A formulation of continuum mechanics as a dimensional reduction of a finite-dimensional dynamical system

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IN THE PAPER a generalized formulation of the continuum mechanics is suggested. The generalization consists in the assumption that the energy balance equation is not satisfied for all subbodies of a body but only for their chosen family. This formulation leads to fields in the continuum which create a finite-dimensional space. With the help of the chosen family of subbodies, a volume of averaging related to the continuum model is defined. This volume is connected with a more elementary dynamical system which takes part in determination of the form of constitutive equations. In general, the mechanical model of the continuum is seen as a dimensional reduction of the more elementary dynamical system related to another continuum or to a discrete set of material points.

1. Introduction

PHYSICAL PHENOMENA related to a microstructure are frequently taken into considerations in mechanical modelling of material behaviour [1, 2, 3].

The evolution of the microstructure can be quite complicated. In such cases it is difficult to postulate the form of the equations, and particularly the form of the constitutive equations for highly averaged models of the continuum.

A good illustration of such a situation is the martensitic transformation related to the shape memory alloys. In small scale we observe different martensite variants, different kinds of moving interfaces, shuffles, internal rotations, stabilization of the martensite etc. These phenomena make a mechanical description in the small scale quite complicated. On the other hand, simpler descriptions can be carried out for a more averaged continuum. However, it is then difficult to determine the form of constitutive equations. This suggests a multiscale approach, where the equations related to a small scale should form the theoretical and numerical base for those related to the larger scale. Such an approach was proposed and discussed in [12, 13, 14].

Considerations related to the model with a small scale create, in turn, new difficulties. The determination of all constants and functions related to material properties of the model in small scale often require complex discrete calculations. Then, a discrete model can form a foundation for the continuous one.

At the moment we have the following problem. All discrete models are finite-dimensional ones. During reformulating them into a continuum model, the description itself undergoes a simplification but all the fields obtained in the continuous body become infinite-dimensional ones. It is expected that continuous model should be dimensionally reduced as compared with a discrete one, and therefore the continuum theory should be finite-dimensional as well.

The next problem is related to the degree of averaging. The notion of the volume of averaging is intuitively intelligible. On the other hand, it is related to physical foundations of the mechanical model. Therefore, the notion of volume of averaging should be introduced and elucidated in detail.

The above mentioned remarks suggest that in considering complicated microstructure, it is difficult to avoid discrete calculations.

There are many efforts to provide discrete foundations for continuum mechanics [7–11] as well as simplifications in the description of complex discrete systems. The statistical mechanics reduces enormous number of degrees of freedom by the statistical averaging [4, 5]. In analytical mechanics, the well known method of constraints reduces the number of degrees of freedom [26]. There is an averaging method known in nonlinear dynamical systems [6] which leads to replacement of the complicated evolution by a simpler one. Thus, simplifications in mathematical description of complicated systems were frequently studied in literature.

The aim of this paper is to give a generalized formulation of the continuum mechanics. This formulation is in a position to adopt the point of view that the continuum appears as a dimensionally reduced discrete system, or another more complicated continuum system. Furthermore, in the frame of this formulation, the notion of volume of averaging is elucidated sufficiently.

2. An idea of a dimensional reduction

The discussion carried out in the introduction suggests that the continuum models should appear as a dimensional reduction of discrete systems. Behaviour of a system of atoms in many cases can be well approximated by a classical system of material particles. It can be obtained with the help of the Born–Oppenheimer approximation [27].

Therefore, at the beginning of our considerations an idea of a dimensional reduction of a dynamical system described by the Hamilton equations will be discussed.

Let us consider a system of N material points with masses m_i, $i \in I_N = \{1, ..., N\}$. The position of the i-th mass is given by $\mathbf{q}_i = \{q_1, q_2, q_3\}$, the velocity by $\mathbf{v}_i = \dot{\mathbf{q}}_i$, and the linear momentum by $\mathbf{p}_i = m_i\mathbf{v}_i$. Let H stand for the Hamiltonian of the system under consideration, and let $\mathbf{f}_i$ be the force related to the i-th point.

Equations of motion for this system of points are are discussed in analytical mechanics and are given in the well known form [26]

$$(2.1) \qquad \frac{d\mathbf{q}_i}{dt} = \frac{\partial H}{\partial \mathbf{p}_i}, \qquad \frac{d\mathbf{p}_i}{dt} = -\frac{\partial H}{\partial \mathbf{q}_i} + \mathbf{f}_i.$$

Let us introduce the concise notations $\mathbf{d}_i = \{\mathbf{q}_i, \mathbf{v}_i\}$, $\mathbf{d} = \{\mathbf{d}_i\}$, $\mathbf{f} = \{\mathbf{f}_i\}$,
$L(\mathbf{d}, \mathbf{f}) = \left\{\dfrac{\partial H}{\partial \mathbf{p}_i}, \dfrac{1}{m_i}\left(-\dfrac{\partial H}{\partial \mathbf{q}_i} + \mathbf{f}_i\right)\right\}$, $i \in I_N$. Then, Eqs. (2.1) can be rewritten
concisely as $\dot{\mathbf{d}} = L(\mathbf{d}, \mathbf{f})$.

The evolution function for the dynamical system defined by (2.1) can be expressed as a generalization of linearized solutions of these equations (see for instance [28]) in the form

$$(2.2) \qquad \chi(\mathbf{d}_0, \mathbf{f})(t) = e^{\int_{t_0}^{t} \frac{\partial L}{\partial \mathbf{d}}(\mathbf{d}, \mathbf{f})dt}\, \mathbf{d}_0\,,$$

where the existence of $\partial L/\partial \mathbf{d}$ is assumed.

We would like to introduce a dynamical system which would have a considerably lower dimension than the original one. Let $\mathcal{M}$ be a manifold consisting of all admissible $\mathbf{d}$. A dimensional reduction relies on introducing a smaller number of variables and on deriving a new appropriate evolution equation. Let $\overline{\mathbf{d}}$ be a variable of such a new kind of a system, and let, by analogy $\overline{\mathcal{M}} = \{\overline{\mathbf{d}}\}$. The connection between these variables can be given with the help of a map $\pi : \mathcal{M} \to \overline{\mathcal{M}}$.

External forces undergo a dimensional reduction as well. Indeed, the reduced dynamical system should be insensitive to some fine features of forces $\{\mathbf{f}_i\}$ related to a more complicated system. Therefore, by analogy, we define $\mathcal{F} = \{\mathbf{f}\}$, $\overline{\mathcal{F}} = \{\overline{\mathbf{f}}\}$ and $\pi_f : \mathcal{F} \to \overline{\mathcal{F}}$.

The map π formally reduces the dimension of the system. However, such a reduction can be accompanied by a simplification of behaviour of the system in some time interval $T = [t_0, t_0 + T]$.

