{r}}) \equiv \mathrm{f}(\underline{\mathrm{r}} + \underline{\mathrm{a}}_\alpha). \tag{4}$$

In the framework of this approach physical value in point $\underline{\mathrm{r}}$ can be represented in three different ways.

$$\mathrm{f}(\underline{\mathrm{r}}) = \mathrm{f}_\alpha(\underline{\mathrm{r}} - \underline{\mathrm{a}}_\alpha) = \mathrm{f}_{-\alpha}(\underline{\mathrm{r}} + \underline{\mathrm{a}}_\alpha) \tag{5}$$

4 Balance of momentum

Let us assume that potential energy per one particle is represented by the following expression

$$\Pi = \Pi(\{\underline{\mathcal{A}}_\alpha\}_{\alpha\in\Lambda}), \tag{6}$$

Here $\{\underline{\mathcal{A}}_\alpha\}_{\alpha\in\Lambda}$ is the set of all vectors $\underline{\mathcal{A}}_\alpha$ for the given particle; Λ is the set of all numbers of particles which interact with the given particle. Potential energy per particle can be represented in the form (6) for the majority of commonly used potentials. In particular, equation (6) is satisfied for pair potentials, embedded atom potential [14], Stillinger-Weber potential [15], Tersoff potential [16].

Let us derive the equation of motion of the particle with radius-vector $\underline{r}$ in the reference configuration. For the sake of simplicity let us consider the case when volumetrical forces are absent. Denote radius-vector of the particle in the current moment of time by $\underline{R}_t$. The following identity is satisfied for $\underline{R}_t$

$$\underline{R}(\underline{r}) = \left\langle \underline{R}_t \right\rangle. \tag{7}$$

Let us denote potential energy per particle α as Π_α, where $\Pi_\alpha = \Pi(\{\underline{\mathcal{A}}_\beta(\underline{r}+\underline{a}_\alpha)\}_{\beta\in\Lambda})$. Using Lagrange approach one can obtain the equation of motion of the reference particle

$$m\ddot{\underline{R}}_t = -\frac{\partial}{\partial \underline{R}_t}\left(\Pi + \sum_\alpha \Pi_\alpha\right) \quad \Rightarrow \quad m\ddot{\underline{u}}_t = -\frac{\partial \Pi}{\partial \underline{u}_t} - \sum_\alpha \frac{\partial \Pi_\alpha}{\partial \underline{u}_t}, \tag{8}$$

where $\underline{u}_t$ is the current displacement of the particle, summation is conducted on the set Λ. Calculating derivatives in equation (8) one can obtain

$$\begin{gathered} \frac{\partial \Pi}{\partial \underline{u}_t} = \sum_\alpha \frac{\partial \underline{\mathcal{A}}_\alpha}{\partial \underline{u}_t} \cdot \frac{\partial \Pi}{\partial \underline{\mathcal{A}}_\alpha} = -\sum_\alpha \frac{\partial \Pi}{\partial \underline{\mathcal{A}}_\alpha}, \\ \left[\frac{\partial \Pi_\alpha}{\partial \underline{u}_t}\right](\underline{r}) = \sum_\beta \frac{\partial \underline{\mathcal{A}}_\beta(\underline{r}+\underline{a}_\alpha)}{\partial \underline{u}_t(\underline{r})} \cdot \left[\frac{\partial \Pi}{\partial \underline{\mathcal{A}}_\beta}\right](\underline{r}+\underline{a}_\alpha) = \left[\frac{\partial \Pi}{\partial \underline{\mathcal{A}}_{-\alpha}}\right](\underline{r}+\underline{a}_\alpha). \end{gathered} \tag{9}$$

