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Model for simultaneous internal and external functional adaptation of bone

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1. Introduction

Remodeling of bone is assumed to be a process induced by the mechanical factor, or, more precisely, by the response of the system to the mechanical stimulation. External load causes the system response (the stress and strain field, and their rates), which provides the signal (called in the following stimulus) to the bone formation/resorption activity. It is assumed, that there exists the remodeling equilibrium state (RE), and if the current state of structure differs from RE, the remodeling takes place, resulting in the modification of the structure. Note that the load external to the bone may be dependent on the bone state, therefore the feed-back mechanism may occur.

Macroscopically the remodeling manifests itself in the evolution of properties of the bone material, as well as in changes of the shape of bone. Remodeling models known from literature usually treat these processes separately, distinguishing the internal remodeling and the surface (or external) remodeling.

Models following the idea described above attempts to simulate cause and effect without a consideration internal mechanisms. Such models are classified as phenomenological, and usually follows the idea of adaptive elasticity, recently vastly reviewed by Cowin [5].

The internal remodeling deals with changes of (averaged) physical properties of bone material, and is related to the formation/resorption process at the surface of trabeculae. It is assumed that the internal remodeling rate is moderated by the internal available specific surface area. A number of authors dealt with the internal remodeling, proposing different stimulus and evolution rules [7, 11, 2, 1, 17, 15], for review see Cowin [4] and Weinans and Prendergast [18].

The surface remodeling describing the changes of the external shape of bone is commonly associated with the formation/resorption activity at the external surface (boundary) of the bone, and is modeled by the rate of boundary geometry. Surface remodeling was considered, for instance, by Cowin [3], Luo et al. [13], van Rietbergen et al. [14]. The models of surface remodeling mentioned above have been developed to simulate the apposition of the new bone, or its local resorption, observed, for instance, after the arthoplasty, or to reflect changes of cross-sections of long bones registered experimentally.

An interesting approach is pesented in [16] where the remodeling process is modeled as a time-dependent shape optimization problem, resulting in extension of the adaptive elesticity theory with insight into microstructure of bone material.

The aim of this paper is to propose the model of bone adaptation that treats both the internal and the external remodeling in the same way. The remodeling is considered as a sole process, which manifests itself through changes of macroscopic properties of the material of bone as well as through variability of the domain occupied by the bone. The same remodeling rule deals with both types of remodeling measures. The approach constitutes the extension of the model for internal remodeling proposed by Tanaka et al. [15] by adding the mechanism of shape modification and deriving the remodeling rule from the hypothesis of optimal response of bone proposed by Lekszycki [12].

The model considered here is purely mechanical and phenomenological. It means that the transmission of mechanical signals and the activity of cells responsible for the bone formation and resorption are described by the set of postulated relations and by the remodeling rule derived from the mechanical hypothesis.

2. Remodeling mechanism

Assume that at the macroscopic level the bone remodeling process reveals itself in changes of apparent density of bone and associated with this process the evolution of its mechanical properties, as well as in changes of the domain occupied by bone. These effects allows to distinguish the internal remodeling related to evolution of bone material, and the external remodeling describing changes of geometry.

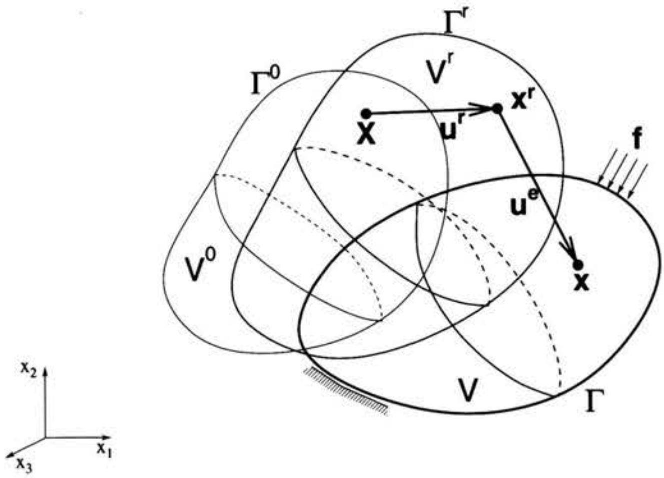

FIGURE 1. Kinematics of the remodeling process

Focus first on the kinematics of the process. It is assumed that due to the external remodeling the load-free configuration evolves. The *initial* load free configuration V^0 with the boundary Γ^0 at the time instant $\tau = t$ takes the *current* configuration V^r with the boundary Γ^r, so the point $\boldsymbol{X} \in V^0$ shifts to the new position $\boldsymbol{x}^r \in V^r$, Fig. 1. This evolution can be described by the *remodeling displacement field* $\boldsymbol{u}^r$ and *remodeling velocities* $\boldsymbol{v}^r$ defined as follows

$$\begin{aligned} \boldsymbol{u}^r &= \boldsymbol{u}^r = \boldsymbol{x}^r - \boldsymbol{X}\,, \\ \dot{\boldsymbol{u}}^r &= \frac{d\boldsymbol{u}^r}{dt} = \frac{d\boldsymbol{x}^r}{dt}\,. \end{aligned} \tag{2.1}$$

The remodeling displacements should be restricted in the way that a rigid body movement is eliminated. Denoting by Γ^0_r the part of the boundary Γ^0 with prescribed remodeling displacements $\bar{\boldsymbol{u}}^r$ these conditions can be written as

$$\boldsymbol{u}^r = \bar{\boldsymbol{u}}^r \quad \text{on} \quad \Gamma^0_r. \tag{2.2}$$

The current configuration V^r is subjected to a mechanical load originated from a muscle action and from an interaction with other tissues, resulting in the elastic deformation. The *current deformed* configuration denote as V and its boundary as Γ. Due to the elastic deformation the point $\boldsymbol{x}^r \in V^r$ shifts to the position $\boldsymbol{x} \in V$, so *elastic displacements* and *velocities* can be defined as

$$\begin{aligned} \boldsymbol{u}^e &= \boldsymbol{u}^r = \boldsymbol{x} - \boldsymbol{x}^r\,, \\ \dot{\boldsymbol{u}}^e &= \frac{d\boldsymbol{u}^e}{dt} = \frac{d\boldsymbol{x}^e}{dt} - \frac{d\boldsymbol{x}^r}{dt}\,. \end{aligned} \tag{2.3}$$

The elastic deformation can be treated as small, therefore the small strain tensor is applied

$$\boldsymbol{\varepsilon}^e = \frac{1}{2}\left(\nabla \boldsymbol{u}^e + \nabla^{\mathrm{T}} \boldsymbol{u}^e\right)\,; \quad \varepsilon^e_{ij} = \frac{1}{2}\left(\frac{\partial u^e_i}{\partial x^r_j} + \frac{\partial u^e_j}{\partial x^r_i}\right) \tag{2.4}$$

and in the following configurations V^r and V are not distinguished.

