On the Continuum Mechanics Approach in Modeling Nanosized Structural Elements

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Abstract During the last 50 years the nanotechnology is established as one of the advanced technologies manipulating matter on an atomic and molecular scale. By this approach new materials, devices or other structures possessing at least one dimension sized from 1 to 100 nm are developed. The question arises how structures composed of nanomaterials should be modeled. Two approaches are suggested—theories which take into account quantum mechanical effects since they are important at the quantum-realm scale or theories which are based on the classical continuum mechanics adapted to nanoscale problems. Here the second approach will be discussed in detail. It will be shown that the classical continuum mechanics (kinematics, stress states analysis, balances and constitutive equations) with some improvements is enough for a sufficient description of the mechanical behavior of nanomaterials and -structures in many situations. After a brief recall of the basics of Continuum Mechanics a theory with surface effects will be discussed.

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1 Introduction

Nanotechnology is related to materials, devices and other structures with at least one dimension sized from 1 to 100 nm. With respect to several applications resulting, for example, in new material properties the questions arise:

- how to model such nanostructures,
- how to design nanodevices, and
- how to predict the new properties.

As usual if the size decreases some effects (for example, surface stresses) are more significant in comparison with effects of materials and devices of conventional size. Such effects are statistical mechanical and quantum mechanical effects among others. They results in significant changes of the properties in comparison with the properties of the bulk material (see [14, 17, 25, 34] among others). This is experimentally established also for the inelastic properties, see, for example, [22, 60].

In recent publications various approaches of modeling are presented. Many contributions are coming from physics and yields in equations which are not similar to the usual equations in the engineering analysis of structures or engineering simulations of the material behavior. By this way we get results describing qualitatively and quantitatively correct the effects related to the nanosize. Since nanoeffects are connected with the size of atoms and molecules molecular modeling codes are used in numerical simulations. The disadvantage of this approach is that the engineering analysis of real nanostructures taking into account the three-dimensional behavior is not trivial.

In contrast to the aforementioned approach in various applications Continuum Mechanics based theories are applied. It can be shown that the classical Continuum Mechanics is unable to simulate the properties of nanostructures in a correct manner [24, 28, 67]. Several improved theories for the analysis of nanostructures are developed, for example,

- Cosserat or micropolar theories,
- Continuum Mechanics theories taking into account surface effects, and
- gradient theories.

It should be noted that these theories can be combined with the classical structural analysis introducing models like beam, rod, plate, shell, etc. as basic one- or two-dimensional models. Now there are developed several theories like, for example, the mechanics of nanocomposites which is widely discussed in the literature (cp. the review [31]). Alternatively, the behavior of the crystal lattice is modeled based on Continuum Mechanics, for example, in [2, 36].

Below we present the basic features of the classical Continuum Mechanics and discuss one possible improvement (the account of surface effects) which is helpful in nanomechanics. Gradient and Cosserat theories will be not discussed. They are presented in [1, 11–13, 15, 37, 40, 65] among others. In the final part there are given briefly some references to applications.

2 Basic Equations in Classical Continuum Mechanics

The classical Continuum Mechanics is based on the continuum assumption. How realistic is this assumption? Up to now there are a lot of discussions. They are based on mathematics (continuous distribution of the field variables and, in addition, of their derivatives) or physics. Continuum Mechanics is the branch of mechanics that deals with the analysis of the behavior of materials and structures modeled as continuous distributed mass (infinite number of material points) instead of discrete particles (presented, for example, by molecular modeling methods). The founder of continuum mechanics was the French mathematician Augustin Louis Cauchy who formulate first relevant models in the 19^{th} century. These models were further generalized by the Cosserat brothers [16], Lord Kelvin, Duhem and Helmholtz among others. However, the classical or the generalized continua are modeled as objects assuming that they completely fill the occupied space. Modeling objects in this way ignores the fact that matter is made of atoms, and so is not continuous. But on length scales much greater than that of inter-atomic distances, such models are highly accurate. Fundamental physical laws such as the balance of mass, the balance of momentum, and the balance of energy may be applied to these models to derive integral or differential equations describing their behavior. The information about the particular material properties is added through the constitutive and, may be, evolution equations.

Continuum Mechanics deals with physical properties of solids and fluids which are independent of any particular coordinate system in which they are observed. These physical properties are then represented by tensors of different rank, which are mathematical objects that have the required property of being independent of the coordinate system. These tensors can be expressed in specific coordinate systems for computational convenience.

In this section we briefly present the basics of Continuum Mechanics. Further information are given in [6, 32] among others. The direct tensor calculus in the sense of [41] is mostly used this chapter.

2.1 Kinematical Equations

A body $\mathcal{B}$ is an assemblage of material points, which is bounded by the boundary points, that means the surface of $\mathcal{B}$. Material bodies are introduced in Continuum Mechanics with the help of the method of sections. By this method the body $\mathcal{B}$ can be separated from the surrounding. The introduction of the surface and the body is arbitrary, which is helpful for the formulation of the balance equations.

The movement of material bodies can be presented by the motion of their material points which should be identified. If the material points are related to points in the Euclidean space $\mathbb{R}^3$ and if one point 0 is fixed in this space, then the position of the material points is determined by the position-vector $\mathbf{x}(t)$ at arbitrary

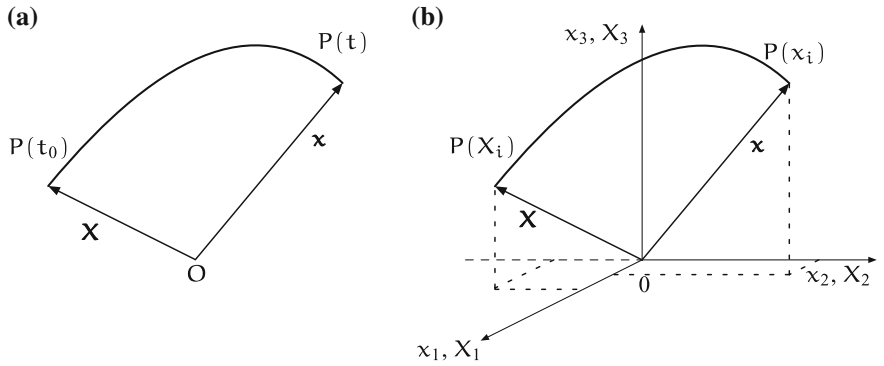

Fig. 1 Movement of a material point: **a** position-vector, **b** Cartesian coordinates

time t. To distinguish the material points of the body $\mathcal{B}$ each of them get a label: at the time $t = t_0$ the material point is characterized by the position-vector $\mathbf{x}(t_0) \equiv \mathbf{X}$. t_0 is the natural initial state, which changes should be computed. In many cases $t_0 = 0$ is assumed.