Here relation $\underline{\mathcal{A}}_\alpha(\underline{r}) = -\underline{\mathcal{A}}_{-\alpha}(\underline{r}+\underline{a}_\alpha)$ was used. Square brackets mean that all expressions in brackets are calculated in one point. Substituting the result into equation of motion (8) one obtains

$$m\ddot{\underline{u}}_t = \sum_\alpha \underline{F}_\alpha, \qquad \underline{F}_\alpha \stackrel{\text{def}}{=} \frac{1}{2}\left(\underline{\mathcal{F}}_\alpha(\underline{r}) - \underline{\mathcal{F}}_{-\alpha}(\underline{r}+\underline{a}_\alpha)\right), \qquad \underline{\mathcal{F}}_\alpha \stackrel{\text{def}}{=} 2\frac{\partial \Pi}{\partial \underline{\mathcal{A}}_\alpha}. \tag{10}$$

Here $\underline{F}_\alpha$ is the force acting between the given particle and particle α. One can prove that the third Newton's law is satisfied for $\underline{F}_\alpha$, i.e. $\underline{F}_\alpha(\underline{r}) = -\underline{F}_{-\alpha}(\underline{r}+\underline{a}_\alpha)$. In the case of pair interactions one has

$$\underline{\mathcal{F}}_\alpha(\underline{r}) = -\underline{\mathcal{F}}_{-\alpha}(\underline{r}+\underline{a}_\alpha) \quad \Rightarrow \quad \underline{F}_\alpha = \underline{\mathcal{F}}_\alpha. \tag{11}$$

Note that $\underline{\mathcal{F}}_\alpha$ can be considered as a force only in this particular case. One can verify this statement on the example of embedded-atom potential [14].

Now let us obtain equation of balance of momentum for equivalent continuum. Let us average (10) and apply long wave assumption. Then the right side of equation (10) take form

$$\begin{gathered} \frac{1}{2}\sum_\alpha \left\langle \underline{\mathcal{F}}_\alpha(\underline{r}) - \underline{\mathcal{F}}_{-\alpha}(\underline{r}+\underline{a}_\alpha)\right\rangle = \frac{1}{2}\sum_\alpha \left\langle \underline{\mathcal{F}}_\alpha\right\rangle(\underline{r}) - \frac{1}{2}\sum_\alpha \left\langle \underline{\mathcal{F}}_\alpha\right\rangle(\underline{r}-\underline{a}_\alpha) \approx \\ \approx \frac{1}{2}\sum_\alpha \left\langle \underline{\mathcal{F}}_\alpha\right\rangle(\underline{r}) - \frac{1}{2}\sum_\alpha \left\langle \underline{\mathcal{F}}_\alpha - \underline{a}_\alpha \cdot \overset{\circ}{\nabla}\, \underline{\mathcal{F}}_\alpha\right\rangle(r) = \frac{1}{2}\overset{\circ}{\nabla} \cdot \left(\sum_\alpha \underline{a}_\alpha \left\langle \underline{\mathcal{F}}_\alpha\right\rangle\right), \end{gathered} \tag{12}$$

Substituting the result into averaged equation (10) and dividing both parts by the volume of elementary cell in the reference configuration one obtains

$$\rho_0 \ddot{\underline{u}} = \overset{\circ}{\nabla} \cdot \left(\frac{1}{2V_0} \sum_\alpha \underline{a}_\alpha \left\langle \underline{\mathcal{F}}_\alpha \right\rangle \right), \qquad \rho_0 \overset{\text{def}}{=} \frac{m}{V_0}. \tag{13}$$

Comparing equation (13) with equation of motion of continual media in Piola form [18] one can conclude that ρ_0 is a density of equivalent continuum in the reference configuration, expression for Piola stress tensor has the following form

$$\underline{\underline{P}} = \frac{1}{2V_0} \sum_\alpha \underline{a}_\alpha \left\langle \underline{\mathcal{F}}_\alpha \right\rangle. \tag{14}$$