Denote by Γ^r_u the part of the boundary Γ^r with prescribed elastic displacements $\bar{\boldsymbol{u}}^e$, and by Γ^r_s the part subjected to surface traction $\boldsymbol{f}$. The boundary conditions can be written in the usual way

$$\begin{aligned} \boldsymbol{u}^e &= \bar{\boldsymbol{u}}^e \quad \text{on} \quad \Gamma^r_u\,, \\ \sigma \boldsymbol{n} &= \boldsymbol{f} \quad \text{on} \quad \Gamma^r_s\,. \end{aligned} \tag{2.5}$$

where $\boldsymbol{\sigma}$ is the stress field and $\boldsymbol{n}$ denotes the unit vector normal to the boundary Γ^r. Denote by $\mathcal{K}$ the set of kinematically admissible displacements

$$\mathcal{K} = \{\boldsymbol{u} \mid \boldsymbol{u} = \bar{\boldsymbol{u}}^e \text{ on } \Gamma^r_u\}\,. \tag{2.6}$$

Applying the virtual work principle we can write the weak form of equilibrium equation

$$\forall \delta\boldsymbol{u} \in \mathcal{K} \quad G\left(h_i,\, \varphi_i,\, \boldsymbol{u}^r,\, \boldsymbol{u}^e;\, \delta\boldsymbol{u}\right) = \int\limits_{V^r} \boldsymbol{\sigma} : \delta\boldsymbol{\varepsilon}\, dV^r - \int\limits_{\Gamma^r} \boldsymbol{f} \cdot \delta\boldsymbol{u}\, d\Gamma^r = 0 \tag{2.7}$$

where $\delta\boldsymbol{\varepsilon}$ are admissible strains defined on the current configuration V^r, namely

$$\delta\boldsymbol{\varepsilon} = \frac{1}{2}\left(\nabla \delta\boldsymbol{u} + \nabla^{\mathrm{T}} \delta\boldsymbol{u}\right)\,; \quad \delta\varepsilon_{ij} = \frac{1}{2}\left(\frac{\partial \delta u_i}{\partial x^r_j} + \frac{\partial \delta u_j}{\partial x^r_i}\right).$$

Note, that the term related to body forces is omitted in (2.7) because obviously the self-weight of bone is much smaller than loads generated by the muscle action, or by the interaction with other tissues.

The incremental equation can be obtained by the time differentiation of the equilibrium equation (2.7), resulting in the following formula

$$\begin{aligned} \forall \delta\boldsymbol{u} \in \mathcal{K} \qquad & \int\limits_{V^r} \left[(\boldsymbol{\sigma} : \delta\boldsymbol{\varepsilon})^{\cdot} + (\boldsymbol{\sigma} : \delta\boldsymbol{\varepsilon})\, \mathrm{div}\, \dot{\boldsymbol{u}}^r\right]\, dV^r \\ & \qquad = \int\limits_{\Gamma^r} \left[\dot{\boldsymbol{f}} + \boldsymbol{f}\left(\mathrm{div}\, \dot{\boldsymbol{u}}^r - \boldsymbol{n} \cdot \nabla^{\mathrm{T}} \dot{\boldsymbol{u}}^r\, \boldsymbol{n}\right)\right] \cdot \delta\boldsymbol{u}\, d\Gamma^r \end{aligned}$$

It can be shown that

$$(\delta\varepsilon_{ij})^{\cdot} = -\frac{1}{2}\left(\frac{\partial\delta u_i}{\partial x_k^r}\frac{\partial\dot{u}_k^r}{\partial x_j^r} + \frac{\partial\delta u_j}{\partial x_k^r}\frac{\partial\dot{u}_k^r}{\partial x_i^r}\right)$$

or in the operator notation

$$(\delta\boldsymbol{\varepsilon})^{\cdot} = -\frac{1}{2}\left(\nabla\delta\boldsymbol{u}\,\nabla\dot{\boldsymbol{u}}^r + \nabla^{\mathrm{T}}\dot{\boldsymbol{u}}^r\,\nabla^{\mathrm{T}}\delta\boldsymbol{u}\right).$$

Applying some properties of symmetric tensors the incremental equilibrium equation can be presented in the form

$$\forall\delta\boldsymbol{u}\in\mathcal{K}$$

$$\int_{V^r}\left[\dot{\boldsymbol{\sigma}}:\delta\boldsymbol{\varepsilon} - \left(\boldsymbol{\sigma}\,\nabla^{\mathrm{T}}\dot{\boldsymbol{u}}^r\right)_s:\delta\boldsymbol{\varepsilon} - \left(\boldsymbol{\sigma}\,\nabla^{\mathrm{T}}\dot{\boldsymbol{u}}^r\right)_w:\delta\boldsymbol{\omega} + (\boldsymbol{\sigma}:\delta\boldsymbol{\varepsilon})\operatorname{div}\dot{\boldsymbol{u}}^r\right]dV^r =$$
$$= \int_{\Gamma^r}\left[\dot{\boldsymbol{f}} + \boldsymbol{f}\left(\operatorname{div}\dot{\boldsymbol{u}}^r + \boldsymbol{n}\cdot\nabla^{\mathrm{T}}\dot{\boldsymbol{u}}^r\,\boldsymbol{n}\right)\right]\cdot\delta\boldsymbol{u}\,d\Gamma^r \tag{2.8}$$