In Cartesian coordinates with the origin O and the basis vectors $\mathbf{e}_i (i = 1, 2, 3)$ the movement of the material point $\mathbf{X}$ can be presented as it follows

$$\mathbf{x} = x_i \mathbf{e}_i, \qquad \mathbf{X} = X_i \mathbf{e}_i, \qquad \mathbf{x}(\mathbf{X}, t_0) = \mathbf{x}_0 \equiv \mathbf{X}, \tag{1}$$

In Fig. 1 is shown the movement of a material point P. The coordinates x_i are Lagrangian coordinates, x_i - Eulerian coordinates. The description of the behavior of the continuum can be related to both the Lagrangian and the Eulerian configurations. For many applications this is sufficient. Sometimes it is necessary to present the continuum in so-called intermediate configurations. Details are given, for example, in [50, 64].

2.1.1 Deformation Gradient and Strain Tensors

The deformation of the continuum can be presented with the help of the equation of motion

$$\mathbf{x} = \mathbf{x}(\mathbf{X}, t)$$

Let us introduce the material deformation gradient

$$\mathbf{F} \equiv [\nabla_{\mathbf{X}} \mathbf{x}(\mathbf{X}, t)]^{\mathrm{T}} \tag{2}$$

describing the transform of a material line element $d\mathbf{X}$ in the reference configuration into a material line element $d\mathbf{x}$ of the actual configuration

$$\mathbf{F} \cdot d\mathbf{X} = d\mathbf{x}$$

$(\ldots)^{\mathrm{T}}$ denotes the transpose of a tensor.

The vice versa transform is given by

$$d\mathbf{X} = \mathbf{F}^{-1} \cdot d\mathbf{x}$$

with

$$\mathbf{F}^{-1} = [\nabla_{\mathbf{x}} \mathbf{X}(\mathbf{x}, t)]^{T}. \tag{3}$$

$(\ldots)^{-1}$ denotes the inverse of a tensor. Note that the motion consist of the motion of the continuum as a rigid body (translation and rotation) and the strains (relative position changes of the material points).

Let us introduce the Green-Lagrange strain tensor which has in the reference configuration for pure rigid body motion the value zero

$$\mathbf{G}(\mathbf{X}, t) = \frac{1}{2}(\mathbf{F}^{T} \cdot \mathbf{F} - \mathbf{I}). \tag{4}$$

$\mathbf{G}$ is a symmetric tensor. In addition, a second strain tensor (Almansi-Hamel strain tensor) related to the actual configuration can be defined as it follows

$$\mathbf{A} = \left(\mathbf{F}^{T}\right)^{-1} \cdot \mathbf{G} \cdot \mathbf{F}^{-1}$$

2.1.2 Displacements, Displacement Gradient, Linearizations

For both configurations we can introduce the displacement vector

$$\mathbf{u}(\mathbf{x}, t) = \mathbf{x}(\mathbf{X}, t) - \mathbf{X}, \qquad \mathbf{u}(\mathbf{X}, t) = \mathbf{x} - \mathbf{X}(\mathbf{x}, t) \tag{5}$$

The displacement gradient can be also computed in both configurations

$$[\nabla_{\mathbf{X}} \mathbf{u}(\mathbf{X}, t)]^{T} \equiv \mathbf{J}, \qquad [\nabla_{\mathbf{x}} \mathbf{u}(\mathbf{x}, t)]^{T} \equiv \mathbf{K}$$

It is easy to show that

$$\mathbf{J} = \mathbf{F} - \mathbf{I}, \qquad \mathbf{K} = \mathbf{I} - \mathbf{F}^{-1}, \tag{6}$$

and the strain tensors can be obtained as it follows

$$\mathbf{G} = \frac{1}{2}(\mathbf{J} + \mathbf{J}^{T} + \mathbf{J} \cdot \mathbf{J}^{T}), \qquad \mathbf{A} = \frac{1}{2}(\mathbf{K} + \mathbf{K}^{T} - \mathbf{K}^{T} \cdot \mathbf{K}) \tag{7}$$

Finally, the strain tensors can be computed

$$\begin{aligned} \mathbf{G} &= \frac{1}{2}\left[(\nabla_{\mathbf{X}} \mathbf{u})^{T} + (\nabla_{\mathbf{X}} \mathbf{u}) + (\nabla_{\mathbf{X}} \mathbf{u}) \cdot (\nabla_{\mathbf{X}} \mathbf{u})^{T}\right], \\ \mathbf{A} &= \frac{1}{2}\left[(\nabla_{\mathbf{x}} \mathbf{u})^{T} + (\nabla_{\mathbf{x}} \mathbf{u}) - (\nabla_{\mathbf{x}} \mathbf{u}) \cdot (\nabla_{\mathbf{x}} \mathbf{u})^{T}\right] \end{aligned} \tag{8}$$

Both strain tensors contain quadratic terms. They describe the geometrical-nonlinear behavior of the continuum. Ignoring quadratic terms we get similar expressions as in Strength of Materials (Cauchy strain tensor). The mathematical consistent linearization of the kinematical relations is presented, for example, in [32].