Let us derive the expression for Cauchy stress tensor. One can show that in actual configuration formula (12) has the following form

$$\begin{aligned} &\frac{1}{2V} \sum_\alpha \left\langle \underline{\mathcal{F}}_\alpha(\underline{R}) - \underline{\mathcal{F}}_{-\alpha}(\underline{R} + \underline{A}_\alpha) \right\rangle = \frac{1}{2V} \sum_\alpha \underline{A}_\alpha \cdot \nabla \left\langle \underline{\mathcal{F}}_\alpha \right\rangle = \\ &= \nabla \cdot \left(\frac{1}{2V} \sum_\alpha \underline{A}_\alpha \left\langle \underline{\mathcal{F}}_\alpha \right\rangle \right) - \sum_\alpha \nabla \cdot \left(\frac{1}{2V} \underline{A}_\alpha \right) \left\langle \underline{\mathcal{F}}_\alpha \right\rangle. \end{aligned} \tag{15}$$

Here ∇, V are nabla-operator and volume of elementary cell in actual configuration. Using formula (3) and Piola's identity [18] one can show that the second term in the right side of equation (15) is equal to zero. Then substituting (15) into equation of motion (10) one obtains

$$\rho \ddot{\underline{u}} = \nabla \cdot \left(\frac{1}{2V} \sum_\alpha \underline{A}_\alpha \left\langle \underline{\mathcal{F}}_\alpha \right\rangle \right), \qquad \rho \overset{\text{def}}{=} \frac{m}{V}. \tag{16}$$

Comparing equation (16) with equation of motion of continuum in Cauchy form one can obtain the following expression for Cauchy stress tensor $\underline{\underline{\tau}}$:

$$\underline{\underline{\tau}} = \frac{1}{2V} \sum_\alpha \underline{A}_\alpha \left\langle \underline{\mathcal{F}}_\alpha \right\rangle. \tag{17}$$

In the case of the absence of thermal motion in the crystal with pair potential the result coincides with expressions proposed in papers [11, 17].

5 Balance of moment of momentum

One can see that tensor $\underline{\underline{\tau}}$ is not symmetrical in the general case. It is known from continual mechanics [19] 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 averaged equation of moment of momentum for elementary cell. Moments will be calculated with respect to the center of the cell determined by vector $\underline{R}$.

$$m \left\langle \underline{\tilde{u}} \times \dot{\underline{\tilde{u}}} \right\rangle^{\cdot} = \frac{1}{2} \left\langle \underline{\tilde{u}} \times \sum_\alpha \left(\underline{\mathcal{F}}_\alpha(\underline{r}) - \underline{\mathcal{F}}_{-\alpha}(\underline{r} + \underline{a}_\alpha) \right) \right\rangle. \tag{18}$$

Let us use the following relation

$$\left\langle \underline{\widetilde{u}}(\underline{r}) \times \underline{\mathcal{F}}_{-\alpha}(\underline{r}+\underline{a}_\alpha) \right\rangle = \left\langle \underline{\widetilde{u}}_{-\alpha} \times \underline{\mathcal{F}}_{-\alpha} \right\rangle (\underline{r}+\underline{a}_\alpha). \tag{19}$$

Substituting formula (19) into equation (18) and using long wave assumption one can obtain

$$m\left\langle \underline{\widetilde{u}} \times \dot{\underline{\widetilde{u}}} \right\rangle^{\cdot} = -\frac{1}{2}\sum_\alpha \left\langle \underline{\widetilde{A}}_\alpha \times \underline{\mathcal{F}}_\alpha \right\rangle + \frac{1}{2}\overset{\circ}{\nabla} \cdot \sum_\alpha \underline{a}_\alpha \left\langle \underline{\widetilde{u}}_\alpha \times \underline{\mathcal{F}}_\alpha \right\rangle. \tag{20}$$

where the relation $\underline{\widetilde{A}}_\alpha = \underline{\widetilde{u}}_\alpha - \underline{\widetilde{u}}$ was used. Let us represent the first expression in the right side in the following form

$$-\frac{1}{2}\sum_\alpha \left\langle \underline{\widetilde{A}}_\alpha \times \underline{\mathcal{F}}_\alpha \right\rangle = -\frac{1}{2}\sum_\alpha \left\langle \underline{\mathcal{A}}_\alpha \times \underline{\mathcal{F}}_\alpha \right\rangle + \frac{1}{2}\sum_\alpha \underline{A}_\alpha \times \left\langle \underline{\mathcal{F}}_\alpha \right\rangle. \tag{21}$$