Let $(\mathcal{M} \times T)_f = \{\chi(\mathbf{d}_0, \mathbf{f})(t) : t \in T, \mathbf{d}_0 \in \mathcal{M}\}$. This set consists of elements which are possible solutions of the equation (2.1) with the initial condition $\mathbf{d}(t_0) = \mathbf{d}_0$ and the given function $\mathbf{f}(t) \in \mathcal{F}_T$, where $\mathcal{F}_T = \{\mathbf{f}(t) : t \in T\}$. In a similar way we define the sets $(\overline{\mathcal{M} \times T})_{\overline{f}} = \{\overline{\chi}(\overline{\mathbf{d}}_0, \overline{\mathbf{f}}) : t \in T, \overline{\mathbf{d}}_0 \in \overline{\mathcal{M}}\}$ and $\overline{\mathcal{F}}_T = \{\overline{\mathbf{f}}(t) : t \in T\}$. With the help of these sets we can introduce new maps $\pi_T : (\mathcal{M} \times T)_f \to (\overline{\mathcal{M} \times T})_{\overline{f}}$ and $\pi_{fT} : \mathcal{F}_T \to \overline{\mathcal{F}}_T$.

For convenience, let us introduce a more general set of all continuous functions with sufficiently high time derivative $C(\overline{\mathbf{d}}_0) = \{\varphi(t) : \varphi : T \to \overline{\mathcal{M}}, \varphi(t_0) = \overline{\mathbf{d}}_0\}$.

The relation between π and π_T lies in the fact that for each $t = \overline{t}$, $\pi_T(\overline{t})$ has the same domain and range as π. Thus, π_T does not introduce new variables.

The evolution function $\overline{\chi} : T \to \overline{\mathcal{M}}$ for the dimensionally reduced dynamical system is unknown. Let us assume that the form of $\overline{\chi}$ can be expressed as

$$(2.3) \qquad \overline{\chi}(\mathbf{C}, \overline{\mathbf{d}}_0, \overline{\mathbf{f}})(t) = e^{\int_{t_0}^{t} \frac{\partial \overline{L}}{\partial \overline{\mathbf{d}}}(\mathbf{C}, \overline{\mathbf{d}}, \overline{\mathbf{f}})dt}\, \overline{\mathbf{d}}_0\,,$$

where $\mathbf{C} \in \mathcal{C}$, with $\mathcal{C}$ being a set of all admissible constants $\mathbf{C}$. Thus, the expression $(\partial \overline{L}/\partial \overline{\mathbf{d}})(\mathbf{C}, \overline{\mathbf{d}}, \overline{\mathbf{f}})$ is postulated to be dependent on $\mathbf{C}$ and operation $\partial/\partial \overline{\mathbf{d}}$ is assumed to be realizable. Consequently, the determination of a dimensionally

reduced dynamical system rests on finding π, π_T, π_f, π_{fT} and the best $\mathbf{C}^* \in \mathcal{C}$. To this end appropriate criteria should be formulated.

We can consider two kinds of dimensionally reduced time processes. The first one is induced by the Hamiltonian system. We have $\chi(\mathbf{d}_0, \mathbf{f})(t) \in (\mathcal{M} \times T)_f$. With the help of the introduced mappings $\{\pi_T, \pi_{fT}\}$, we obtain induced process $\pi_T(\chi(\mathbf{d}_0, \mathbf{f})(t))$ which belongs to a new set $(\pi\mathcal{M} \times T)_{\overline{f}}$. The second time process is related to the evolution function $\overline{\chi}(\mathbf{C}, \overline{\mathbf{d}}_0, \overline{\mathbf{f}})(t)$ which is parametrized by $\mathbf{C}$. Let us assume that for each $\mathbf{C}$ the evolution function $\overline{\chi}$ is determined. Then we are able to define a new set $(\overline{\mathcal{M}}_C \times T)_{\overline{f}} = \{\overline{\chi}(\mathbf{C}, \overline{\mathbf{d}}_0, \overline{\mathbf{f}})(t) : t \in T, \overline{\mathbf{d}}_0 \in \overline{\mathcal{M}}\}$ and two injections $i : (\pi\mathcal{M} \times T)_{\overline{f}} \to C$ and $i_c : (\overline{\mathcal{M}}_c \times T)_{\overline{f}} \to C$.

Now we have a possibility to compare two processes introduced previously. To this end, a metric on C has to be introduced. Thus, let $\varrho : C \times C \to R^+ \cup \{0\}$ be a metric on C.

With the help of the assumption (2.3) we can generate a family of processes dependent on $\mathbf{C}$ in the form $\overline{\chi}(\mathbf{C}, \overline{\mathbf{d}}_0, \overline{\mathbf{f}})(t)$, $\mathbf{C} \in \mathcal{C}$, $\overline{\mathbf{d}}_0 = \pi(\mathbf{d}_0)$, $\overline{\mathbf{f}} = \pi_{fT}(\mathbf{f})$, where $\mathbf{d}_0$ and $\mathbf{f}$ are applied to determine the Hamiltonian process $\chi(\mathbf{d}_0, \mathbf{f})(t)$.

Let us define a function

$$(2.4) \qquad h(\overline{\mathbf{d}}_0, \overline{\mathbf{f}}) = \inf_{\mathbf{C} \in \mathcal{C}} \varrho(i_c(\chi(\mathbf{C}, \overline{\mathbf{d}}_0, \overline{\mathbf{f}})(t)),\ i(\pi_T(\chi(\mathbf{d}_0, \mathbf{f})(t))).$$

By $\mathbf{C}^*$ we denote the constant $\mathbf{C} \in \mathcal{C}$ which minimizes the function h. Accordingly, $\mathbf{C}^* = \mathbf{C}^*(\overline{\mathbf{d}}_0, \overline{\mathbf{f}})$. A satisfactory approximation should have the property that $\mathbf{C}^*$ displays a weak dependence on $\overline{\mathbf{d}}_0$ and $\overline{\mathbf{f}}$. It depends, in turn, on an assumed function π_T for the dimensional reduction. Finally,

$$(2.5) \qquad \overline{\mathbf{C}} = \mathrm{Av}\{\mathbf{C}^* : \mathbf{C}^* = \mathbf{C}^*(\overline{\mathbf{d}}_0, \overline{\mathbf{f}}),\ \overline{\mathbf{d}}_0 \in \overline{\mathcal{M}},\ \overline{\mathbf{f}} \in \overline{\mathcal{F}}_T\},$$

where Av means an averaging operation. Thus, $\overline{\mathbf{C}}$ determines the evolution function of the reduced system $\overline{\chi}(\overline{\mathbf{C}})(t)$.