2.2 Stress State

The external actions on the continuum can by classified as volume or surface actions. They can be pure mechanical, thermal, electromagnetic, etc. Here we focus our attention on mechanical actions, which can split as known from the General Mechanics (Statics) into forces and moments. Then we can introduce:

- mass or volume forces and moments and
- surface forces and moments.

In general the actions are continuously distributed in the volume or on the surface functions. They are introduced as models since they cannot observed directly (only the response of the actions can be measured). It is easy to show that line and concentrated single actions are limit cases of the volume and surface actions. These limit cases are the result of the different order of the three spatial dimensions or of the two dimensions of the surface.

Any material body is characterized by a continuous mass density distribution $\rho(\mathbf{x})$. The mass or volume actions are also continuous functions applied to any material point of the body. Examples of volume forces are the gravitational force, the force of inertia, the Coriolis force among others. The sources of these forces are out of the body, that means they are external (far-distance) forces. By analogy one can introduce sources for volume moments.

Volume forces are related to volume or mass. By $\mathbf{k}^{\mathrm{V}}$ the volume force density and by $\mathbf{k}^{\mathrm{m}} \equiv \mathbf{k}$ the mass force density are denoted (in what is following $\mathbf{k}$ is used instead of $\mathbf{k}^{\mathrm{m}}$). It holds

$$\rho(\mathbf{x},\mathrm{t})\mathbf{k}(\mathbf{x},\mathrm{t}) = \mathbf{k}^{\mathrm{V}} \tag{9}$$

In the case of volume moments the analogous equation is valid

$$\rho(\mathbf{x},\mathrm{t})\mathbf{l}^{\mathrm{m}}(\mathbf{x},\mathrm{t}) = \rho(\mathbf{x},\mathrm{t})\mathbf{l}(\mathbf{x},\mathrm{t}) = \mathbf{l}^{\mathrm{V}} \tag{10}$$

with $\mathbf{l}^{\mathrm{m}}(\mathbf{x},t)$ as the mass moment density and $\mathbf{l}^{\mathrm{V}}(\mathbf{x},t)$ as the volume moment density.

External surface loads are acting on surfaces. Such loads are named contact loads. The surface can be the surface of a material body with a volume A(V), but also common interfaces between the parts of the body or between two different bodies. External surface loads are existing also between solids and fluids, for example, the hydrostatic pressure of the fluid on a solid surrounded by the fluid. The surface loads can be split again into surface forces and surface moments. The

surface forces are related to the surface and result in the force stress vector $\mathbf{t}$, the surface moments by analogy result in the moment stress vectors $\boldsymbol{\mu}$. The following limits are valid [5, 27]

$$\mathbf{t} = \lim_{\triangle A \to 0} \frac{\triangle \mathbf{f}}{\triangle A}, \qquad \boldsymbol{\mu} = \lim_{\triangle A \to 0} \frac{\triangle \mathbf{m}}{\triangle A} \tag{11}$$

$\triangle \mathbf{f}$ and $\triangle \mathbf{m}$ are the resulting force vector and the resulting moment vector applied on the surface element $\triangle A$. It should be mentioned that $\triangle A$ is oriented $\triangle \mathbf{A} = \mathbf{n} \triangle A$ with $\mathbf{n}$ as the unit normal vector. This results later in the necessity to introduce stress tensors.

The resulting force $\mathbf{f}^R$ acting on the continuum can be computed by integration of the volume and surface forces

$$\mathbf{f}^R = \int_V \rho \mathbf{k} \, dV + \int_A \mathbf{t} \, dA \tag{12}$$

The resulting moment with respect to the coordinate origin 0 can be estimated by analogy

$$\mathbf{m}_0^R = \int_V \rho(\mathbf{l}^m + \mathbf{x} \times \mathbf{k}) dV + \int_A (\boldsymbol{\mu} + \mathbf{x} \times \mathbf{t}) dA \tag{13}$$

In the classical Continuum Mechanics the volume moment densities and the moment stress vectors are ignored. In this case the last one equation can be rewritten

$$\mathbf{m}_0^R = \int_V \rho(\mathbf{x} \times \mathbf{k}) dV + \int_A (\mathbf{x} \times \mathbf{t}) dA \tag{14}$$

2.2.1 Cauchy's Stress Vector and Tensor

As the result of the action of outer forces on the continuum one gets a stress state in the continuum. It can be estimated with the help of the cutting principle and the static equilibrium statement. If $\Delta \mathbf{f}$ is the resulting force vector on the surface element ΔA (both are presented in the actual configuration), the following definition is valid

$$\lim_{\Delta A \to 0} \frac{\Delta \mathbf{f}}{\Delta A} \equiv \mathbf{t}(\mathbf{x}, \mathbf{n}, t)$$

All stress vectors $\mathbf{t}$ in the point P define the stress state. In material testing one has to distinguish two different stress definitions. The first one relates the force to the surface in the reference configuration (engineering stress), the second one to

the surface in the actual configuration (true stress). In Continuum Mechanics we have more possibilities: the force can be given in both configurations and the surface can be presented in both configurations. In addition, one can introduce intermediate configurations.