Dividing both parts of (21) by V and using the expression (17) for Cauchy stress tensor one obtains

$$-\frac{1}{2V}\sum_\alpha \left\langle \underline{\widetilde{A}}_\alpha \times \underline{\mathcal{F}}_\alpha \right\rangle = -\frac{1}{2V}\sum_\alpha \left\langle \underline{\mathcal{A}}_\alpha \times \underline{\mathcal{F}}_\alpha \right\rangle + \underline{\underline{E}} \cdot \times \underline{\underline{\tau}}. \tag{22}$$

Substituting the right side of equation (22) into equation (20) one has

$$\underline{\underline{E}} \cdot \times \underline{\underline{\tau}} = \frac{1}{2V}\sum_\alpha \left\langle \underline{\mathcal{A}}_\alpha \times \underline{\mathcal{F}}_\alpha \right\rangle + \rho\left\langle \underline{\widetilde{u}} \times \dot{\underline{\widetilde{u}}} \right\rangle^{\cdot} - \frac{1}{2V}\sum_\alpha \underline{a}_\alpha \cdot \overset{\circ}{\nabla} \left\langle \underline{\widetilde{u}}_\alpha \times \underline{\mathcal{F}}_\alpha \right\rangle. \tag{23}$$

Let us consider the right side of equation (23). The first term is equal to zero for the majority of known potentials. This statement is proved in the appendix in the case when potential energy per particle is represented in form

$$\Pi = \Pi(\{\mathcal{A}_\alpha\}_{\alpha\in\Lambda}, \{\underline{\mathcal{A}}_\beta \cdot \underline{\mathcal{A}}_\gamma\}_{\beta,\gamma\in\Lambda}). \tag{24}$$

In other words, potential energy depends on the distances between particles and angles between bonds of the particle with its neighbors. The second term in equation (23) is equal to zero only on the average over the space. In order to show this let us conduct the following reasoning. Obviously, the following identity is satisfied

$$\rho\left\langle \underline{\widetilde{u}} \times \dot{\underline{\widetilde{u}}} \right\rangle^{\cdot} = \rho\left\langle (\underline{R}+\underline{\widetilde{u}}) \times \dot{\underline{\widetilde{u}}} \right\rangle^{\cdot}. \tag{25}$$

The right side of this equation is the derivative of the part of moment of momentum which corresponds to thermal motion. Moment of momentum is calculated with respect to the 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 (25) are equal to zero. As a result the following identity is satisfied on the average over space.

$$\underline{\underline{\tau}}^A = -\frac{1}{2V}\sum_\alpha \underline{a}_\alpha \cdot \overset{\circ}{\nabla} \left\langle \underline{\widetilde{u}}_\alpha \underline{\mathcal{F}}_\alpha \right\rangle^A. \tag{26}$$

Here index A means an antisymmetrical part of the tensor. One can see that the antisymmetrical part of the stress tensor (17) has the same order as terms which are neglected in long wave approximation. Therefore $\underline{\underline{\tau}}^A$ is small in comparison with the symmetrical part and stress tensor can be considered as approximately symmetrical.

Thus, averaging operator proposed above can not be arbitrary. It should include spatial averaging. Otherwise tensor $\underline{\underline{\tau}}$ will not be symmetrical and the usage of formula (17) in calculations can lead to incorrect results. Note that all reasoning mentioned above is satisfied only for the potentials that can be represented in form (24). Evidently one cannot prove that the first term in equation (23) is equal to zero in the case if arbitrary potential like (6). Therefore stress tensor (17) is not symmetrical in the general case.