Thus, as a result of the dimensional reduction, we have obtained a new dynamical system. Let us characterize the main elements of the dimensional reduction. First, we have to choose new variables represented by $\overline{\mathbf{d}}$. Similarly, the forces are also dimensionally reduced to the $\overline{\mathbf{f}}$. Next, we have to assume or to infer the form of expression $(\partial\overline{L}/\partial\overline{\mathbf{d}})(\mathbf{C}, \overline{\mathbf{d}}, \overline{\mathbf{f}})$. This equation creates a skeleton of a new dynamical system SDS which can be characterized by $SDS(\mathbf{C}) = \{\overline{\mathbf{d}}, \overline{\mathbf{f}}, (\partial\overline{L}/\partial\overline{\mathbf{d}})(\mathbf{C}, \overline{\mathbf{d}}, \overline{\mathbf{f}})\}$. We should also determine the family of maps $\{\pi\} = \{\pi, \pi_T, \pi_f, \pi_{fT}\}$. Dimensionally reduced dynamical system $RDS(\overline{\mathbf{C}})$ is obtained with the help of an approximation method app given by (2.4), (2.5). Consequently, the dimensional reduction operation can be characterized by $DR = \{SDS, \{\pi\}, app\}$. Finally, the pair $\{EDS, DR\}$ leads to $RDS(\overline{\mathbf{C}})$, where EDS is the elementary dynamical system determined in (2.1).

Continuum models should be such dynamical systems which describe a material behaviour. Thus, they should appear as dimensionally reduced dynamical

systems describing a behaviour of a set of atoms which constitute the material of the body. Therefore, in the paper, just such a formulation of continuum mechanics is discussed.

3. A generalized formulation of continuum mechanics

The continuum mechanics has been developed by creating its precise mathematical foundations. These problems were widely discussed in the literature, for instance in [15, 16, 17, 18, 19].

In this paper we propose a generalization of the formulation of the continuum theory. This generalization is based on weakening of an assumption that the energy balance equation is satisfied for each subbody of the body B. It is assumed here that this is the case only for a distinguished family of subbodies of B. Such a theory comprises the traditional formulation as well, since the distinguished family of subbodies can, in particular, consist of all subbodies of B.

Let us note that for discrete system, energy depends on a finite number of variables wich are related to positions and velocities of particles of the discrete system. During a dimensional reduction the number of variables decreases. Such a new variable represents usually a group of particles from its discrete set. This leads to justification of the theorem that the balance of energy can be introduced for the finite subbodies of the whole body only.

Let us consider a set B and a family of its subsets which create a countable additive field S.

DEFINITION 1. *The body B is a space with a positive measure $M : S \to R^+ \cup \emptyset$. The measure M is called the mass.*

DEFINITION 2. *The body B is the continuous body if it is endowed with a structure defined by a non-empty class C of maps which satisfy the following axioms:*

a. *The members of C are invertible maps from B onto open subsets of the Euclidean space.*

b. *If κ, $\gamma \in C$, then $\kappa \circ \gamma^{-1}$ is a homeomorphism in E^3.*

c. *If $\kappa \in C$, λ is a homeomorphism in E^3 and Range κ = Dom λ, then $\lambda \circ \kappa \in C$.*

The members of C are called the placements of B. The range $\kappa(B)$, $\kappa \in C$, is called the region occupied by B in the placement κ.

The function $\lambda = \gamma \circ \kappa^{-1}$ is called the displacement function between placement κ and γ. The last definition follows from [19].

DEFINITION 3. *The continuous map of the time interval $[0, T]$ onto the set C is called the motion of the body B.*

Let $\chi(\mathbf{X}, t)$ be a motion of the body $\mathcal{B}$, where $\mathbf{X} \in \mathcal{B}$. The velocity $\mathbf{v}$ is defined as $\mathbf{v} = \dfrac{\partial}{\partial t} \chi(\mathbf{X}, t)$.

Let $\mathcal{K} = \{K_i : K_i \in \mathcal{S}, i \in I\}$, $I = \{1, 2, ..., N\}$, $K_i \cap K_j = \emptyset$ for each $i, j \in I$ and $\bigcup_{i \in I} K_i = \mathcal{B}$. Thus, $\mathcal{K} \subset \mathcal{S}$ is a subfamily of subsets of $\mathcal{B}$ which represents a decomposition of the body into subsets K_i, $i \in I$.

Let us consider a function $\overline{\chi} : \mathcal{K} \to R^3$, $\overline{\chi}(K_h) = \chi_h \in R^3$. Let $I_h^a \subset I$, $h \in I$ and $\{\chi_m\}$ be a set of values of the function $\overline{\chi}$ for $m \in I_h^a$. We can define the set $\Phi_a = \{a_h : a_h : \{\chi_m\} \to R^p, m \in I_h^a, p \in N\}$. Then, we introduce a function $a : \mathcal{K} \to \Phi_a$, $a(K_h) = a_h$.

The function $\overline{\chi}$ assigns a set of discrete values of the field χ_h, $h \in I$ to the body $\mathcal{B}$ with the help of the family $\mathcal{K}$. Similarly, the function a assigns a set of discrete values of the field a_h, $h \in I$. However, a_h depends on the finite set of values χ_m, $m \in I_h^a$. The definition of the finite set is introduced with the help of a set of indices I_h^a. This set in turn, contains numbers of elements of $\mathcal{K}$ which have influence on the value of a_h. Usually, it will be some neighbourhood sets K_i for K_h. Thus, the functions $\overline{\chi}$ and a together can express nonlocal properties of χ_h.

Let $\overline{V}_D = \{\{\overline{\chi}, a\} : \{\chi_h, a_h\}, h \in I\}$. Let us define the space V_κ of displacement functions χ_κ of the body $\mathcal{B}$ with respect to a configuration κ as $V_\kappa = \{\chi_\kappa : \chi_\kappa = \lambda \circ \kappa^{-1}, \lambda, \kappa \in \mathcal{C}\}$. Let furthermore, $\alpha : \overline{V}_D \to V_\kappa$ be a linear function and $\chi_\kappa^\mathcal{K} = \alpha(\{\chi_h, a_h\})$.

Let us consider a Cartesian coordinate system. Then, $\mathbf{X} = (X_1, X_2, X_3)$. We define a function $C_\kappa : \mathcal{K} \to R^3$, $C_\kappa(K_h) = \mathbf{X}_h$. We assume that in particular cases the function a_h can be expressed as $a_h = \{a_{1h}, ..., a_{Lh}\}$. In this case we assume that the function α satisfies also the following conditions

$$\chi_\kappa^\mathcal{K}(\mathbf{X}_h) = \chi_h, \qquad (a_{ih})_{kl_1...l_m} = \frac{\partial^i (\chi_\kappa^\mathcal{K})_k}{\partial^{i_1} X_{l_1}...\partial^{i_m} X_{l_m}}(\mathbf{X}_h),$$

$$i_1 + ... + i_m = i, \qquad i \in \{1, 2, ..., L\}, \qquad k, l_1, ..., l_m \in I_3 = \{1, 2, 3\}.$$

Then, $(a_{1h})_{kl} = \dfrac{\partial (\chi_\kappa^\mathcal{K})_k}{\partial X_l}$ can be interpreted as an approximation of the gradient of deformation and we can consider $((a_{1h})^{-1})_{kl}$ as well.