Let us define at first the Cauchy stress tensor: if the force is given in the actual configuration and the surface element too, we have the so-called true stress vector $\mathbf{t}$. In this case the Cauchy stress tensor is given by (Cauchy's theorem)

$$\mathbf{t}(\mathbf{x}, \mathbf{n}, \mathrm{t}) = \mathbf{n} \cdot \mathbf{T}(\mathbf{x}, \mathrm{t}) \tag{15}$$

Based on this definition the first equilibrium Eq. (12) can be transformed into

$$\int_{\mathrm{V}} \rho \mathbf{k} \, \mathrm{dV} + \int_{\mathrm{A}} \mathbf{n} \cdot \mathbf{T}(\mathbf{x}, \mathrm{t}) \, \mathrm{dA} = \mathbf{0}. \tag{16}$$

Applying the Gauss-Ostrogradsky theorem (divergence theorem)

$$\int_{\mathrm{A}} \mathbf{t} \, \mathrm{dA} = \int_{\mathrm{A}} \mathbf{n} \cdot \mathbf{T} \, \mathrm{dA} = \int_{\mathrm{V}} \nabla_{\mathbf{x}} \cdot \mathbf{T} \, \mathrm{dV}, \tag{17}$$

finally one gets

$$\int_{\mathrm{V}} (\rho \mathbf{k} + \nabla_{\mathbf{x}} \cdot \mathbf{T}) \mathrm{dV} = \mathbf{0}. \tag{18}$$

and in the case of smooth fields the differential equilibrium equation

$$\nabla_{\mathbf{x}} \cdot \mathbf{T} + \rho \mathbf{k} = \mathbf{0} \tag{19}$$

Adding the inertial term $-\ddot{\mathbf{x}} \mathrm{dM} = -\ddot{\mathbf{x}} \rho \mathrm{dV}$ in the sense of Newton/d'Alembert to the integral equilibrium, after similar manipulations the following local equation is valid

$$\rho \ddot{\mathbf{x}} = \nabla_{\mathbf{x}} \cdot \mathbf{T} + \rho \mathbf{k}. \tag{20}$$

This is the first Cauchy-Euler equation of motion.

In the classical Continuum Mechanics from the moment equilibrium it follows that the stress tensor must be a symmetric tensor

$$\mathbf{T} = \mathbf{T}^{\mathrm{T}}$$

2.2.2 Stress Vectors and Tensors After Piola-Kirchhoff

The first Piola-Kirchhoff stress tensor can be defined on the base of the following stress vector. If we relate the actual force vector $\Delta \mathbf{f}$ to the surface element $\Delta \mathrm{A}_0$ in the reference configuration we get the first Piola-Kirchhoff stress vector

$$\lim_{\Delta A_0 \to 0} \frac{\Delta \mathbf{f}}{\Delta A_0} = {}^{\mathrm{I}}\mathbf{t}$$

From this definition it follows

$$ {}^{I}\mathbf{t} = \mathbf{n}_0 \cdot {}^{\mathrm{I}}\mathbf{P} \tag{21}$$

The Cauchy stress tensor and the first Piola-Kirchhoff stress tensor are interlinked by the following equations

$$\mathbf{T} = (\det \mathbf{F})^{-1}\mathbf{F} \cdot {}^{\mathrm{I}}\mathbf{P}, \qquad {}^{\mathrm{I}}\mathbf{P} = (\det \mathbf{F})\mathbf{F}^{-1} \cdot \mathbf{T} \tag{22}$$

The first Piola-Kirchhoff stress tensor is in the general case no more a symmetric tensor. The differential equations of motion for the forces and the moments with respect to the first Piola-Kirchhoff tensor can be formulated

$$\rho_0 \ddot{\mathbf{x}} = \nabla_{\mathbf{X}} \cdot {}^{\mathrm{I}}\mathbf{P} + \rho_0 \mathbf{k}, \qquad {}^{\mathrm{I}}\mathbf{P} \cdot \mathbf{F}^{\mathrm{T}} = \mathbf{F} \cdot {}^{\mathrm{I}}\mathbf{P}^{\mathrm{T}}. \tag{23}$$

The unsymmetric tensor ${}^{\mathrm{I}}\mathbf{P}$ is not convenient, if we want to combine the stresses with the strains which are presented by a symmetric tensor. Let us introduce a "fictive" force vector

$$\mathrm{d}\mathbf{f}_0 = \mathbf{F}^{-1} \cdot \mathrm{d}\mathbf{f}. \tag{24}$$

With the help of this vector by analogue the second Piola-Kirchhoff tensor, which is a symmetric tensor, can be defined. The following relation between the first and the second Piola-Kirchhoff tensor is valid

$${}^{\mathrm{II}}\mathbf{P} = {}^{\mathrm{I}}\mathbf{P} \cdot \left(\mathbf{F}^{-1}\right)^{\mathrm{T}}$$

2.3 Balance Equations

The balance equation are fundamental equation in the Continuum Mechanics. They are valid for all materials, etc. that means they do not contain any specific information on the properties of the continuum. The following balances are detailed presented, for example, in [32, 49, 58, 63].

2.3.1 General Global and Local Equations in the Case of Smooth Fields

The actual state of the continuum is given by volume integrals of densities of the mechanical state variables. The external action should be presented by volume and surface integrals of the volume and surface action densities. This holds true for both configurations.

The general form of the balance equation can be introduced as it follows. $\Psi(\mathbf{x},\mathrm{t})$ and $\Psi_0(\mathbf{X},\mathrm{t})$ are densities of a scalar mechanical variable with respect to the volume elements dV and dV_0 in the actual and the reference configurations. The integration over the volume results in an additive (extensive) variable $\mathrm{Y}(\mathrm{t})$

$$\mathrm{Y}(\mathrm{t}) = \int\limits_{\mathrm{V}} \Psi(\mathbf{x},\mathrm{t})\mathrm{dV} = \int\limits_{\mathrm{V}_0} \Psi_0(\mathbf{X},\mathrm{t})\mathrm{dV}_0 \tag{25}$$

The material time derivative of $\mathrm{Y}(\mathrm{t})$ is the rate of changes of $\Psi_0(\mathbf{x},\mathrm{t})$. The changes have the origins in the action of the surrounding on the continuum. In the actual configuration we assume

$$\frac{\mathrm{D}}{\mathrm{Dt}}\mathrm{Y}(\mathrm{t}) = \frac{\mathrm{D}}{\mathrm{Dt}}\int\limits_{\mathrm{V}} \Psi(\mathbf{x},\mathrm{t})\mathrm{dV} = \int\limits_{\mathrm{A}} \Phi(\mathbf{x},\mathrm{t})\mathrm{dA} + \int\limits_{\mathrm{V}} \Xi(\mathbf{x},\mathrm{t})\mathrm{dV} \tag{26}$$

and in the reference configuration

$$\frac{\mathrm{D}}{\mathrm{Dt}}\mathrm{Y}(\mathrm{t}) = \frac{\mathrm{D}}{\mathrm{Dt}}\int\limits_{\mathrm{V}_0} \Psi_0(\mathbf{X},\mathrm{t})\mathrm{dV}_0 = \int\limits_{\mathrm{A}_0} \Phi_0(\mathbf{X},\mathrm{t})\mathrm{dA}_0 + \int\limits_{\mathrm{V}_0} \Xi_0(\mathbf{X},\mathrm{t})\mathrm{dV}_0 \tag{27}$$