6 Comparison with known expressions for Cauchy stress tensor

Different expressions connecting Cauchy stress tensor with parameters of discrete systems are proposed in literature. Relatively full reviews on this topic can be found in papers [9], [17]. In paper [9] it was shown that the majority of known expressions can be represented in the form proposed in paper [7]. Let us find the relation between this expression and formula (17). Let us write down the equation of thermal motion of the reference particle. It has the following form

$$m\ddot{\underline{\tilde{u}}} = \frac{1}{2}\sum_{\alpha}\left(\underline{\tilde{\mathcal{F}}}_{\alpha}(\underline{r}) - \underline{\tilde{\mathcal{F}}}_{-\alpha}(\underline{r}+\underline{a}_{\alpha})\right). \tag{27}$$

Multiplying both part of the given equation by $\underline{\tilde{u}}$ and averaging it one obtains

$$m\left\langle\underline{\tilde{u}}\dot{\underline{\tilde{u}}}\right\rangle^{\cdot} - m\left\langle\dot{\underline{\tilde{u}}}\dot{\underline{\tilde{u}}}\right\rangle = -\frac{1}{2}\sum_{\alpha}\left\langle\underline{\tilde{A}}_{\alpha}\underline{\tilde{\mathcal{F}}}_{\alpha}\right\rangle + \frac{1}{2}\sum_{\alpha}\underline{a}_{\alpha}\cdot\overset{\circ}{\nabla}\left\langle\underline{\tilde{u}}_{\alpha}\underline{\tilde{\mathcal{F}}}_{\alpha}\right\rangle. \tag{28}$$

The derivation of this formula is similar with the derivation of equation (20). Dividing both parts by volume V and using expressions (17), (21) one can obtain

$$\rho\left\langle\underline{\tilde{u}}\dot{\underline{\tilde{u}}}\right\rangle^{\cdot} - \rho\left\langle\dot{\underline{\tilde{u}}}\dot{\underline{\tilde{u}}}\right\rangle = \underline{\underline{\tau}} - \frac{1}{2V}\sum_{\alpha}\left\langle\underline{\mathcal{A}}_{\alpha}\underline{\mathcal{F}}_{\alpha}\right\rangle + \frac{1}{2V}\sum_{\alpha}\underline{a}_{\alpha}\cdot\overset{\circ}{\nabla}\left\langle\underline{\tilde{u}}_{\alpha}\underline{\tilde{\mathcal{F}}}_{\alpha}\right\rangle. \tag{29}$$

On the one hand this expression can be used for the proof of symmetry of Cauchy stress. Thereto one can calculate vector invariant of both parts of equation (29). On the other hand one can consider stationary state of the crystal[1]. In this case one obtains

$$\underline{\underline{\tau}} = \frac{1}{2V}\sum_{\alpha}\underline{A}_{\alpha}\left\langle\underline{\mathcal{F}}_{\alpha}\right\rangle = \frac{1}{2V}\sum_{\alpha}\left\langle\underline{\mathcal{A}}_{\alpha}\underline{\mathcal{F}}_{\alpha}\right\rangle - \rho\left\langle\dot{\underline{\tilde{u}}}\dot{\underline{\tilde{u}}}\right\rangle. \tag{30}$$

Thus in the particular case formulae (17) is similar with the expression used in papers [7, 9].

