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Thermo-mechanical effects in perfect crystals with arbitrary multibody potential

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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.

Introduction

Determination of the connection between parameters of discrete and continual systems is one of the challenging problems for modern physics. Various methods of transition from discrete system to equivalent continual exist. Long wave assumption is used in [1]. The concept of quasicontinuum is proposed in [2]. Localization functions are used in [3, 4]. 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. In papers [3, 4] 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. Fourier transformation was used in [5] 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 [1] was proposed in papers [6, 7, 8]. In book [6] it was used for derivation of expressions for stress tensors for ideal crystals with pair interactions. Thermal motion was neglected. The influence of thermal oscillations on mechanical properties was considered in [6, 7] for one dimensional case and generalized for three dimensional case in [8].

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

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present paper derivations are conducted for arbitrary multibody 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 [6, 7] 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. Relation with known expressions for Cauchy stress tensor is discussed.

Method

Hypotheses and designations

Let us consider discrete system of interacting particles which form perfect simple crystal lattice in $d = 1, 2$ 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 [5, 7], and long wave assumption [1]. First let us focus on decomposition. In practice different types of averaging, such as time averaging, spatial averaging are used for decomposition. In paper [5] 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 $\langle f \rangle$ and thermal component $\tilde{f}$ of physical value f that are connected by the following expression

$$f = \langle f \rangle + \tilde{f}. \tag{1}$$

The second important statement is long wave assumption [1]. 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.

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 material points of equivalent continuum in reference and actual configurations as $\underline{r}$ and $\underline{R}$ 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 $\underline{a}_\alpha$. The numbering will be conducted in such a manner

that $\underline{a}_\alpha$ has the following property: $\underline{a}_\alpha = -\underline{a}_{-\alpha}$. The same vectors in actual configuration $\underline{\mathcal{A}}_\alpha$ will be represented as a sum of averaged component $\underline{A}_\alpha$ and thermal component $\underline{\tilde{A}}_\alpha$.

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

$$\Pi = \Pi\left(\{\underline{\mathcal{A}}\alpha\}_{\alpha\in\Lambda}\right). \tag{2}$$

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 (2) for the majority of commonly used potentials. In particular, equation (2) is satisfied for pair potentials, embedded atom potential [9], Stillinger-Weber potential [10], Tersoff potential [11].

Derivation of expressions for thermo-mechanical parameters

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

$$m\ddot{\underline{u}}_t = -\frac{\partial\Pi}{\partial\underline{u}_t} - \sum_\alpha \frac{\partial\Pi_\alpha}{\partial\underline{u}_t}, \tag{3}$$

where $\underline{u}_t$ is the current displacement of the particle, summation is conducted on the set Λ. Calculating derivatives in equation (3) one can obtain

$$m\ddot{\underline{u}}_t = \sum_\alpha \underline{F}_\alpha, \quad \underline{F}_\alpha \overset{def}{=} \frac{1}{2}\left(\underline{\mathcal{F}}_\alpha(\underline{r}) - \underline{\mathcal{F}}_{-\alpha}(\underline{r}+\underline{a}_\alpha)\right), \quad \underline{\mathcal{F}}_\alpha \overset{def}{=} 2\frac{\partial\Pi}{\partial\underline{\mathcal{A}}_\alpha}. \tag{4}$$

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 $\underline{F}_\alpha = \underline{\mathcal{F}}_\alpha$. 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 [9].

Now let us obtain equation of balance of momentum for equivalent continuum. Let us average equation (4) and apply long wave assumption. Also let us use the following expression

$$\left\langle \underline{\underline{\mathcal{F}}}_\alpha \right\rangle (\underline{r} + \underline{a}_\alpha) \approx \left\langle \underline{\underline{\mathcal{F}}}_\alpha \right\rangle (\underline{r}) + \underline{a}_\alpha \cdot \overset{0}{\nabla} \left\langle \underline{\underline{\mathcal{F}}}_\alpha \right\rangle (\underline{r}). \tag{5}$$

Here long wave assumption was used. Substituting (5) into averaged equation (4) and comparing the result with equation of motion of continual media in Piola form one can obtain the expression for Piola stress tensor $\underline{\underline{P}}$. Similarly one can obtain the expression for Cauchy stress tensor $\underline{\underline{\tau}}$. As a result one has the following formulae

$$\underline{\underline{P}} = \frac{1}{2V_0} \sum_\alpha \underline{a}_\alpha \left\langle \underline{\underline{\mathcal{F}}}_\alpha \right\rangle, \quad \underline{\underline{\tau}} = \frac{1}{2V} \sum_\alpha \underline{A}_\alpha \left\langle \underline{\underline{\mathcal{F}}}_\alpha \right\rangle. \tag{6}$$

One can see that tensor $\underline{\underline{\tau}}$ is not symmetrical in the general case. Necessary conditions of the symmetry will be discussed later.