Φ and Φ_0 are scalar surface densities of the external actions in both configurations, $\boldsymbol{\Xi}$ and $\boldsymbol{\Xi_0}$ are the volume densities, D/Dt denotes the material derivative. This basic idea can be applied also to tensor fields. Let us introduce the general balance equation in the actual configuration

$$\frac{\mathrm{D}}{\mathrm{Dt}}\int\limits_{\mathrm{V}} {}^{(\mathrm{n})}\boldsymbol{\Psi}(\mathbf{x},\mathrm{t})\mathrm{dV} = \int\limits_{\mathrm{A}} \mathbf{n}(\mathbf{x},\mathrm{t}) \cdot {}^{(\mathrm{n}+1)}\boldsymbol{\Phi}(\mathbf{x},\mathrm{t})\mathrm{dA} + \int\limits_{\mathrm{V}} {}^{(\mathrm{n})}\boldsymbol{\Xi}(\mathbf{x},\mathrm{t})\mathrm{dV} \tag{28}$$

${}^{(\mathrm{n})}\boldsymbol{\Psi}(\mathbf{x},\mathrm{t})$ is the balance variable (tensor of rank n), ${}^{(\mathrm{n}+1)}\boldsymbol{\Phi}(\mathbf{x},\mathrm{t})$ is the flux term (tensor of rank n + 1) and ${}^{(\mathrm{n})}\boldsymbol{\Xi}(\mathbf{x},\mathrm{t})$ is the source/drain term (tensor of rank n). For the reference configuration similar balance equation can be formulated

$$\begin{aligned}\frac{\mathrm{D}}{\mathrm{Dt}}\int\limits_{\mathrm{V}_0} {}^{(\mathrm{n})}\boldsymbol{\Psi}_0(\mathbf{X},\mathrm{t})\mathrm{dV}_0 &\equiv \frac{\partial}{\partial \mathrm{t}}\int\limits_{\mathrm{V}_0} {}^{(\mathrm{n})}\boldsymbol{\Psi}_0(\mathbf{X},\mathrm{t})\mathrm{dV}_0 \\ &= \int\limits_{\mathrm{A}_0} \mathbf{n}_0(\mathbf{X},\mathrm{t}) \cdot {}^{(\mathrm{n}+1)}\boldsymbol{\Phi}_0(\mathbf{X},\mathrm{t})\mathrm{dA}_0 + \int\limits_{\mathrm{V}_0} {}^{(\mathrm{n})}\boldsymbol{\Xi}_0(\mathbf{X},\mathrm{t})\mathrm{dV}_0\end{aligned} \tag{29}$$

Note that instead of the mass densities the volume densities can be used.

If the smoothness requirements are fulfilled the local general balance equation can be given for the actual configuration

$$\frac{\mathrm{D}}{\mathrm{Dt}}[\boldsymbol{\Psi}(\mathbf{x},\mathrm{t})\rho] = \nabla_{\mathbf{x}} \cdot \boldsymbol{\Phi}(\mathbf{x},\mathrm{t}) + \boldsymbol{\Xi}(\mathbf{x},\mathrm{t})\rho \tag{30}$$

and for the reference configuration

$$\frac{\partial}{\partial \mathrm{t}}[\boldsymbol{\Psi}_0(\mathbf{X},\mathrm{t})\rho_0] = \nabla_{\mathbf{X}} \cdot \boldsymbol{\Phi}_0(\mathbf{X},\mathrm{t}) + \boldsymbol{\Xi}(\mathbf{X},\mathrm{t})\rho_0 \tag{31}$$

2.3.2 Mechanical Balance Equations

In the literature as usual 4 or 5 balances are presented (some authors do not accept the entropy balance and discuss the second law of thermodynamics separately). Here we present the 5 balances (mass, momentum, moment of momentum, energy and entropy) in an unique form.

Mass Balance

The mass is a characteristic property of the continuum and can be computed by a volume integral over the density in both configurations

$$\mathrm{m} = \int_{\mathrm{V}} \rho(\mathbf{x},\mathrm{t})\mathrm{dV} = \int_{\mathrm{V}_0} \rho_0(\mathbf{X})\mathrm{dV}_0 \tag{32}$$

If there is no mass flux and source/drain term in the general balance equation the mass is constant for any time t (mass conversation). The mass conservation as usual is accepted for solids.

$\rho \mathrm{d}V$ and $\rho_0 \mathrm{dV}_0$ are the mass of a material point in the actual and the reference configuration. If they are the same it follows

$$\rho \det \mathbf{F} = \rho_0 \Rightarrow \frac{\rho_0}{\rho} = \det \mathbf{F},$$

If $\rho_0 = \rho$ the value $\det \mathbf{F} = 1$ (incompressibility condition).