[1]In such state the average components of all physical values are constant in time and space

7 Balance of energy

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

$$\rho_0\mathcal{E} = \frac{1}{2}\rho_0\Big\langle(\dot{\underline{u}} + \dot{\tilde{\underline{u}}})^2\Big\rangle + \frac{1}{V_0}\Big\langle\Pi(\{\underline{\mathcal{A}}_\alpha\}_{\alpha\in\Lambda})\Big\rangle, \tag{31}$$

Here $\mathcal{E}$ is mass density of the total energy. Let us represent $\mathcal{E}$ as sum of densities of kinetic $\mathcal{K}$ and internal $\mathcal{U}$ energies. $\mathcal{K}$ is kinetic energy of average motions. $\mathcal{U}$ is potential energy plus kinetic energy of thermal motion. Then $\mathcal{K}$ and $\mathcal{U}$ has the following form

$$\rho_0\mathcal{E} = \rho_0\mathcal{K} + \rho_0\mathcal{U}, \quad \rho_0\mathcal{K} = \frac{1}{2}\rho_0\dot{\underline{u}}^2, \quad \rho_0\mathcal{U} = \frac{1}{2}\rho_0\Big\langle\dot{\tilde{\underline{u}}}^2\Big\rangle + \frac{1}{V_0}\Big\langle\Pi(\{\underline{\mathcal{A}}_\alpha\}_{\alpha\in\Lambda})\Big\rangle. \tag{32}$$

Differentiating $\mathcal{K}$ and $\mathcal{U}$ with respect to time one obtains

$$\begin{aligned}
&\rho_0\dot{\mathcal{K}} = \rho_0\ddot{\underline{u}}\cdot\dot{\underline{u}} = \Big(\overset{\circ}{\nabla}\cdot\underline{\underline{P}}\Big)\cdot\dot{\underline{u}},\\
&\rho_0\dot{\mathcal{U}} = \rho_0\Big\langle\dot{\tilde{\underline{u}}}\cdot\ddot{\tilde{\underline{u}}}\Big\rangle + \frac{1}{2V_0}\sum_\alpha\Big\langle\underline{\mathcal{F}}_\alpha\Big\rangle\cdot\dot{\underline{A}}_\alpha + \frac{1}{2V_0}\sum_\alpha\Big\langle\underline{\mathcal{F}}_\alpha\cdot\dot{\tilde{\underline{A}}}_\alpha\Big\rangle.
\end{aligned} \tag{33}$$

Where differentiation rule for multivariable function was used: $\dot{\Pi} = \sum_\alpha \frac{\partial\Pi}{\partial\underline{\mathcal{A}}_\alpha}\cdot\dot{\underline{\mathcal{A}}}_\alpha$. Let us consider terms in right side of (33) separately. The first term in the right side of equation (33) can be transformed as follows

$$\begin{aligned}
&\rho_0\Big\langle\dot{\tilde{\underline{u}}}\cdot\ddot{\tilde{\underline{u}}}\Big\rangle = \frac{1}{2V_0}\sum_\alpha\Big\langle(\underline{\mathcal{F}}_\alpha(\underline{r}) - \underline{\mathcal{F}}_{-\alpha}(\underline{r}+\underline{a}_\alpha))\cdot\dot{\tilde{\underline{u}}}(\underline{r})\Big\rangle =\\
&= \frac{1}{2V_0}\sum_\alpha\Big\langle\Big[\underline{\mathcal{F}}_\alpha\cdot\dot{\tilde{\underline{u}}}\Big](\underline{r}) - \Big[\underline{\mathcal{F}}_{-\alpha}\cdot\dot{\tilde{\underline{u}}}_{-\alpha}\Big](\underline{r}+\underline{a}_\alpha)\Big\rangle \approx -\frac{1}{2V_0}\sum_\alpha\Big\langle\underline{\mathcal{F}}_\alpha\cdot\dot{\tilde{\underline{A}}}_\alpha - \underline{a}_\alpha\cdot\overset{\circ}{\nabla}\Big(\underline{\mathcal{F}}_\alpha\cdot\dot{\tilde{\underline{u}}}_\alpha\Big)\Big\rangle.
\end{aligned} \tag{34}$$