where

$$\delta\boldsymbol{\omega} = \frac{1}{2}\left(\nabla\,\delta\boldsymbol{u} - \nabla^{\mathrm{T}}\delta\boldsymbol{u}\right),$$

and $\left(\boldsymbol{\sigma}\,\nabla^{\mathrm{T}}\dot{\boldsymbol{u}}^r\right)_s$ and $\left(\boldsymbol{\sigma}\,\nabla^{\mathrm{T}}\dot{\boldsymbol{u}}^r\right)_w$ are respectively the symmetric and skew-symmetric part of the tensor product $\boldsymbol{\sigma}\,\nabla^{\mathrm{T}}\dot{\boldsymbol{u}}^r$, namely

$$\begin{aligned}\left(\boldsymbol{\sigma}\,\nabla^{\mathrm{T}}\dot{\boldsymbol{u}}^r\right)_s &= \frac{1}{2}\left(\boldsymbol{\sigma}\,\nabla^{\mathrm{T}}\dot{\boldsymbol{u}}^r + \nabla\dot{\boldsymbol{u}}^r\,\boldsymbol{\sigma}\right),\\ \left(\boldsymbol{\sigma}\,\nabla^{\mathrm{T}}\dot{\boldsymbol{u}}^r\right)_s &= \frac{1}{2}\left(\boldsymbol{\sigma}\,\nabla^{\mathrm{T}}\dot{\boldsymbol{u}}^r - \nabla\dot{\boldsymbol{u}}^r\,\boldsymbol{\sigma}\right).\end{aligned}$$

The remodeling process is associated with the production/resorption of mass of bone. The total mass of bone at the time instant t is the integral of density over the remodeled domain,

$$M = \int_{V^r}\rho\,dV^r. \tag{2.9}$$

Variations of mass are related to changes of density, and also to the evolution of domain described by the remodeling displacement field $\boldsymbol{u}^r$. Therefore the mass rate can be expressed as

$$\dot{M} = \frac{dM}{dt} = \frac{d}{dt}\int_{V^r}\rho\,dV^r = \int_{V^r}\left(\dot{\rho} + \rho\operatorname{div}\dot{\boldsymbol{u}}^r\right)dV^r. \tag{2.10}$$

3. Stimulus and remodeling rule

Tanaka et al. [15] elaborated the model of internal remodeling belonging to the family of models following the Cowin and Hegedus idea of adaptive elasticity [6, 10], for review see Cowin [5]. The substantial difference from other models is the concept of modeling of the transmission of mechanical stimulus to bone cells, and dependence of the final stage of bone on the actual load history. In the model of Tanaka the remodeling manifests itself through the changes of apparent density. The bone is assumed to be isotropic and linearly elastic, therefore the stiffness tensor can be expressed as $\boldsymbol{C} = \boldsymbol{C}(E, \nu)$ with the Poisson ratio $\nu =$ const and the Young modulus E related to the apparent density ρ through the power law

$$E = E_0 \left(\frac{\rho}{\rho_0} \right)^k. \tag{3.1}$$

The relation above has been derived theoretically for the foam-like structures [9] and is commonly used in modeling of trabecular bone. Experimental identifications provide the factor k ranging from 1 to 3.

Following Fyhrie and Carter [8], the specific strain power (strain power per unit mass) was proposed as the stimulus of remodeling, namely

$$S = \left| \frac{\boldsymbol{\sigma} \cdot \dot{\boldsymbol{\varepsilon}}^e}{\rho} \right|, \tag{3.2}$$

and the local remodeling equilibrium was defined as follows

$$\begin{aligned} RE &= \rho - \rho_r\left(R_n\right) = 0 && \text{– no remodeling,} \\ RE &= \left|\rho - \rho_r\left(R_n\right)\right| \neq 0 && \text{– remodeling,} \end{aligned} \tag{3.3}$$

where $\rho_r(R_n)$ is an internal state function, that indicates the desired value of apparent density resulting from the actual load history. In the following this function will be called the *reference density*. R_n is the signal function discussed later on. The remodeling rule proposed in [15] can be presented in the form

$$\dot{\rho} = \alpha\left(\rho\right)\left[\alpha_f\langle\rho_r - \rho\rangle + \alpha_r\langle\rho - \rho_r\rangle\right] \tag{3.4}$$

where $\langle\cdot\rangle$ denotes Macaulay bracket defined as $\langle x\rangle = xU(x)$ where $U(x)$ is the unit step function, $\alpha\left(\rho\right)$ is the function taking into account the free surface of trabecular bone where the process of bone formation/resorption take place, and α_f, α_r are the formation and resorption coefficients, respectively. The term $\rho - \rho_r(R_n)$ is used as the remodeling driving force, therefore this remodeling rule assures that the apparent density changes toward the reference density value, and the change is proportional to the current difference between the apparent density and the reference one.

The signal function R_n reflects the history of mechanical stimulation, and is defined as the solution of the following set of subsequent differential equations

$$\begin{aligned} \dot{R}_0 &= P(S) - r_0 R_0^l, \\ \dot{R}_i &= r_i (R_{i-1} - R_i), \quad i = 1, \dots, n \\ R_i(t=0) &= \bar{R}_i, \quad i = 0, \dots, n \end{aligned} \tag{3.5}$$

Here $P(S)$ denotes the prescribed function of mechanical stimulus, $l, r_0, \dots, r_n$ are model parameters, and $\bar{R}_i, i = 0, \dots, n$ denote initial values of signal functions R_i. For detailed discussion of this transformation, including the initial conditions, see Tanaka et al. [15].

Our aim now is to extend the approach described above to the simultaneous internal and external remodeling. The remodeling rule is derived by applying the hypothesis of optimal response of bone, developed by Lekszycki [12]. The main idea of the hypothesis can be formulated descriptionally as follows:

the biological activity uses the remodeling ability in such a way, that the system approaches the remodeling equilibrium as quickly as possible.