Balance of Momentum

Let us introduce the momentum vector $\mathbf{p}$

$$\mathbf{p}(\mathbf{x},\mathrm{t}) = \int_{\mathrm{m}} \mathbf{v}(\mathbf{x},\mathrm{t})\mathrm{dm} = \int_{\mathrm{V}} \mathbf{v}(\mathbf{x},\mathrm{t})\rho(\mathbf{x},\mathrm{t})\mathrm{dV} \tag{33}$$

with the velocity in the actual configuration $\mathbf{v}(\mathbf{x},\mathrm{t})$. The balance of momentum is defined

$$\frac{\mathrm{D}}{\mathrm{Dt}}\int\limits_{\mathrm{V}} \mathbf{v}(\mathbf{x},\mathrm{t})\rho(\mathbf{x},\mathrm{t})\mathrm{dV} = \int\limits_{\mathrm{A}} \mathbf{t}(\mathbf{x},\mathbf{n},\mathrm{t})\mathrm{dA} + \int\limits_{\mathrm{V}} \mathbf{k}(\mathbf{x},\mathrm{t})\rho(\mathbf{x},\mathrm{t})\mathrm{dV} \tag{34}$$

In the reference configuration the following equation holds

$$\frac{\partial}{\partial \mathrm{t}}\int\limits_{\mathrm{V}_0} \mathbf{v}(\mathbf{X},\mathrm{t})\rho_0(\mathbf{X})\mathrm{dV}_0 = \int\limits_{\mathrm{A}_0} {}^{\mathrm{I}}\mathbf{t}(\mathbf{X},\mathbf{n}_0,\mathrm{t})\mathrm{dA}_0 + \int\limits_{\mathrm{V}_0} \mathbf{k}(\mathbf{X},\mathrm{t})\rho_0(\mathbf{X})\mathrm{dV}_0 \tag{35}$$

Assuming the smoothness of all fields the local balances of momentum can be derived

$$\nabla_{\mathbf{x}} \cdot \mathbf{T}(\mathbf{x},\mathrm{t}) + \rho(\mathbf{x},\mathrm{t})\mathbf{k}(\mathbf{x},\mathrm{t}) = \rho(\mathbf{x},\mathrm{t})\frac{\mathrm{D}\mathbf{v}(\mathbf{x},\mathrm{t})}{\mathrm{Dt}}, \tag{36}$$

$$\nabla_{\mathbf{X}} \cdot {}^{\mathrm{I}}\mathbf{P}(\mathbf{X},\mathrm{t}) + \rho_{\mathbf{0}}(\mathbf{X})\mathbf{k}(\mathbf{X},\mathrm{t}) = \rho_{\mathbf{0}}(\mathbf{X})\frac{\partial \mathbf{v}(\mathbf{X},\mathrm{t})}{\partial \mathrm{t}} \tag{37}$$

These are again the so-called first Eulerian equations of motion.

Balance of Moment of Momentum

Let us define the global moment of momentum vector with respect to the origin O

$$\mathbf{l}_{\mathrm{O}}(\mathbf{x},\mathrm{t}) = \int\limits_{\mathrm{V}} \mathbf{x} \times \rho(\mathbf{x},\mathrm{t})\mathbf{v}(\mathbf{x},\mathrm{t})\mathrm{dV}$$

The balance of moment of momentum

$$\frac{\mathrm{D}}{\mathrm{Dt}}\int\limits_{\mathrm{V}} [\mathbf{x} \times \rho(\mathbf{x},\mathrm{t})\mathbf{v}(\mathbf{x},\mathrm{t})]\mathrm{dV} = \int\limits_{\mathrm{V}} [\mathbf{x} \times \rho(\mathbf{x},\mathrm{t})\mathbf{k}(\mathbf{x},\mathrm{t})]\mathrm{dV} + \int\limits_{\mathrm{A}} [\mathbf{x} \times \mathbf{t}(\mathbf{x},\mathbf{n},\mathrm{t})]\mathrm{dA}$$

After some manipulations the symmetry of the Cauchy stress tensor $\mathbf{T} = \mathbf{T}^{\mathrm{T}}$ can be established. Performing similar manipulations for the reference configuration ${}^{\mathrm{I}}\mathbf{P} \cdot \mathbf{F}^{\mathrm{T}} = \mathbf{F}^{\mathrm{T}} \cdot {}^{\mathrm{I}}\mathbf{P}$ is the consequence of the balance of moment of momentum.

Balance of Energy

With the kinetic energy $\mathcal{K}$ and the inner energy $\mathcal{U}$

$$\mathcal{K} = \frac{1}{2}\int_{\mathrm{V}} \mathbf{v}\cdot\mathbf{v}\rho \mathrm{dV}, \qquad \mathcal{U} = \int_{\mathrm{V}} \mathrm{u}\rho \mathrm{dV} \tag{38}$$

and the power of the external forces

$$\mathcal{P}_{\mathrm{a}} = \int_{\mathrm{A}} \mathbf{t}\cdot\mathbf{v}\mathrm{dA} + \int_{\mathrm{V}} \mathbf{k}\cdot\mathbf{v}\rho \mathrm{dV} \tag{39}$$

one gets the following balance of energy

$$\frac{\mathrm{D}}{\mathrm{Dt}}\int_{\mathrm{V}} \left(\frac{1}{2}\mathbf{v}\cdot\mathbf{v} + \mathrm{u}\right)\rho \mathrm{dV} = \int_{\mathrm{A}} \mathbf{t}\cdot\mathbf{v}\mathrm{dA} + \int_{\mathrm{V}} \mathbf{k}\cdot\mathbf{v}\rho \mathrm{dV} \tag{40}$$

Taking into account the local balance of momentum after some manipulations the energy balance can be presented as

$$\frac{\mathrm{D}}{\mathrm{Dt}}\int_{\mathrm{V}} \mathrm{u}\rho \mathrm{dV} = \int_{\mathrm{V}} \mathbf{T}\cdot\cdot(\nabla_{\mathbf{x}}\mathbf{v})^{\mathrm{T}} \mathrm{dV} \tag{41}$$

or in the local form

$$\dot{\mathrm{u}}\rho = \mathbf{T}\cdot\cdot(\nabla_{\mathbf{x}}\mathbf{v})^{\mathrm{T}} = \mathbf{T}\cdot\cdot\mathbf{D} \tag{42}$$

with $\mathbf{D}$ as the symmetric part of the velocity gradient tensor. The similar expression for the reference configuration relates the second Piola-Kirchhoff tensor to the rate of the Green-Lagrange strain tensor

$$\rho_0\dot{\mathrm{u}} = {}^{\mathrm{II}}\mathbf{P}\cdot\cdot\dot{\mathbf{G}} \tag{43}$$

Balance of Entropy

Let us assume pure mechanical behavior. The entropy balance results in usual conclusions. For the further statements we do not need these conclusion and we pass on the detailed analysis of the entropy balance.