The second term can be represented as follows

$$\frac{1}{2V_0}\sum_\alpha\Big\langle\underline{\mathcal{F}}_\alpha\Big\rangle\cdot\dot{\underline{A}}_\alpha = \frac{1}{2V_0}\sum_\alpha\Big\langle\underline{\mathcal{F}}_\alpha\Big\rangle\cdot(\dot{\underline{u}}(\underline{r}+\underline{a}_\alpha) - \dot{\underline{u}}(\underline{r})) \approx \underline{\underline{P}}\cdot\cdot\Big(\dot{\underline{u}}\,\overset{\circ}{\nabla}\Big). \tag{35}$$

Substituting results of derivations (34), (35) into equation (33) one can obtain the following expression for $\rho_0\dot{\mathcal{U}}$:

$$\rho_0\dot{\mathcal{U}} = \underline{\underline{P}}\cdot\cdot\Big(\dot{\underline{u}}\,\overset{\circ}{\nabla}\Big) + \overset{\circ}{\nabla}\cdot\left(\frac{1}{2V_0}\sum_\alpha\underline{a}_\alpha\Big\langle\underline{\mathcal{F}}_\alpha\cdot\dot{\tilde{\underline{u}}}_\alpha\Big\rangle\right). \tag{36}$$

Let us compare equation (36) with equation of balance of energy for continuum [19]. Let us demand the equivalence of discrete system and continuum. Then heat flux in the reference configuration $\underline{h}$ has the following form

$$\underline{h} = -\frac{1}{2V_0}\sum_\alpha\underline{a}_\alpha\Big\langle\underline{\mathcal{F}}_\alpha\cdot\dot{\tilde{\underline{u}}}_\alpha\Big\rangle. \tag{37}$$

Using equation for connection between fluxes in different configurations [20]

$$\underline{H} = \frac{V_0}{V}\left(\underline{R}\,\overset{\circ}{\nabla}\right)\cdot\underline{h},$$

one obtains the expression for heat flux in actual configuration $\underline{H}$:

$$\underline{H} = -\frac{1}{2V}\sum_{\alpha}\underline{A}_{\alpha}\left\langle\underline{\mathcal{F}}_{\alpha}\cdot\dot{\underline{\tilde{u}}}_{\alpha}\right\rangle. \tag{38}$$

8 Conclusion

Generalization of approach for transition from discrete system to equivalent continuum proposed in [11] was conducted. Two main principles were used for transition: decomposition of motions into continual and thermal parts, and long wave assumption [5]. The decomposition was conducted by means of averaging operator of general type. Kinematics of discrete system was considered. Connection between vectors connecting neighboring atoms in two configurations was obtained. It was shown that the connection is similar with equation for vectors $\mathrm{d}\underline{r}$ and $\mathrm{d}\underline{R}$ which is used in continual mechanics. Potential of general type was used for description of interactions. It was proposed to represent potential energy per particle as function of all vectors connecting the given particle with its neighbors. Equation of motion for some particle was obtained. Transition from this equation to equation of motion for continual system was conducted. Expressions connecting Cauchy and Piola stress tensor with parameters of discrete system were obtained. It was shown that in general case the discrete analog of Cauchy stress tensor can be unsymmetrical. The symmetry was proven in the case when potential energy per particle depends on distances between the particle and her neighbors and angles between bonds created by the particle. Also it was shown that spatial averaging is required for symmetry of the stress tensor. Thus it was proven that averaging operator can not be taken arbitrary. It was shown that expression for Cauchy stress tensor is similar with expression proposed in papers [7, 9]. Equation of balance of energy was considered. The given equation was transformed to the form similar to equation of balance of energy for continuum. As a result the expression for connection between heat flux and parameters of discrete system was obtained.

9 Appendix

It was shown that the fulfilment of the following expression is necessary for the symmetry of the discrete analog of Cauchy stress tensor

$$\sum_{\alpha}\underline{\mathcal{A}}_{\alpha}\times\underline{\mathcal{F}}_{\alpha} = 0. \tag{39}$$

For the sake of simplicity averaging operator will be omitted in this paragraph. In the case of pair interactions $\underline{\mathcal{F}}_{\alpha}$ is force between the reference particle and particle number α. Obviously $\underline{\mathcal{F}}_{\alpha}$ and $\underline{\mathcal{A}}_{\alpha}$ are collinear therefore identity (39) is satisfied.