Let us express the hypothesis mathematically in terms of the model considered. First we need to define the control functional of remodeling describing the deviation of the actual state of bone from the *remodeling equilibrium*. Therefore the functional should depend on actual values of remodeling parameters as well as on the expected state of remodeling equilibrium. Note that in the Tanaka's model the latter is dependent on the load history.

Next an optimization problem controlling the adaptation process should be stated with the rate of the control functional as the objective and rates of remodeling variables as design parameters. Such an optimization problem allows to specify the steepest approaching of remodeling equilibrium.

Assume, that at each point of bone the external remodeling is described by remodeling displacements $\boldsymbol{u}^r$, while the internal remodeling is associated with the apparent density ρ. Collect all remodeling variables in the n-element column vector $\boldsymbol{v} = \{\rho, (\boldsymbol{u}^r)^{\mathrm{T}}\}^{\mathrm{T}}$, and their rates in the column vector $\dot{\boldsymbol{v}} = \{\dot{\rho}, (\dot{\boldsymbol{u}}^r)^{\mathrm{T}}\}^{\mathrm{T}}$. Define at each point of the structure the *local characteristic function of remodeling* $F[\rho - \rho_r(R_n)]$ describing locally the deviation of actual state from the remodeling equilibrium. The function $F(y)$ should hold the following conditions

$$\begin{aligned} &F : \mathcal{R} \longrightarrow \mathcal{R} \\ &\forall y \in \mathcal{R} \quad F(y) \geq 0, \\ &F(y) = 0 \implies y = 0, \\ &y \neq 0 \implies \frac{dF}{dy} \operatorname{sign}(y) > 0 \end{aligned}$$

The function F equals zero when the remodeling equilibrium locally takes place ($\rho = \rho_r$) and increases monotonically with increasing $|\rho - \rho_r|$. Note that when the remodeling equilibrium is attained in whole bone then

$$\forall \boldsymbol{x}^r \in V^r \quad F(\rho - \rho_r) = 0$$

and at this stage the apparent density at distinct points may differ, because the reference density ρ_r depends on the history of mechanical stimulus at point. The mean value of function F,

$$G = \frac{1}{V^r} \int\limits_{V^r} F(\rho - \rho_r)\, dV^r \tag{3.6}$$

provides the information about the deviation from remodeling equilibrium in whole bone. From the definition of F we can conclude that

$$\begin{aligned} &G = 0 \qquad \text{if} \quad \forall \boldsymbol{x}^r \in V^r \quad F = 0\,, \\ &G > 0 \qquad \text{otherwise,} \end{aligned} \tag{3.7}$$

it means that $G = 0$ only if at all points the remodeling equilibrium takes place.

Mentioned above properties of G make this functional suitable to be the control functional for the hypothesis of optimal response of bone. The hypothesis requires, that the evolution of bone is realized in the way that minimizes the rate of the control functional $\dot{G} = dG/dt$. Differentiating the functional G we obtain

$$\dot{G} = \frac{1}{V^r} \int\limits_{V^r} \left[\frac{\partial F}{\partial \rho} \dot{\rho} + \frac{\partial F}{\partial \rho_r} \frac{\partial \rho_r}{\partial R_n} \dot{R}_n + \left(F(\rho - \rho_r) - G\right) \operatorname{div} \dot{\boldsymbol{u}}^r \right] dV^r, \tag{3.8}$$

and the variation of $\dot{G}$ with respect to rates of remodeling variables can be expressed as

$$\hat{\delta}_{\dot{v}} \dot{G} = \frac{1}{V^r} \int\limits_{V^r} \left[\frac{\partial F}{\partial \rho} \hat{\delta} \dot{\rho} + \frac{\partial F}{\partial \rho_r} \frac{\partial \rho_r}{\partial R_n} \hat{\delta}_{\dot{v}} \dot{R}_n + \left(F(\rho - \rho_r) - G\right) \operatorname{div} \hat{\delta} \dot{\boldsymbol{u}}^r \right] dV^r. \tag{3.9}$$

The overhat in the symbol $\hat{\delta}_{\dot{v}}(\,)$ has been introduced in order to distinguish the variation with respect to rates of remodeling variables from the kinematically admissible fields $\delta \boldsymbol{u}$, $\delta \boldsymbol{\varepsilon}$.

Focus now on the variation $\hat{\delta}_{\dot{v}} R_n$. Varying the system of differential equations (3.5) with respect to rates of remodeling variables $\dot{\boldsymbol{v}}$ we can write

$$\begin{aligned} &\hat{\delta}_{\dot{v}} \dot{R}_0 = \frac{\partial P}{\partial S}\, \hat{\delta}_{\dot{v}} S \;-\, r_0\, l\, R_0^{l-1}\, \hat{\delta}_{\dot{v}} R_0 \\ &\hat{\delta}_{\dot{v}} \dot{R}_i = r_i \left(\hat{\delta}_{\dot{v}} R_{i-1} - \hat{\delta}_{\dot{v}} R_i \right), \quad i = 1, \ldots, n \\ &\hat{\delta}_{\dot{v}} R_i \Big|_{t=0} = \hat{\delta}_{\dot{v}} \bar{R}_i\,, \quad i = 0, \ldots, n, \end{aligned} \tag{3.10}$$

and in view of (3.2) we have

$$\hat{\delta}_{\dot{v}} S = \operatorname{sign}\left(\tilde{S}\right) \frac{1}{\rho} \left(\hat{\delta}_{\dot{v}} \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}}^e + \boldsymbol{\sigma} : \hat{\delta}_{\dot{v}} \dot{\boldsymbol{\varepsilon}}^e \right) \tag{3.11}$$

where $\tilde{S} = \left(\boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}}^e \right) / \rho$. In order to determine the variation $\hat{\delta}_{\dot{v}} \boldsymbol{\sigma}$ examine the equation of equilibrium (2.7). Neither the external load f nor the remodeled domain V^r depend on the velocity of remodeling variables $\dot{\boldsymbol{v}}$. It implies that

$$\hat{\delta}_{\dot{v}} \boldsymbol{\sigma} \,=\, 0\,, \qquad \hat{\delta}_{\dot{v}} \boldsymbol{\varepsilon}^e \,=\, 0 \tag{3.12}$$