2.4 Constitutive Modeling: Elastic Material

Let us assume elastic material behavior. In this case the constitutive equations are functions of the stress and strain tensors. Considering the material objectivity principle the following equation holds

$$^{\mathrm{II}}\mathbf{P}(\mathbf{X},\mathrm{t}) = \mathbf{g}(\mathbf{G},\mathbf{X},\mathrm{t})$$

That is adequate to the case of simple materials since the deformation state is defined only by the deformation gradient $\mathbf{F}(\mathbf{X},\mathrm{t})$.

For any isotropic tensor function $\mathbf{f}(\mathbf{A})$ the relations

$$\mathbf{Q}\cdot\mathbf{f}(\mathbf{A})\cdot\mathbf{Q}^{\mathrm{T}} = \mathbf{f}(\mathbf{Q}\cdot\mathbf{A}\cdot\mathbf{Q}^{\mathrm{T}})$$

are valid for the orthogonal tensor $\mathbf{Q}$ and the representation holds

$$\mathbf{f}(\mathbf{A}) = \phi_0\mathbf{I} + \phi_1\mathbf{A} + \phi_2\mathbf{A}^2$$

That means for the isotropic elastic material the constitutive equation can suggested as it follows

$$^{\mathrm{II}}\mathbf{P} = \psi_0\mathbf{I} + \psi_1\mathbf{G} + \psi_2\mathbf{G}^2$$

The ψ_i are functions of the invariants of $\mathbf{G}$.

3 Additional Equations Taking into Account Surface Effects

Let us assume purely elastic behavior for the bulk material and the surface. The theory of elasticity with surface stresses is presented, for example, in the review [18]. This theory is based on the assumption that together with the stress tensor determined in the bulk material and on its surface additional surface stresses act on the surface or on the part of the surface. The surface stress tensor is a generalization of the scalar surface tension in fluid mechanics [38] to deformable solids. The introduction of surface stresses permits an adequate modeling of size effects observed in tests of nanomaterials [18, 19].

First mathematical studies of surface stresses were performed by Laplace [39], Young [66], Gibbs [23] among others (see the surveys [21, 48, 53, 55, 56]). The mechanics of deformable solids with surface stresses is developed, for example, in [29, 30, 46, 52–54, 59]. The model proposed in [30] is equivalent to a deformable body with an fixed elastic membrane on the surface. The surface stress tensor acts in this membrane. This model is extended in [59] considering surface flexural stiffness and it can be regarded in the simplest case as a Kirchhoff-Love type shell on the body surface. In [33, 61, 62] surface effects are analyzed applying an approach in analogue to the classical Continuum Mechanics. Another theory for nano-scaled films developed in [43, 44] is based on the classical thin plate theory assuming the Kirchhoff hypothesis or its generalization, but the surface layers are modeled by a continuum theory of surface elasticity. Surface effects are analyzed also on the base of Cosserat-type or micropolar theories [17, 20, 35, 45, 51, 53].

3.1 Kinematical Equations

The simplest continuum model in the case that the properties of the bulk material and surface effects are taken into account can be formulated as it follows. The continuum occupies the domain $V \in \mathbb{R}^3$ bounded by the surface A. The surface A consist of two parts: on A_1 prescribed the displacements $\mathbf{u}$, on A_2 the tractions. If the continuum is fixed the equation

$$\mathbf{u}|_{A_1} = \mathbf{0}$$

is valid. On the rest the traction vector and maybe surface stresses are acting.

For the sake of simplicity we restrict ourself to the geometrical-linear theory. In this case it is not necessary to distinguish between the actual and the reference configuration:

$$\mathbf{X} \approx \mathbf{x}, \qquad \nabla_{\mathbf{X}} \approx \nabla_{\mathbf{x}} \equiv \nabla$$

The displacement vector $\mathbf{u}$ can serve as the fundamental quantity in the strain estimation. The strain tensors Eq. (8) are reduced to

$$\mathbf{G} \approx \mathbf{A} \approx \boldsymbol{\varepsilon} \equiv \frac{\boldsymbol{I}}{\boldsymbol{2}}\left[\nabla\mathbf{u} + (\nabla\mathbf{u})^{\mathrm{T}}\right] \tag{44}$$

In addition, for the modeling of surface effects we assume that surface effects are related also to the geometrical-linear theory. Then the following strain tensor can be suggested

$$\boldsymbol{\epsilon} \equiv \frac{1}{2}\left[\widetilde{\nabla}\mathbf{u} \cdot \widetilde{\mathbf{I}} + \widetilde{\mathbf{I}} \cdot (\widetilde{\nabla}\mathbf{u})^{\mathrm{T}}\right] \tag{45}$$

Here $\widetilde{\nabla}$ denotes the nabla operator defined on the surface only

$$\widetilde{\nabla} = \nabla - \mathbf{nn} \cdot \nabla$$

and $\widetilde{\mathbf{I}}$ is the two-dimensional unit tensor: $\widetilde{\mathbf{I}} = \mathbf{I} - \mathbf{nn}$.

The presented theory can be extended to the case of geometrical-nonlinear kinematical relations. That means the fundamental quantity for both the bulk and the surface behavior is the deformation gradient. Details of such theory are given, for example, in [9].

3.2 Stress state

The stress state in the continuum is defined by the stress tensor. With respect to the assumptions of the previous subsection it is not necessary to distinguish between the Cauchy and the Piola-Kirchhoff stress tensors. The stress tensor for the bulk

behavior is denoted by $\boldsymbol{\sigma}$. In addition, on the surface A_3 the stress tensor $\boldsymbol{\tau}$ is acting. Note that $A = A_1 \cup A_2 \cup A_3$ with A_2 as part of the surface on which only the tractions are acting and A_3 as part of the surface on which, in addition, the surface stresses are acting.