DEFINITION 4. *The displacement function associated with the family of sets $\mathcal{K}$ is a function $\chi_\kappa^\mathcal{K}$ of the form $\chi_\kappa^\mathcal{K} = \alpha(\{\chi_h, a_h\})$.*

The function α assigns a displacement function field $\chi_\kappa^\mathcal{K}$ to the set of discrete values. The aim of this function is to introduce a continuous field χ on the body $\mathcal{B}$. Thus, the space of such fields $\operatorname{Im} \alpha \subset V_\kappa$ is finite-dimensional, where $\operatorname{Im} \phi$ means the image of a function ϕ.

DEFINITION 5. *The motion of the body $\mathcal{B}$ associated with the family of sets $\mathcal{K}$ is a continuous map $\chi_t : [0, T] \to \{\chi_\kappa^\mathcal{K}\}$.*

We also introduce a function $\overline{T}$ on $\mathcal{K}$, which will represent temperature, as $\overline{T} : \mathcal{K} \to R$, $\overline{T}(K_h) = T_h$. Let $I_h^b \subset I$ and $\{T_n\}$ be a set of values of the function $\overline{T}$ for $n \in I_h^b$. We define a set $\Phi_b = \{b_h : b_h : \{T_n\} \to R^q, n \in I_h^b, q \in N\}$. Similarly as for the function a, we introduce a function $b : \mathcal{K} \to \Phi_b$, $b(K_h) = b_h$. Let $\overline{V}_T = \{\{\overline{T}, b\} : \{\overline{T}, b\} = \{T_h, b_h\}, h \in I\}$, $V_T = \{T(\mathbf{X}) : \mathbf{X} \in \mathcal{B}\}$. Let us consider a function $\beta : \overline{V}_T \to V_T$ which is linear by definition and $T^{\mathcal{K}} = \beta(\{T_h, b_h\})$. We assume also that $T^{\mathcal{K}}(\mathbf{X}_h) = T_h$ and $\dfrac{\partial T^{\mathcal{K}}}{\partial X_l}(\mathbf{X}_h) = b_h$.

DEFINITION 6. *The temperature field $T^{\mathcal{K}}$ associated with the family $\mathcal{K}$ is the field obtained with the help of function β as $T^{\mathcal{K}} = \beta(\{T_h, b_h\})$.*

Thus, we have obtained a finite-dimensional space of temperature fields Im $\beta \subset V_T$ in the body $\mathcal{B}$.

Let us consider the functions: the internal energy E_t, the entropy S_t, the energy flux W_t, the power of inertia forces P_t, the entropy flux H_t, the energy source R_t, and the entropy source N_t. Here $E_t : \mathcal{K} \to R$, $S_t : \mathcal{K} \to R$, $W_t : \partial \mathcal{K} \to R$, $P_t : \mathcal{K} \to R$, $H_t : \partial \mathcal{K} \to R$, $R_t : \mathcal{K} \to R$, $N_t : \mathcal{K} \to R$, where $\partial \mathcal{K}$ is the family of sets $K_i \cap \partial \mathcal{B}$. These functions are determined for any time instant, thus they represent some processes. It is also assumed that they are differentiable enough with respect to time.

Neglecting at the moment the detailed representations of these functions, we assume the energy balance equation in the form

(3.1) $$\dot{E}_t(\mathcal{B}) - \dot{P}_t(\mathcal{B}) + W_t(\partial \mathcal{B}) - R_t(\mathcal{B}) = 0,$$

where

$$\mathcal{B} = \bigcup_i K_i, \qquad K_i \in \mathcal{K}, \qquad \partial \mathcal{B} = \bigcup_j K_j \cap \partial \mathcal{B}.$$

The second law of thermodynamics is expressed with the help of the entropy balance equation and takes the form

(3.2) $$\dot{S}_t(\mathcal{B}) + H_t(\partial \mathcal{B}) - N_t(\mathcal{B}) \geq 0.$$

We introduce also the function $\Psi_t : \mathcal{K} \to R$ which is interpreted as the free energy.

4. An example of a continuum with finite-dimensional fields

An example of a finite-dimensional continuum presented here is connected with a special choice of the family $\mathcal{K}$, functions which appear in (3.1), (3.2), the variables and the form of constitutive equations.

Let $\mathcal{K} = \{K_i\}$, $i \in I$ be a division of the body $\mathcal{B}$ into a sum of geometrical complexes K_i which have a cubicoid form. Let the coordinate axes $\{X_1, X_2, X_3\}$

be prependicular to the faces of cuboids in the undeformed state. We can introduce a discrete field on the set of complexes K_i. Then, we assign a value of a field to the center of gravity of each K_i, $i \in I$.

We have introduced discrete fields related to the family $\mathcal{K}$. Thus, the following expressions will be helpful in what follows:

$$D_2(y_m) = \frac{1}{2\Delta}(y_{m+1} - y_{m-1}),$$

(4.1) $$A(y_m) = \frac{1}{2}(y_{m+1} + y_{m-1}),$$

$$D_2(y_m z_m) = D_2(y_m)A(z_m) + D_2(z_m)A(y_m),$$

where Δ is a distance between centers of neighbourhood complexes K_m. It is assumed that, for simplicity, Δ is the same for the whole body. Let $D_{2i}(y_h) = (1/2\Delta)(y_{h_{i2}} - y_{h_{i1}})$, $i = 1, 2, 3$, where h_{i2}, h_{i1} stand, respectively, for indices of two neighbourhood complexes for K_h in the direction X_i. By analogy, we introduce also $A_i(y_h) = (1/2)(y_{h_{i2}} + y_{h_{i1}})$.

Let $p_h = \{p_{hi}, \ i \in I_3\}$ be a discrete field assigned to the center of K_h. By means of the above formulas we can introduce a discrete version of the Gauss theorem which is convenient for our purposes

(4.2) $$\sum_{h \in I} D_{2i}(p_{hi}) \approx \sum_{h \in I} \sum_{s_h \in I_h} p_{s_h i} N_{s_h i},$$

where $p_{s_h i}$ is the same field p_h which has been assigned to the center of face S_{s_h} of the complex K_h, N_{s_h} are components of the unit vector normal to the face S_{s_h}. Furthermore, $p_{hi} = J(a_{1h}^{-1})_{ik}\bar{p}_{hk}$ is a connection between vectors dependent on space and material variables.

In general we assume that $p_{s_h i} = \lambda(p_{hi}, \ p_{li})$, where h, l are indices related to complexes which have common face S_{s_h}. λ is a function chosen in such a way that the formula (4.2) would be satisfactorily satisfied.