because in view of (3.1) the stiffness tensor depends only on the remodeling variables $\boldsymbol{v}$ themselves, but does not depend of their rates $\dot{\boldsymbol{v}}$. Apply now the incremental equilibrium equation (2.8). In view of (3.1) and (3.12) we obtain

$$\begin{aligned} &\forall \delta \boldsymbol{u} \in \mathcal{K}, \\ &\int\limits_{V^r} \left[\boldsymbol{C} \hat{\delta}_{\dot{v}} \dot{\boldsymbol{\varepsilon}}^e : \delta \boldsymbol{\varepsilon} \,+\, \left(\frac{\partial \boldsymbol{C}}{\partial \rho} \hat{\delta} \dot{\rho} \right) \boldsymbol{\varepsilon} : \delta \boldsymbol{\varepsilon} \,-\, \left(\boldsymbol{\sigma}\, \nabla^{\mathrm{T}} \hat{\delta} \dot{\boldsymbol{u}}^r \right)_s : \delta \boldsymbol{\varepsilon} \,+ \right. \\ &\qquad \left. -\, \left(\boldsymbol{\sigma}\, \nabla^{\mathrm{T}} \hat{\delta} \dot{\boldsymbol{u}}^r \right)_w : \delta \boldsymbol{\omega} + (\boldsymbol{\sigma} : \delta \boldsymbol{\varepsilon})\, \operatorname{div} \hat{\delta} \dot{\boldsymbol{u}}^r \right] dV^r = \\ &\quad = \int\limits_{\Gamma^r} \left[\frac{\partial \boldsymbol{f}}{\partial \boldsymbol{v}} \hat{\delta} \dot{\boldsymbol{v}} + \boldsymbol{f} \left(\operatorname{div} \hat{\delta} \dot{\boldsymbol{u}}^r - \boldsymbol{n} \cdot \nabla^{\mathrm{T}} \hat{\delta} \dot{\boldsymbol{u}}^r\, \boldsymbol{n} \right) \right] \cdot \delta \boldsymbol{u}\, d\Gamma^r. \end{aligned} \tag{3.13}$$

If relations $\boldsymbol{C} = \boldsymbol{C}(\rho)$ and $\boldsymbol{f} = \boldsymbol{f}(\boldsymbol{v})$ are prescribed, the equation (3.13) constitutes the boundary-value problem with unknown $\hat{\delta}_{\dot{v}} \dot{\boldsymbol{\varepsilon}}^e$.

Introducing the quantities $\tilde{\boldsymbol{\sigma}}_0$, $\tilde{\boldsymbol{q}}$ and $\tilde{\boldsymbol{f}}$ defined as follows

$$\begin{aligned} \tilde{\boldsymbol{\sigma}}_0 : \delta \boldsymbol{\varepsilon} \;&=\; - \left[(\partial \boldsymbol{C} / \partial \rho)\, \hat{\delta} \dot{\rho} \right] \boldsymbol{\varepsilon}^e : \delta \boldsymbol{\varepsilon} + \left(\boldsymbol{\sigma}\, \nabla^{\mathrm{T}} \hat{\delta} \dot{\boldsymbol{u}}^r \right)_s : \delta \boldsymbol{\varepsilon} - (\boldsymbol{\sigma} : \delta \boldsymbol{\varepsilon})\, \operatorname{div} \hat{\delta} \dot{\boldsymbol{u}}^r, \\ \tilde{\boldsymbol{q}} \cdot \delta \boldsymbol{u} \;&=\; \left(\boldsymbol{\sigma}\, \nabla^{\mathrm{T}} \hat{\delta} \dot{\boldsymbol{u}}^r \right)_w : \delta \boldsymbol{\omega}\,, \\ \tilde{\boldsymbol{f}} \cdot \delta \boldsymbol{u} \;&=\; \frac{\partial \boldsymbol{f}}{\partial \boldsymbol{v}} \hat{\delta} \dot{\boldsymbol{v}} - \boldsymbol{f} \left(\operatorname{div} \hat{\delta} \dot{\boldsymbol{u}}^r + \boldsymbol{n} \cdot \nabla^{\mathrm{T}} \hat{\delta} \dot{\boldsymbol{u}}^r\, \boldsymbol{n} \right). \end{aligned}$$

Equation (3.13) can be expressed in the form

$$\int\limits_{V^r} \left\{ \left[C \left(\hat{\delta}_{\dot{v}} \varepsilon^e \right) - \tilde{\sigma}_0 \right] : \delta\varepsilon - \tilde{q} \cdot \delta u \right\} dV^r - \int\limits_{\Gamma^r} \left(\tilde{f} \cdot \delta u \right) d\Gamma^r = 0 \,. \tag{3.14}$$

The remodeling process is subjected to a number of restrictions arising from the nature of remodeling process, such as the number of bone cells, the capability of single cell to form or resorbe the bone, the ability to transport substances for bone formation or products of bone resorption, etc.. These restrictions have to be introduced to the model as the constraints of the resulting optimal design problem. The manner of their formulation determines the variant of remodeling rule. Nevertheless, these limitations are not discussed in detail. It is assumed that they can be modeled with constraints constituting the extension of the remodeling rule (3.4).