By analogy to the classical continuum the following equilibrium equation can be introduced

$$\nabla \cdot \boldsymbol{\sigma} + \rho \mathbf{k} = \mathbf{0} \qquad \forall \mathbf{X} \in V \tag{46}$$

In addition, on the surface A_3 (the following equilibrium is assumed

$$(\mathbf{n} \cdot \boldsymbol{\sigma} - \widetilde{\nabla} \cdot \boldsymbol{\tau})|_{A_3} = \mathbf{t} \tag{47}$$

$\mathbf{t}$ is the surface load vector. The other boundary conditions are

$$\mathbf{u}|_{A_1} = \mathbf{u}_0, \quad \mathbf{n} \cdot \boldsymbol{\sigma}|_{A_2} = \mathbf{t} \tag{48}$$

3.3 Constitutive Equations

For the bulk material the standard constitutive equations can be assumed

$$\boldsymbol{\sigma} = \frac{\partial u}{\partial \boldsymbol{\varepsilon}} \tag{49}$$

By analogy the surface stress tensor can be introduce as

$$\boldsymbol{\tau} = \frac{\partial \widetilde{u}}{\partial \boldsymbol{\epsilon}} \tag{50}$$

The inner (strain) energy density u is a function of $\boldsymbol{\varepsilon}$ and the surface strain energy density $\widetilde{u}$ is a function of ϵ. The main problem is to make a constitutive assumptions for both energy densities.

In the simplest case, assuming isotropic linear-elastic material behavior, one gets for the bulk material

$$u = \frac{1}{2}\lambda \mathrm{tr}^2 \boldsymbol{\varepsilon} + \mu \boldsymbol{\varepsilon} \cdot \cdot \boldsymbol{\varepsilon} \tag{51}$$

and for the surface

$$\widetilde{u} = \frac{1}{2}\widetilde{\lambda} \mathrm{tr}^2 \boldsymbol{\epsilon} + \widetilde{\mu} \boldsymbol{\epsilon} \cdot \cdot \boldsymbol{\epsilon}. \tag{52}$$

λ and μ are the Lamé parameters for the bulk material, $\widetilde{\lambda}$ and $\widetilde{\mu}$ are the Lamé parameters for the surface. It is easy to show that $\boldsymbol{\sigma}$ and $\boldsymbol{\tau}$ can be computed as it follows

$$\boldsymbol{\sigma} = \lambda \mathbf{I} \mathrm{tr}\boldsymbol{\varepsilon} + 2\mu\boldsymbol{\varepsilon}, \qquad \boldsymbol{\tau} = \widetilde{\lambda}\widetilde{\mathbf{I}}\mathrm{tr}\boldsymbol{\epsilon} + 2\widetilde{\mu}\boldsymbol{\epsilon}. \tag{53}$$

Other constitutive equations are discussed in the literature. For example, in [8] linear isotropic viscoelastic behavior is introduced. In [9] nonlinear isotropic elastic material behavior is assumed. In both cases the constitutive equations are established similar to the aforementioned approach.

4 Applications

The presented here theory can be applied to the analysis of nanostructures. In many cases theses structures can be modeled as plate- or shell-like structures. Such modeling results in a simplified analysis in comparison to the 3D applications because instead of three spatial coordinates describing the problem we have now only two.

The establishment of two-dimensional plate and shell equations can be performing using

- engineering hypothesis,
- mathematical techniques and
- the direct approach.

These three approaches are discussed briefly in [3, 4, 10, 26, 47]. The applications discussed in this section are based on the through-the-thickness integration introduced, for example, in [42].

In [7] the through-the-thickness integration is applied to the case of linear isotropic elastic behavior for the bulk material and on the surface. An additional term is introduced to consider residual surface stresses. The full set of governing palte/shell equations is deduced in the local form:

- kinematical relations based on an independent translation vector and an independent rotations vector and which consist of the in-plane strain tensor, the out-of-plane strain tensor and the transverse shear strain vector,
- equilibrium equations for the forces and moments (stress resultants) which are similar to the Reissner-Mindlin type theories, but taking into account surface effects, and
- two-dimensional constitutive equations for the stress resultants added by the terms related to to surface effects.

The plate equations are observed neglecting the influence of the shell curvature radii in the governing equations. In addition, the theory presented in [7] can be classified as a 5-parameter-theory. The surface stress influence is clearly seen in the effective stiffness expressions, which are expresses by the bulk and the surface properties. The improved stiffness parameters consist of material properties and the thickness. For the classical case (no surface effects) if the thickness tends to zero the stiffness tends to zero too. In the case if we take surface stresses into

account the stiffness parameter can increase or decrease. This tendency is significant for the prediction of the stiffness of nanostructures.

The previous theory is extended in [8] to linear viscoelastic material behavior using the Laplace transform and correspondence principle. As in the elastic case the transverse shear stiffness plays a specific role and must be computed carefully. It is established that the surface behavior is not affected by the transverse shear behavior with respect to the thinness of the influence zone.

5 Outlook

It was shown that the Continuum Mechanics allows the description of the mechanical behavior of nanomaterials, -structures or -devices. For this purpose it is necessary to extend slightly the classical theory by

- introducing nonclassical continuum models (for example, the micropolar),
- introducing instead of the simple material assumption higher gradients and
- introducing additional terms describing surface effects.

On the advantages of the first and second items is reported widely in the literature. Here the last item was discussed briefly.

Further investigations should be focused on

- the extension of the experimental data base which is necessary for the estimation of the constitutive parameters,
- the comparison of various approaches for a better understanding of the advantages, disadvantages of each approach and
- the consistent Continuum Mechanics formulation (balance equation, constitutive equations) and
- the extension of other types of inelastic material behavior.

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