Let us introduce a function a_h of the form $a_h = \{D_{21}(\chi_h), D_{22}(\chi_h), D_{23}(\chi_h)\}$, $\chi_h = \{\chi_{hn}\}$, $n \in I_3 = \{1, 2, 3\}$, $h \in I$. Thus, $a_h = \{a_{hni}\}$, n, $i \in I_3$.

We assume the following representations for functions related to the energy balance equation and the second law of thermodynamics:

(4.3) $$E(K_h) = E_h, \qquad E(K_h) = \Psi_h + S_h T_h,$$

(4.4) $$\dot{E}(K_h) = \dot{E}_h, \qquad \dot{E}(K_h) = \dot{\Psi}_h + \dot{S}_h T_h + S_h \dot{T}_h,$$

(4.5) $$W(\partial K_h) = \sum_{s_h} q_{s_h i} N_{s_h i} - \sum_{s_h} p_{s_h i} \dot{\chi}_{s_h i},$$

(4.6) $$P(K_h) = -m_h \ddot{\chi}_{hi} \dot{\chi}_{hi} + D_{2m}(i_{hmn} \ddot{a}_{hkn})\dot{\chi}_{hk},$$

(4.7) $$R(K_h) = R_{eh} + f_{hi}\dot{\chi}_{hi},$$

$$(4.8) \qquad S(K_h) = S_h, \qquad \dot{S}(K_h) = \dot{S}_h,$$

$$(4.9) \qquad H(\partial K_h) = \sum_{sh} \frac{1}{T_{sh}} q_{shi} N_{shi},$$

$$(4.10) \qquad N(K_h) = \frac{1}{T_h} R_{eh},$$

where m_h is a mass assigned to the complex K_h, i_{hnm} is an inertia tensor related to K_h. $f_h = \{f_{hi}\}$ and R_{eh} are a force and a heat source related to K_h. $q_{sh} = \{q_{shi}\}$ and $p_{sh} = \{p_{shi}\}$ are a heat flux and a surface force related to the surface S_{sh}. Let us note that the expression (4.6) is obtained with the help of definition of the kinetic energy $E_k = \int \varrho \dot{x}_i \dot{x}_i dV$.

We assume that the energy balance equation is fulfilled for each $K_h \in \mathcal{K}$ separately. Then, the energy balance equation takes the form

$$(4.11) \qquad \dot{\Psi}_h + \dot{S}_h T_h + S_h \dot{T}_h + m_h \ddot{\chi}_{hi} \dot{\chi}_{hi}$$
$$- D_{2m}(i_{hmn} \ddot{a}_{hkn}) \dot{\chi}_{hk} - R_{eh} + \sum_{sh} q_{shi} N_{shi} - f_{hi} \dot{\chi}_{hi} - \sum_{sh} p_{shi} \dot{\chi}_{shi} = 0.$$

The term $\dot{\Psi}_h$ can be expressed as

$$(4.12) \qquad \dot{\Psi}_h = \frac{\partial \Psi_h}{\partial a_{hni}} \dot{a}_{hni} + \frac{\partial \Psi_h}{\partial T_h} \dot{T}_h = \frac{\partial \Psi_h}{\partial a_{hni}} D_{2i}(\dot{\chi}_{hn}) + \frac{\partial \Psi_h}{\partial T_h} \dot{T}_h$$
$$= D_{2i}\left(\frac{\partial \Psi_h}{\partial a_{hni}} \dot{\chi}_{hn}\right) - D_{2i}\left(\frac{\partial \Psi_h}{\partial a_{hni}}\right) A_i(\dot{\chi}_{hn}) + \frac{\partial \Psi_h}{\partial T_h} \dot{T}_h,$$

where the properties given by the formula (4.1) have been used. The summation convention does not concern the index i in A_i. Furthermore, we assume that $A_i(\dot{\chi}_{hn}) \approx \dot{\chi}_{hn}$.

With the help of (4.12) and the discrete Gauss theorem (4.2), we can transform (4.11) into the form

$$(4.13) \qquad \left[-D_{2i}\left(\frac{\partial \Psi_h}{\partial a_{hni}}\right) - f_{hn} + m_h \ddot{\chi}_{hn} - D_{2m}(i_{hmp} \ddot{a}_{hnp})\right] \dot{\chi}_{hn}$$
$$+ \left(\frac{\partial \Psi_h}{\partial T_h} + S_h\right) \dot{T}_h + \dot{S}_h T_h$$
$$+ D_{2i}(q_{hi}) - R_{eh} + \sum_{sh} \left(\frac{\partial \Psi_{sh}}{\partial a_{shni}} N_{shi} - p_{shn}\right) \dot{\chi}_{shn} = 0.$$

Then assuming that an arbitrary time process $\dot{\chi}_h$ is admissible, we obtain from (4.13) the following system of equations:

$$(4.14) \qquad -D_{2i}\left(\frac{\partial \Psi_h}{\partial a_{hni}}\right) - f_{hn} + m_h \ddot{\chi}_{hn} - D_{2m}(i_{hmp} \ddot{a}_{hnp}) = 0,$$

$$(4.15) \qquad\qquad S_h = -\frac{\partial \Psi_h}{\partial T_h},$$

$$(4.16) \qquad\qquad \dot{S}_h T_h + D_{2i}(q_{hi}) - R_{eh} = 0$$

and

$$(4.17) \qquad\qquad \frac{\partial \Psi_{s_h}}{\partial a_{s_h ni}} N_{s_h i} - p_{s_h n} = 0.$$

The Clausius – Duhem inequality can be expressed with the help of (3.2), (4.8) – (4.10) as

$$(4.18) \qquad\qquad \dot{S}_h - R_{eh}\frac{1}{T_h} + D_{2i}\left(q_{hi}\frac{1}{T_h}\right) \geq 0.$$

Taking into account dissipative processes and introducing internal state variables ξ_h we can generalize Eqs. (4.14)–(4.16) to the form

$$(4.19) \qquad -D_{2i}\left(\frac{\partial \Psi_h}{\partial a_{hni}} + t^d_{hni}\right) - f_{hn} + m_h \ddot{\chi}_{hn} - D_{2m}(i_{hmp}\ddot{a}_{hnp}) = 0,$$

$$(4.20) \qquad\qquad S_h = -\frac{\partial \Psi_h}{\partial T_h} + S^d_h,$$

$$(4.21) \qquad \dot{S}_h T_h + D_{2i}(\overline{q}_{hi}) - R_{eh} + S^d_h \dot{T}_h - t^d_{hni}\dot{a}_{hni} + \frac{\partial \Psi_h}{\partial \xi_h}\dot{\xi}_h = 0.$$