The left-hand-side of Eq.(3.4) actually describes the local mass production, and this production is controlled by the difference $\rho - \rho_r$. Let us follow this idea, adopting it to the case of multiparameter remodeling. The local mass production can be expressed in terms of rates of remodeling parameters. Denote the measure of the local (specific) mass production as $m(\dot{v})$ In real bone both the formation and the resorption processes take place on distinct free surfaces of trabeculae. Nevertheless, the model considered in this paper deals with macroscopic, averaged properties of bone. It justifies the assumption that at the given point x^r both resorption and formation could take place simultaneously. Denote the measure of formed mass (positive) as $\langle m(\dot{v}) \rangle_+$, and the measure of resorbed mass (negative) as $\langle m(\dot{v}) \rangle_-$. Let $m(\dot{v})$ be a homogeneous function of remodeling variables of rank one. Then these measures can be expressed as

$$\begin{aligned} \langle m(\dot{v}) \rangle_+ &= \sum_i \left\langle \frac{\partial m}{\partial \dot{v}_i} \dot{v}_i \right\rangle , \\ \langle m(\dot{v}) \rangle_- &= - \sum_i \left\langle - \frac{\partial m}{\partial \dot{v}_i} \dot{v}_i \right\rangle , \end{aligned} \tag{3.15}$$

where $\langle \cdot \rangle$ is the Macaulay bracket. In order to follow the idea of Eq.(3.4) postulate

$$\begin{aligned} \langle m(\dot{v}) \rangle_+ &\leq \gamma_f F \left(rho - \rho_r \right) , \\ \langle m(\dot{v}) \rangle_- &\geq -\gamma_r F \left(\rho - \rho_r \right) , \end{aligned} \tag{3.16}$$

where $\gamma_f = \alpha(\rho)\alpha_f$ and $\gamma_r \alpha(\rho)\alpha_r$ are the formation and the resorption coefficient, respectively. The conditions (3.16) constitute a polyhedron in the

n-dimensional space of rates of remodeling variables $\dot{\boldsymbol{v}}$ with corners at

$$\dot{\boldsymbol{v}} = \{0,\ldots,0,\dot{v}_i,0,\ldots,0\}\,, \quad i=1,\ldots,n$$
$$\text{such that } \langle\, m\left(\{0,\ldots,0,\dot{v}_i,0,\ldots,0\}\right)\rangle_+ = \gamma_f F\,,$$

$$\dot{\boldsymbol{v}} = \{0,\ldots,0,\dot{v}_i,0,\ldots,0\}\,, \quad i=1,\ldots,n$$
$$\text{such that } \langle\, m\left(\{0,\ldots,0,\dot{v}_i,0,\ldots,0\}\right)\rangle_- = -\gamma_r F\,,$$

$$\dot{\boldsymbol{v}} = \{0,\ldots,0,\dot{v}_i,0,\ldots,0,\dot{v}_j,0,\ldots,0\}\,, \quad i=1,\ldots,n\,,\ \ j=1,\ldots,n\,,\ \ i\neq j$$
$$\text{such that} \quad \langle\, m\left(\{0,\ldots,0,v_i,0,\ldots,0,v_j,0,\ldots,0\}\right)\rangle_+ = \gamma_f F\,,$$
$$\langle\, m\left(\{0,\ldots,0,v_i,0,\ldots,0,\dot{v}_j,0,\ldots,0\}\right)\rangle_- = -\gamma_r F\,. \tag{3.17}$$

Introduce the function $M_1(\dot{\boldsymbol{v}})$ such that $M_1(\dot{\boldsymbol{v}},F)=0$ if $\dot{\boldsymbol{v}}$ belongs to the polyhedron defined above, $M_1(\dot{\boldsymbol{v}},F)<0$ if $\dot{\boldsymbol{v}}$ is inside the polyhedron, and $M_1(\dot{\boldsymbol{v}},F)>0$ if $\dot{\boldsymbol{v}}$ is outside. The conditions (3.16) are equivalent to

$$M_1(\dot{\boldsymbol{v}},F) \le 0\,. \tag{3.18}$$

The numerical implementation of the constraint (3.18) may cause some problems due to the non-smoothness of the limit surface $M_1=0$. Nevertheless an alternate constraint can be proposed by replacing the limit polyhedron with the second rank limit surface circumscribed on the polyhedron. Denoting this surface as $M_2(\dot{\boldsymbol{v}},F)$ instead of (3.18) we obtain the condition

$$M_2(\dot{\boldsymbol{v}},F) \le 0\,. \tag{3.19}$$

If the measure of the mass production can be expressed as

$$m(\dot{\boldsymbol{v}}) = \frac{\partial m}{\partial \dot{v}_i}\dot{v}_i = \theta_i \dot{v}_i$$

then the limit surface takes the form

$$M_2(\dot{\boldsymbol{v}},F) = a_{ij}\dot{v}_i\dot{v}_j + a_i\dot{v}_i - b = 0 \tag{3.20}$$

or in the matrix form

$$M_2(\dot{\boldsymbol{v}},F) = \dot{\boldsymbol{v}}^{\mathrm{T}}\boldsymbol{A}\dot{\boldsymbol{v}} + \boldsymbol{a}\cdot\dot{\boldsymbol{v}} - b = 0 \tag{3.21}$$

where

$$A_{ij} = a_{ij}\,, \quad \boldsymbol{a} = \{a_1,\ldots,a_n\}^{\mathrm{T}}$$

and

$$a_{ij} = \begin{cases} \theta_i\theta_j & \text{if} \quad i = j \\ \frac{1}{2}\theta_i\theta_j & \text{if} \quad i \neq j \end{cases}, \qquad a_i = -\left|\theta_i\right|(\gamma_f - \gamma_r)\,F\,, \qquad b = \gamma_f\gamma_r F^2. \tag{3.22}$$

An additional constraint results from the fact that the apparent density is a non-negative quantity. Therefore introduce the lower bound of the apparent density $\rho_{\min}$ such that $\rho \geq \rho_{\min}$. Applying also the condition (2.2) define the set of admissible remodeling velocities as

$$K^v = \left\{ \dot{\boldsymbol{v}} = \{\dot{\rho}, \dot{\boldsymbol{u}}^r\} \mid \dot{\boldsymbol{u}}^r = \dot{\bar{\boldsymbol{u}}}^r \; on \; \Gamma_r^0\,, \;\; \langle\rho_{\min} - \rho\rangle\,\dot{\rho} \geq 0 \right\}. \tag{3.23}$$

Now the optimization problem controlling the remodeling process can be state as follows

$$\begin{aligned} &\text{Find} && \min_{\dot{\boldsymbol{v}} \in \mathcal{K}^v} \dot{G} \\ &\text{subject to} && M_k\left(\dot{\boldsymbol{v}}, F\right) \leq 0. \end{aligned} \tag{3.24}$$

Remind that the functional $\dot{G}$ is defined in (3.8). In view of (3.8), (3.10) and (3.11) the objective functional $\dot{G}$ is linear with respect to $\dot{\boldsymbol{v}}$, and the feasible space limited by constraints is convex. Therefore the solution of the minimization problem *always* exists, and is located at the boundary of the feasible space. The remodeling rule derived here is schematically illustrated in Fig. 2 for two remodeling variables. Figure 2(a) presents the rule with the polyhedral limit surface $M_1(\dot{\boldsymbol{v}}, F) = 0$. In this case the resulting remodeling velocity is placed at the corner of the polyhedron through which passes the line orthogonal to the vector $\partial\dot{G}/\partial\dot{\boldsymbol{v}}$ and external to the polyhedron. In Figure 2(b) is shown the rule with ellipsoidal limit surface. The remodeling velocity is determined by the tangent to the ellipsoid which is orthogonal to the vector $\partial\dot{G}/\partial\dot{\boldsymbol{v}}$.