Let us show that the identity (39) is satisfied in the case when potential energy per particle has form (24). Substituting (24) into (39) one obtains

$$\begin{aligned}\sum_{\alpha} \underline{\mathcal{A}}_{\alpha} \times \underline{\mathcal{F}}_{\alpha} &= 2 \sum_{\alpha} \underline{\mathcal{A}}_{\alpha} \times \left(\sum_{\varepsilon} \frac{\partial \Pi}{\partial \mathcal{A}_{\varepsilon}} \frac{\mathrm{d}\mathcal{A}_{\varepsilon}}{\mathrm{d}\underline{\mathcal{A}}_{\alpha}} + \sum_{\beta,\gamma} \frac{\partial \Pi}{\partial (\underline{\mathcal{A}}_{\beta} \cdot \underline{\mathcal{A}}_{\gamma})} \frac{\mathrm{d}\underline{\mathcal{A}}_{\beta} \cdot \underline{\mathcal{A}}_{\gamma}}{\mathrm{d}\underline{\mathcal{A}}_{\alpha}} \right) = \\ &= 2 \sum_{\alpha} \underline{\mathcal{A}}_{\alpha} \times \sum_{\beta,\gamma} \frac{\partial \Pi}{\partial (\underline{\mathcal{A}}_{\beta} \cdot \underline{\mathcal{A}}_{\gamma})} \left(\delta_{\alpha\beta} \underline{\mathcal{A}}_{\gamma} + \delta_{\alpha\gamma} \underline{\mathcal{A}}_{\beta} \right),\end{aligned} \tag{40}$$

where δ is Kronecker's symbol. Using the definition of Kronecker's symbol one can conduct the following transformations

$$\begin{aligned}\sum_{\alpha} \underline{\mathcal{A}}_{\alpha} \times \underline{\mathcal{F}}_{\alpha} &= 2 \sum_{\alpha,\gamma} \frac{\partial \Pi}{\partial (\underline{\mathcal{A}}_{\alpha} \cdot \underline{\mathcal{A}}_{\gamma})} \underline{\mathcal{A}}_{\alpha} \times \underline{\mathcal{A}}_{\gamma} + 2 \sum_{\alpha,\beta} \frac{\partial \Pi}{\partial (\underline{\mathcal{A}}_{\alpha} \cdot \underline{\mathcal{A}}_{\beta})} \underline{\mathcal{A}}_{\alpha} \times \underline{\mathcal{A}}_{\beta} = \\ &= 2 \sum_{\alpha,\beta} \frac{\partial \Pi}{\partial (\underline{\mathcal{A}}_{\alpha} \cdot \underline{\mathcal{A}}_{\beta})} \underline{\mathcal{A}}_{\alpha} \times \underline{\mathcal{A}}_{\beta} + 2 \sum_{\alpha,\beta} \frac{\partial \Pi}{\partial (\underline{\mathcal{A}}_{\beta} \cdot \underline{\mathcal{A}}_{\alpha})} \underline{\mathcal{A}}_{\beta} \times \underline{\mathcal{A}}_{\alpha} = 0,\end{aligned} \tag{41}$$

where the the following relation was used $\frac{\partial \Pi}{\partial (\underline{\mathcal{A}}_{\beta} \cdot \underline{\mathcal{A}}_{\alpha})} = \frac{\partial \Pi}{\partial (\underline{\mathcal{A}}_{\alpha} \cdot \underline{\mathcal{A}}_{\beta})}$.

Thus in the case when potential energy per particle is given by the formula (24) the identity (39) is satisfied.

10 Aknowlegments

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