The constitutive equations should be assumed for the functions $r_h = \{\Psi_h,\ S_h,\ \mathbf{t}_h,\ \mathbf{q}_h\}$ and $\mathbf{t}_h = (\partial \Psi_h/\partial a_h) + \mathbf{t}^d_h$. The constitutive equations will then depend on the variables $\mathbf{h}_h = \{\chi_h,\ a_h,\ T_h,\ b_h\}$ and ξ_h. We assume that the equations take the form

$$(4.22) \qquad\qquad \Psi_h = \Psi_h(\mathbf{C}_\psi,\ \mathbf{h}_h,\ \xi_h),$$
$$(4.23) \qquad\qquad S_h = S_h(\mathbf{C}_s,\ \mathbf{h}_h,\ \xi_h),$$
$$(4.24) \qquad\qquad \mathbf{t}_h = \mathbf{t}_h(\mathbf{C}_t,\ \mathbf{h}_h,\ \xi_h),$$
$$(4.25) \qquad\qquad \mathbf{q}_h = \mathbf{q}_h(\mathbf{C}_q,\ \mathbf{h}_h,\ \xi_h),$$
$$(4.26) \qquad\qquad \dot{\xi}_h = A_h(\mathbf{C}_A,\ \mathbf{h}_h,\ \xi_h),$$

where $\mathcal{C} = \{\mathbf{C}:\ \mathbf{C} = \{\mathbf{C}_\psi,\ \mathbf{C}_s,\ \mathbf{C}_t,\ \mathbf{C}_q,\ \mathbf{C}_A\}\}$ are constants which define these constitutive equations.

The generalization in our formulation rests on the fact that our theory is formulated for a given subfamily $\mathcal{K}$. In the particular case when $\mathcal{K} = \mathcal{S}$ we obtain the classical continuum theory.

It is possible to carry out two different procedures for obtaining a continuous field from the discrete one given on the family $\mathcal{K}$.

The first procedure, called further the A-procedure, consists in the interpolation of the sets of the discrete values. It can be performed with the help of maps α, β introduced above, which replace the discrete fields $\{\chi_h, \ a_h, \ T_h, \ b_h\}$ by some continuous ones.

We should also introduce some additional maps which will be useful for interpolation of the remaining variables which appear in our description. Thus, let us introduce the following spaces

$$\overline{V}_\varrho = \{m : \ m = \{m_h\}, \ h \in I\}, \qquad V_\varrho = \{\varrho(\mathbf{X}) : \ \mathbf{X} \in \mathcal{B}\},$$

$$\overline{V}_r = \{r : \ r = \{\Psi_h, \ S_h, \ \mathbf{t}_h, \ \mathbf{q}_h\}, \ h \in I\},$$

$$V_r = \{r(\mathbf{X}) : \ r(\mathbf{X}) = \{\psi(\mathbf{X}), \ s(\mathbf{X}), \ \mathbf{t}(\mathbf{X}), \ \mathbf{q}(\mathbf{X})\}, \ \mathbf{X} \in \mathcal{B}\},$$

$$\overline{V}_\xi = \{\xi : \ \xi = \{\xi_h\}, \ h \in I\}, \qquad V_\xi = \{\xi(\mathbf{X}) : \ \mathbf{X} \in \mathcal{B}\},$$

$$\overline{V}_f = \{\{\mathbf{f}, \ R_e, \ \mathbf{p}\} : \{\mathbf{f}_h, \ R_{eh}, \ \mathbf{p}_h\}, \ h \in I\},$$

$$V_f = \{\{\mathbf{f}(\mathbf{X}), \ r_e(\mathbf{X}), \ \mathbf{p}(\mathbf{X})\} : \ \mathbf{X} \in \mathcal{B}\}.$$

Let us consider the following maps which act on the introduced spaces $\rho :$ $\overline{V}_\varrho \to V_\varrho, \ \mu : \overline{V}_r \to V_r, \ \mu_\xi : \overline{V}_\xi \to V_\xi, \ \nu : \overline{V}_f \to V_f$. The introduced maps are linear by assumption and with the help of these maps, discrete fields are replaced by continuous ones. However, in order to obtain satisfactory approximation, the continuous fields obtained above should satisfactorily fulfill the following conditions

$$m_h = \int\limits_{\check{K}_h} \varrho \, dV \,, \qquad \Psi_h = \int\limits_{\check{K}_h} \varrho\psi \, dV \,, \qquad S_h = \int\limits_{\check{K}_h} \varrho s \, dV \,,$$

$$D_{2i}(t_{hni}) = \int\limits_{\check{K}_h} t_{ij,i} \, dV = \int\limits_{\partial \check{K}_h} t_{nk} N_k \, dA \,,$$

(4.27)
$$D_{2i}(q_{hi}) = \int\limits_{\check{K}_h} q_{i,i} \, dV = \int\limits_{\partial \check{K}_h} q_k N_k \, dA \,,$$

$$f_h = \int\limits_{\check{K}_h} f \, dV \,, \qquad R_{eh} = \int\limits_{\check{K}_h} r_e \, dV \,, \qquad p_{s_h i} = \int\limits_{\partial \check{K}_h} p_i \, dA \,,$$

where $q_{hk} = J(a_h^{-1})_{kl}\bar{q}_{hl}$, $t_{hni} = J(a_h^{-1})_{il}\bar{t}_{hnl}$ are quantities determined with respect to the reference configuration. Finally, we obtain continuous finite-dimensional fields on the continuum with the help of the A-procedure.

The second procedure, called further the L-procedure, is connected with a limit transition. Let $\mathcal{B} = \bigcup_{i \in I} K_i$, $K_i \in \mathcal{K}$ be a division of the body $\mathcal{B}$. Let us consider a sequence of $\{\mathcal{K}_m\}$, $m = 1, 2, 3, \ldots$ of such divisions and $\mathcal{K}_1 = \mathcal{K}$. Thus, for each m, $\mathcal{B} = \bigcup_{i \in I_m} K_{mi}$, $K_{mi} \in \mathcal{K}_m$. Let us assume that constants $\mathbf{C}$ are already determined for the family $\mathcal{K}$.

For each $\mathcal{K}_m$ we introduce the sets of indices I_{mh}^a, I_{mh}^b. Consequently, we have sequences $\{I_m\}$, $\{\mathcal{K}_m\}$, $\{I_{mh}^a\}$, $\{I_{mh}^b\}$, $h \in I_m$, $m = 1, 2, 3, \ldots$. With the help of these sequences we can carry out a limit L for the equations (4.18)–(4.21) and the constitutive equations (4.22)–(4.26). However, in order to make this operation realizable, let us assume that variables which appear in (4.18)–(4.21) have representations in the form given by (4.27). We assume also that during this operation $\lim_{m \to \infty} \delta(K_{mi}) = 0$, where δ is a diameter of the set K_{mi}. It is assumed that the constants related to the constitutive equations do not undergo any change.