Let us derive the expression for heat flux. 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

$$\rho_0 E = \rho_0 K + \rho_0 U, \ \rho_0 K = \frac{1}{2} \rho_0 \dot{\underline{u}}^2, \ \rho_0 U = \frac{1}{2} \rho_0 \left\langle \dot{\underline{\tilde{u}}}^2 \right\rangle + \frac{1}{2V_0} \sum_\alpha \left\langle \Pi_\alpha \left(\{ \underline{\underline{\mathcal{F}}}_\alpha \}_{\alpha \in \Lambda} \right) \right\rangle \tag{7}$$

Here E, K, U are mass densities of the total, kinetic and internal energies respectively. Differentiating K and U with respect to time one can obtain the following expression for $\rho_0 \dot{U}$:

$$\rho_0 \dot{U} = \underline{\underline{P}} \cdot\cdot \left(\underline{u} \overset{0}{\nabla} \right)^{\cdot} + \overset{0}{\nabla} \cdot \left(\frac{1}{2V_0} \sum_\alpha \underline{a}_\alpha \left\langle \underline{\underline{\mathcal{F}}}_\alpha \cdot \dot{\underline{\tilde{u}}}_\alpha \right\rangle \right) \tag{8}$$

Comparing equation (9) with equation of balance of energy for continuum one obtains the expression for heat flux in the reference configuration $\underline{h}$. Using the known connection between fluxes in different configurations one can obtain the expression for heat flux in the actual configuration $\underline{H}$. The results are as follows

$$\underline{h} = -\frac{1}{2V_0} \sum_\alpha \underline{a}_\alpha \left\langle \underline{\underline{\mathcal{F}}}_\alpha \cdot \dot{\underline{\tilde{u}}}_\alpha \right\rangle, \quad \underline{H} = -\frac{1}{2V} \sum_\alpha \underline{A}_\alpha \left\langle \underline{\underline{\mathcal{F}}}_\alpha \cdot \dot{\underline{\tilde{u}}}_\alpha \right\rangle. \tag{9}$$

Results and Discussion

Different expressions connecting Cauchy stress tensor with parameters of discrete systems are proposed in literature. Full reviews on this topic can be found in papers [4, 5]. In paper [5] it was shown that the majority of known expressions can be represented in the form proposed in paper [3]. Let us find the relation between this expression and the second of formulae (6). Let us write down the equation of thermal motion of the reference particle. It has the following form

$$m\ddot{\underline{\tilde{u}}} = \frac{1}{2}\sum_{\alpha}\left(\underline{\tilde{\mathcal{F}}}_{\alpha}(\underline{r}) - \underline{\tilde{\mathcal{F}}}_{-\alpha}(\underline{r}+\underline{a}_{\alpha})\right), \tag{10}$$

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

$$\rho\left\langle\underline{\tilde{u}}\dot{\underline{\tilde{u}}}\right\rangle^{\cdot} - \rho\left\langle\dot{\underline{\tilde{u}}}\dot{\underline{\tilde{u}}}\right\rangle = \underline{\underline{\tau}} - \frac{1}{2V}\sum_{\alpha}\left\langle\underline{\mathcal{A}}_{\alpha}\underline{\mathcal{F}}_{\alpha}\right\rangle + \frac{1}{2V}\overset{0}{\nabla}\cdot\left(\sum_{\alpha}\underline{a}_{\alpha}\left\langle\underline{\mathcal{F}}_{\alpha}\underline{\tilde{u}}_{\alpha}\right\rangle\right) \tag{11}$$

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 (11).

$$\underline{\underline{E}}\cdot\times\underline{\underline{\tau}} = \rho\left\langle\underline{\tilde{u}}\times\dot{\underline{\tilde{u}}}\right\rangle^{\cdot} + \frac{1}{2V}\sum_{\alpha}\left\langle\underline{\mathcal{A}}_{\alpha}\times\underline{\mathcal{F}}_{\alpha}\right\rangle - \frac{1}{2V}\overset{0}{\nabla}\cdot\left(\sum_{\alpha}\underline{a}_{\alpha}\left\langle\underline{\mathcal{F}}_{\alpha}\times\underline{\tilde{u}}_{\alpha}\right\rangle\right) \tag{12}$$

The first expression in the right side of this equation is equal to the derivative of moment of momentum, which corresponds to thermal motion. Let the averaging operator includes spatial averaging over significantly big volume and let us assume that thermal motion does not lead to macroscopic rotation of the volume. Then the first term in (12) is equal to zero. One can show that the second term is equal to zero as well in the case, when potential energy has form $\Pi = \Pi\left(\{\underline{\mathcal{A}}\alpha\}_{\alpha\in\Lambda}, \left\{\underline{\mathcal{A}}\beta\cdot\underline{\mathcal{A}}\gamma\right\}_{\beta,\gamma\in\Lambda}\right)$. Therefore one can conclude that in this particular case $\|\underline{\underline{\tau}}^{A}\| \ll \|\underline{\underline{\tau}}^{S}\|$. Thus spatial averaging is necessary for symmetry of the stress tensor.

On the other hand one can consider stationary state[1]. In this case one obtains

$$\underline{\underline{\tau}} = \frac{1}{2V}\sum_{\alpha}\underline{A}_{\alpha}\left\langle\underline{\mathcal{F}}_{\alpha}\right\rangle = \frac{1}{2V}\sum_{\alpha}\left\langle\underline{\mathcal{A}}_{\alpha}\underline{\mathcal{F}}_{\alpha}\right\rangle - \rho\left\langle\dot{\underline{\tilde{u}}}\dot{\underline{\tilde{u}}}\right\rangle. \tag{13}$$

Thus in the particular case formulae (6) is similar with the expression used in papers [3, 4].

Conclusions

Generalization of approach for transition from discrete system to equivalent

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

continuum proposed in [6] was conducted. Two main principles were used for transition: decomposition of motions into continual and thermal parts, and long wave assumption [1]. The decomposition was conducted by means of averaging operator of general type. It was proposed to represent potential energy per particle as function of all vectors connecting the given particle with its neighbors. Transition from the equation of motion of discrete system to equation of motion for continuum was conducted. Expressions connecting Cauchy and Piola stress tensor with parameters of discrete system were obtained. It was shown that in the 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 its 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 [3, 4]. Equation of balance of energy was considered. The expression for connection between heat flux and parameters of discrete system was obtained.

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