In order to find the solution in the case of M_1 for instance the linear programming can be applied. In the case of M_2 let us use the optimality conditions method. Construct the Lagrangian of the problem (3.24), namely

$$\mathcal{L} = \dot{G} - \frac{1}{V^r}\int\limits_{V^r} \eta M_2\left(\dot{\boldsymbol{v}}, F\right) dV^r \tag{3.25}$$

where η is the Lagrange multiplier. The actual rates of remodeling variables can be found as the stationary point of the Lagrangian $\mathcal{L}$. The stationarity

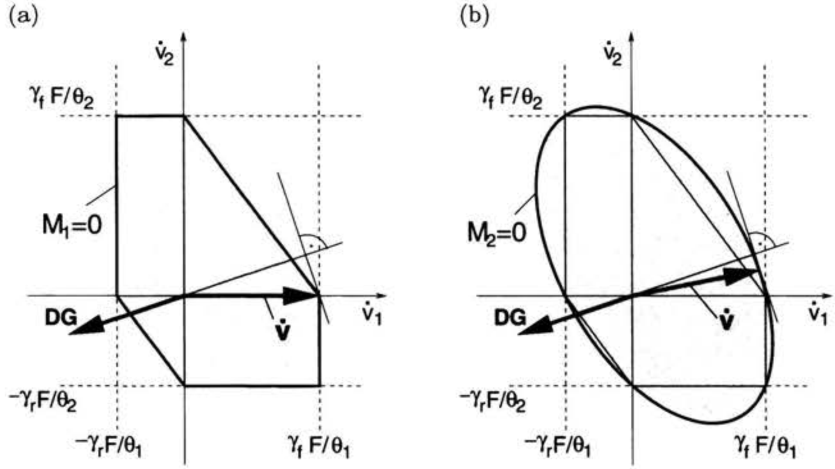

FIGURE 2. Remodeling rule, (a) polyhedral limit surface, (b) ellipsoidal limit surface. $DG = \partial \dot{G}/\partial \dot{v}$.

condition leads to

$$\forall \left\{ \hat{\delta}\dot{v} \in \mathcal{K}^v, \hat{\delta}\eta \right\}$$
$$\delta\mathcal{L} = \hat{\delta}_{\dot{v}}\dot{G} - \frac{1}{V^r} \int_{V^r} \left[\eta \frac{\partial M_2}{\partial \dot{v}} \hat{\delta}\dot{v} + \hat{\delta}\eta M_2 (\dot{v}, F) \right] dV^r = 0 \tag{3.26}$$

providing localized equations

$$\forall\, x^r \in V^r , \ \ \forall \left\{ \hat{\delta}\dot{v} \in \mathcal{K}^v, \hat{\delta}\eta \right\}$$
$$\frac{\partial F}{\partial v} \hat{\delta}\dot{v} + \frac{\partial F}{\partial \rho_r} \frac{\partial \rho_r}{\partial R_n} \hat{\delta}_{\dot{v}} R_n + (F - G) \operatorname{div} \hat{\delta}\dot{u}^r - \eta \frac{\partial M_2}{\partial \dot{v}} \hat{\delta}\dot{v} = 0$$
$$\hat{\delta}\eta\, M_2 (\dot{v}, F) = 0 \tag{3.27}$$

and $\hat{\delta}_{\dot{v}} R_n$ is specified in (3.10).

Note that the measure of mass production can be identified with the expression under the integral (3.1). In this case

$$m(\dot{v}) = \dot{\rho} + \rho \operatorname{div} \dot{u}^r .$$

4. Illustrative example

In order to illustrate the behavior of the model proposed we adopt the example presented in [15]. The rectangle of width a_1 and height a_2 is freely

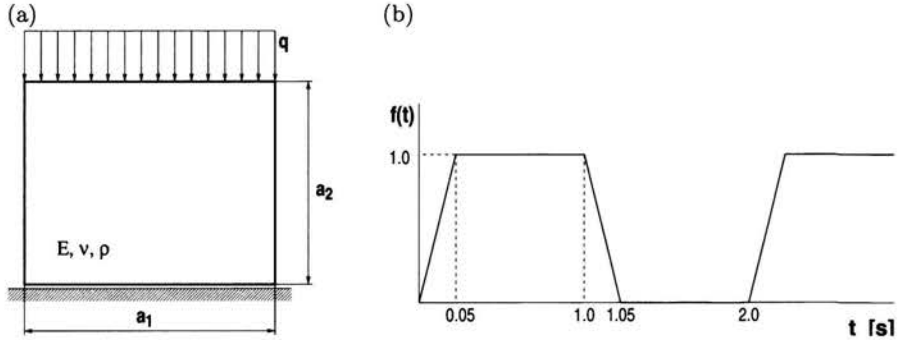

FIGURE 3. Scheme of load and support (a) and the diagram of one cycle of time history of load (b).

supported at the bottom edge and is loaded by the uniformly distributed cyclic force at its upper edge,

$$q = \bar{q} f(t) = \frac{q_0}{a1} f(t), \quad q_0 = \text{const}.$$

The apparent density ρ and the width of the rectangle a_1 are chosen as the remodeling variables. Values of parameters of the model and the history of load follow [15]. The results of simulation of remodeling process are shown in Fig. 4, presenting the evolution of remodeling variables in time. During the first simulation the amplitude of load is constant (q0=const, solid line). The initial conditions are set in the way, that the remodeling equilibrium occurs.