During this limit transition $\mathbf{h}_h \to \mathbf{h}$ appears, where $\mathbf{h} = \{\chi_i, (\partial \chi_i / \partial X_n), T, (\partial T / \partial X_n)\}$ in the considered case. The final form of this limit depends on the previously assumed functions a_h, b_h. In particular, limits connected with these functions can lead also to higher gradients of χ and T.

The limit form of Eqs. (4.18)–(4.21) can be obtained by dividing them first by volume of K_h marked by V_h. Next, during the limit transition we obtain $i_{hmn} \to 0$, $(m_h/V_h) \to \varrho$, $D_{2i}(q_{hi}) \to \mathrm{Div}\,\mathbf{q}$, $D_{2i}(t_{hni}) \to \mathrm{Div}\,\mathbf{t}$. Finally, we obtain the well known expressions for the local forms of balance equations and the Clausius–Duhem inequality [16].

Let us note that the L procedure leads to the infinite-dimensional fields on the continuum. However, the starting point of this procedure has decisive meaning. Namely, the first element $\mathcal{K}_1$ of the sequence $\{\mathcal{K}_m\}$ is assumed. This element influences the final form of the constitutive equations.

The first element of the sequence $\{\mathcal{K}_m\}$ will be related to the volume of averaging. This problem will be discussed in the next section. The volume of averaging is especially connected with the form of the constitutive equations.

5. Volume of averaging related to the continuum model

The primary motivation for discussing the continuum theory suggested in the paper is to create a possibility of determining the equations of the continuum (for instance (4.18)–(4.26)) from a more elementary level. This elementary level can be connected with a discrete system of material points or with a continuum which is much more complicated.

Let us assume that on the more elementary level, the behaviour of a body is described by a dynamical system. Let $\mathbf{d}$ be a variable of this system, $V = \{\mathbf{d}\}$ is a set of admissible values of this variable, and let $\varphi : [0, T] \to V$ be an evolution function of the dynamical system.

On the other hand, let $\overline{\mathbf{d}} = \{\{\chi_h,\ a_h,\ \dot{\chi}_h,\ \dot{a}_h,\ T_h,\ b_h,\ \xi_h\}\ :\ h \in I\}$, $\overline{V} = \{\overline{\mathbf{d}}\}$, $\overline{\mathbf{f}} = \{\mathbf{f}_h,\ R_{eh},\ \mathbf{p}_h\}$ and let $\overline{\varphi} : [0,\ T] \to \overline{V}$ be an evolution function which is determined by equations (4.18)–(4.26).

At this moment we can return to notations from the Sec. 2 where we have defined two dynamical systems and a dimensional reduction method. The SDS introduced in Sec. 2 can be now identified with $SDS(\mathbf{C}) = \{\mathcal{K},\ \overline{\mathbf{d}},\ \overline{\mathbf{f}},\ \{BE,\ r(\mathbf{C})\}\}$, where $\mathcal{K}$ is the previously discussed family of subsets of the body and influences the option of variables $\overline{\mathbf{d}}$ and forces $\overline{\mathbf{f}}$. BE means the set of balance equations (4.18)–(4.21) and $r(\mathbf{C})$ represents the parametrized family of constitutive equations (4.22)–(4.26). The pair $\{BE,\ r(\mathbf{C})\}$ corresponds to $\dfrac{\partial \overline{\mathbf{L}}}{\partial \overline{\overline{\mathbf{d}}}}(\mathbf{C})$ which describes evolution of SDS. The dimensional reduction method has the same form as previously $DR = \{SDS,\ \{\pi\},\ app\}$.

In this section we discuss the continuum dynamical system CDS which should be obtained as a result of the dimensional reduction. This system can be characterized by $CDS(\mathbf{C}) = SDS(\mathbf{C})$. Thus, we can choose an elementary dynamical system EDS which can be a discrete or a continuous one but more complicated than $SDS(\mathbf{C})$. Then, $\{EDS,\ DR\}$ creates an $RDS(\overline{\mathbf{C}}) = CDS(\overline{\mathbf{C}})$.

Now, we are able to define a volume of averaging related to the continuum model. Let $\mathcal{K}$ be a family of sets K_i and $\mathcal{B} = \bigcup_i K_i$, $K_i \cap K_j = \emptyset$. Let φ be a dynamical system whereby the discrete field related to $\mathcal{K}$ is determined. Next, let the L-procedure or the A-procedure be applied in order to attain the continuum model. Then, the average of values $\mu(K_i)$ represents a volume of averaging for the continuum model obtained, where μ is the volume measure.

In a natural way, we can generalize this approach to a multiscale description. Then, $(CDS)_n = \{(CDS)_{n-1}, (DR)_{n-1}\}$, where $(CDS)_{n-1}$ represents the more elementary dynamical system and $(DR)_{n-1}$ means a dimensional reduction which is then applied.

6. Volume of averaging connected with the martensitic transformation

The martensitic transformation, especially the one related to the shape memory alloys, exhibits a complicated structure and moving interfaces. As it has been discussed previously, different scales should be taken into account in a mechanical modelling of this transformation. Let us try to discuss what these scales should mean.

In a small scale, we can observe the single martensite variants. They can create fine twins or selfaccomodating groups. In a larger scale, such structures usually create a complicated composition. However, in a large scale a coalescence of martensite variants can appear, and only one martensite variant is also possible.

Let us consider, for instance, the CuAl alloy. We observe twenty four martensite variants which create six selfaccomodating groups [22]. In Fig. 1, the struc-
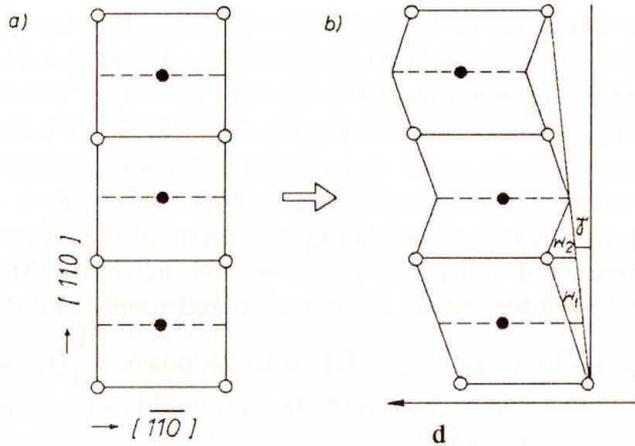
FIG. 1. Structure of austenite and martensite in CuAl alloy.

ture of austenite and martensite unit for CuAl alloy is shown. They have nine atomic layers which characterize this unit and define fully this martensite variant. The austenite structure and stress-induced martensite variants for CuAlNi alloy is shown in Fig. 2, where eighteen atom layers define the martensite unit [23]. Consequently, a linear dimension which characterizes the small volume of averaging in the considered cases should exceed the dimension of the martensite unit and should be between 10^{-9} m and 10^{-8} m. On this level of description, single martensite variants and single interfaces will be distinguished.

In Fig. 3 the selfaccomodating group is shown for CuAl alloy. In this structure different kinds of single martensite variants are composed. Another structure related to the fine twinning of martensite for CuAlNi alloy is shown in Fig. 4. Compositions of this kind of structures bring a considerable nonhomogeneity. Therefore, the scale of averaging for theories which do not distinguish different martensite variants should be connected with such a volume in which the composition of martensities can be approximated by a homogeneous structure. Taking into account observable structures [24, 25], one should assume that the linear dimension related to the volume of averaging is between 10^{-6} m and 10^{-4} m for models with the larger scale.

In papers [12, 13] a continuum model related to the small volume of averaging is introduced. As a consequence of this kind of averaging shuffles are taken into considerations. They are introduced with the help of the relative displacement vectors $\mathbf{w}_\lambda$ which are shown in Fig. 1. The role of shuffles is valid on this level of description. They take place in determining the martensite variants. They have also some influence on the kind of internal rotation of the martensite variant towards the habit plane. Thus, the dynamical system related to this model has variable $\mathbf{d} = \{\mathbf{x}, \dot{\mathbf{x}}, \mathbf{w}_\lambda, \dot{\mathbf{w}}_\lambda, T, \alpha, \beta, \delta\}$, where α, β, δ are internal variables related to dissipation connected with shuffles, related to jumps of the creating
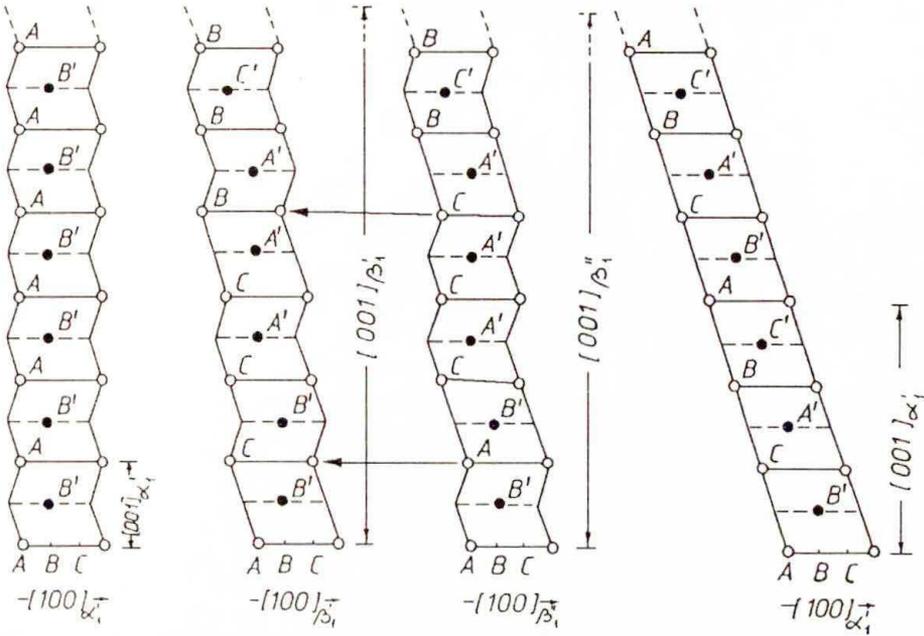
FIG. 2. Structure of stress-induced martensite in CuAlNi alloy.
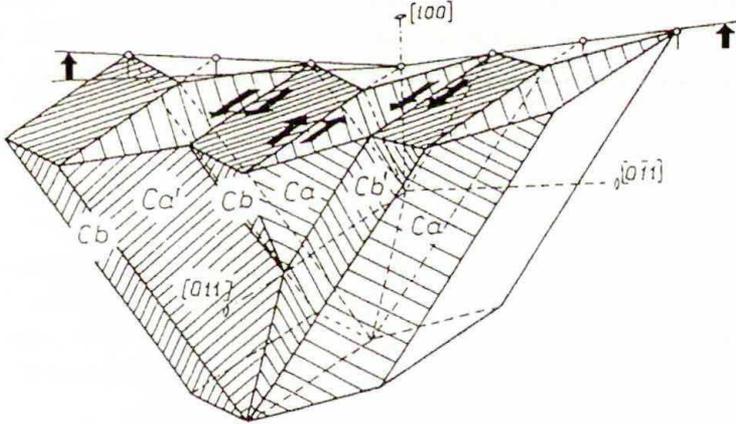
FIG. 3. The selfaccomodating group of martensite variants in CuAl alloy.

martensitic structure over an anergetic barrier and stabilization of the martensite, respectively.

On the other hand, we can introduce variable $\bar{d}$ given in previous section, where ξ can be in particular connected with the mass of martensite in the whole structure. Then, the model of larger scale of averaging is considered. Such models have been discussed in literature [20, 21].
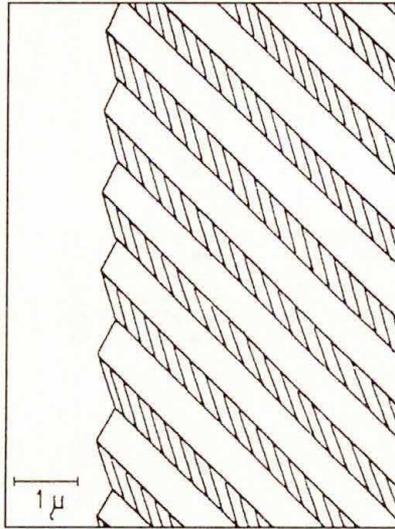
FIG. 4. The fine twinning which appears in CuAlNi alloy.

With the help of the procedure given in Sec. 4, a connection between these two models could be determined. However, such procedure will certainly be not simple. It requires, first, precise identification of the constants and functions related to material properties for the model with the small scale. Then, another difficult problem appears. This is connected with a satisfactory form of approximation given by (2.4), a form of dependence of functions in (4.22)–(4.26) on $\mathbf{C}$ and choosing an appropriate kind of internal variables ξ.

7. Final remarks

The suggested formulation of continuum mechanics makes it possible to obtain a continuum model as a dimensional reduction of a discrete system. It seems to be convenient to consider a discrete dynamical system as a physical basis for continuum model. Furthermore, multiscale approach for continuum description can also be introduced in this way.

The main stress has been laid on the description of dynamics. It is displayed by the introduced method of dynamical reduction by means of maps π_T, π_{fT}, and by introduction of internal state variables in dimensionally reduced systems. Such an approach is suggested by the example of a moving microstructure in case of the martensitic transformation. Then, it is difficult to use, for instance, the homogenization method since we do not know the dynamical laws of microstructure evolution.

Furthermore, it is hoped that the suggested procedure will be convenient in determination of the constants and functions connected with the material consid-

ered. It is valid especially for small scale of the averaging models. Then, we have not too many possibilities to obtain such constants and functions experimentally.

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