However, due to loading the internal function ρ_r increases, causing the remodeling process that takes place until the saturation is achieved. The other curves were obtained for different load history. The amplitude of load was constant in the time interval $\langle 0, t_1 \rangle$. At the time instant t_1 the amplitude of load is reduced to half of its value, and at t_2 it regains its primary magnitude. Two cases are presented, the first with $t_1 = 100$ [days], $t_2 = 200$ [days] (dotted line), and the second for which $t_1 = 150$ [days], $t_2 = 300$ [days] were assumed (dashed line). In these simulations the remodeling variables trace the solid curve until the time instant t_1, next decrease after the load amplitude reduction and since t_2 they increased again attaining practically the saturation value depicted by the solid line. The increase of the apparent density is accompanied with the increase of the width of the sample. Note

(a)

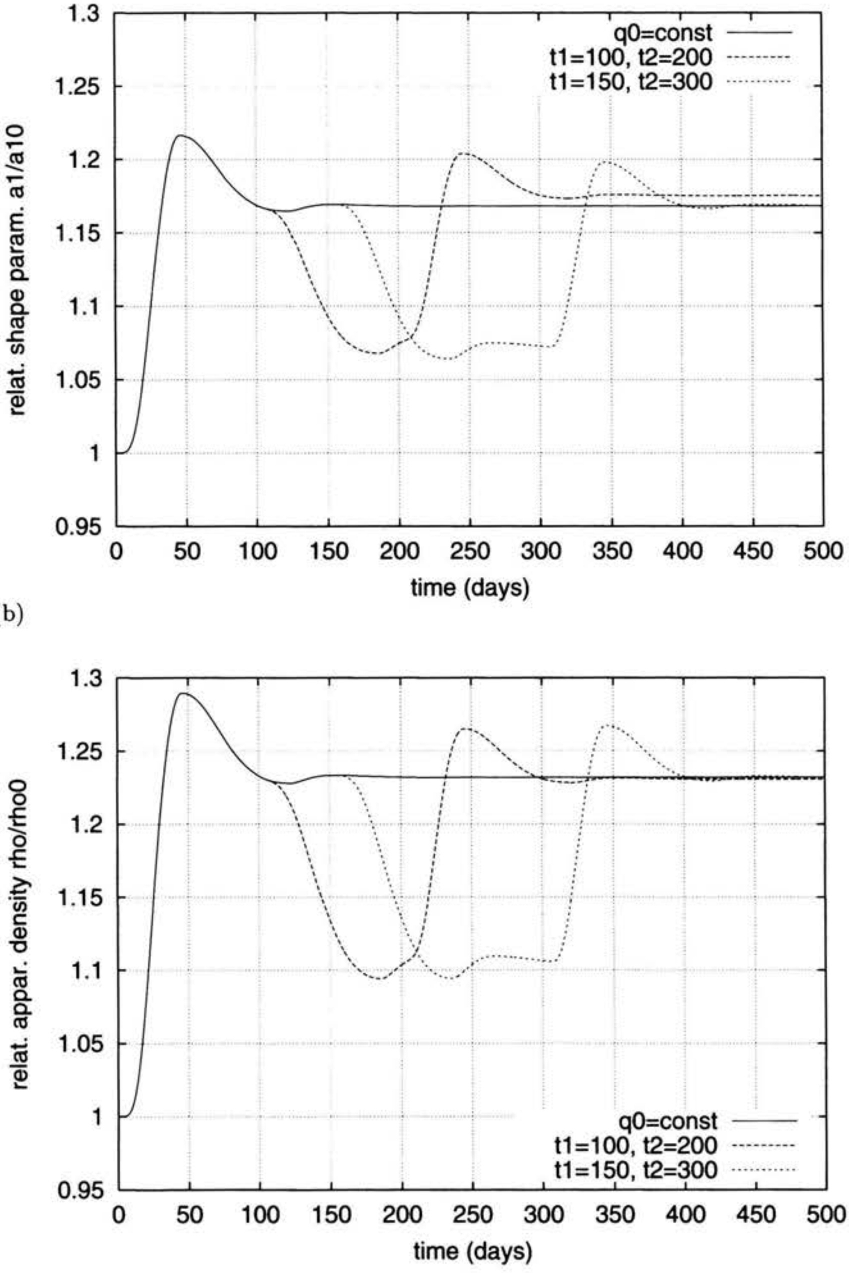

FIGURE 4. Differences in path of evolution induced by different loading history, (a) width a_1, (b) apparent density.

that overstep before attaining the saturation values can be observed. Such behavior is caused by the delay of signal transmission specific for the system of differential equations (3.5).

5. Concluding remarks

The rule of remodeling proposed in this paper deals with the simultaneous internal and external remodeling. The model constitutes the extension of the contribution of Tanaka et al. [15] by adding the mechanism of external remodeling. In previous contributions separate remodeling mechanisms have been proposed for external and internal remodeling. The elaborated remodeling rule is common for both kinds of remodeling.

The remodeling rule has been derived basing on th hypothesis of optimal response of bone. The hypothesis allows to formulate different remodeling laws by the suitable selection of the control functional and of remodeling constraints. Other models derived from the hypothesis of optimal response of bone can be found in [12].

Behavior of the model is illustrated using a simple example containing one material and one shape remodeling variable. The example shows that the numerical stability of the model is satisfactory. As it could be expected, the saturation of remodeling parameters is observed for prescribed, constant load level, and occur to be not dependent of the history of load changes. In simulation presented here the model parameters identified in [15] were used. However the model requires a careful identification based on experiments in which the internal properties and the shape of bone are recorded.

The proposed rule belongs to the group of phenomenological models, following the idea of Cowin's adaptive elasticity. The internal mechanisms and physiology of the process are not considered, as the aim of the work was to propose relatively simple model with limited number of parameters, useful in numerical simulation of real musculo-skeletal systems.

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