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OPTIMALITY CONDITIONS IN MODELING OF BONE ADAPTATION PHENOMENON

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Continuous bone remodeling consists in simultaneous resorption of tissues and synthesis of a new matrix. If, due to variable external or internal conditions, the equilibrium is disrupted, significant rearrangements of the micro-structure and bone shape are possible. Many mathematical and computational models of this adaptation phenomenon can be assingned one of the two categories; namely, theoretical models originating from the theory of adaptive elasticity and computational models making use of the optimization theory.
In the present paper the approach based on the hypothesis of optimal response of a bone is proposed. It enables derivation of various adaptation laws associated with extremum of the objective functional under a set of appropriate constraints and makes a bridge between the aforementioned categories. In order to illustrate possible application of the proposed general approach the specific formulation is presented and mathematical relations governing the adaptation process are derived. Four numerical examples illustrating some of possible applications of the presented relations are included.

Key words: remodeling, adaptation law, objective functional, constraints, trabecular structure

1. Introduction

The ability of a bone to adapt its internal structure and external shape according to environmental conditions has long been known. In general, the three classes of changes can be distinguished: growth, remodeling and morphogenesis, see e.g. Taber (1995). The growth is associated with variation in a bone volume and is composed of surface and volumetric changes. Remodeling is characterized by changes of local properties of a tissue. The morphogenesis is defined as a change of shape with a constant volume. But in fact the mentioned classes overlap each other and in the present paper the term "remodeling" is used to express the variations of internal structure and the shape with or without volume changes.

In normal situation the living bone undergoes continuous changes. The mass transportation, simultaneous resorption and deposition of tissues result in the equilibrium state, i.e. in spite of extraordinary complexity of the processes continuously taking place "inside the bone" at the macro level no significant changes are observed. This is a commonly accepted fact, confirmed by observations, that bone remodeling depends upon its mechanical loading. Besides, many other factors; e.g., hormonal, genetic and metabolic effects, influence this process. There probably exists some range of values of parameters defining environmental conditions as loading or boundary conditions for which the internal activities of bone stuff result in a stable state. In the case when the external conditions exceed these bounds, some of the effects predominate and remodeling takes place. This self-regulatory process is very important as it enables adaptation of the organism to variable external conditions. But sometimes it may work against us. An evident example is the situation after arthroplasty. A part of bone carrying the load is suddenly cut off and replaced by the implant. This results in a change of stress distribution and in consequence – in remodeling of internal structure and external shape. In some subdomains the bone resorbs what can, after a sufficiently long period of time, lead to loosening of the implant. In that context the problem of prediction of long-term adaptation process and associated changes of the bone structure is crucial (see e.g. one of the presented in the following sections illustrative examples).

Although Wolff's law, Wolff (1892) has been already known for more than century, the problem of a precise formulation of mathematical relations governing the adaptation process of tissues continues to attract researchers. In fact, answers to many problems associated with adaptation phenomena are still unknown. On the other hand, the knowledge about mechanisms of bone remodeling due to adaptation to variable environmental conditions is of great practical importance. This fact, together with rapidly increasing computational possibilities, results in growing scientific activity in this area.

The mechanism governing the bone adaptation is still not completely known. Since the bone represents a very complex structure no mathematical model can describe at present all of the effects which may contribute to remodeling. Thus the choice should be made to investigate the most significant relations. If only mechanical loading and its effects for remodeling is considered the situation is much simpler. According to Cowin et al. (1991) the mechanical state of tissue is sensed by osteocytes. Then this information is processed according to the adaptation law coded somewhere and, transferred to actor cells – osteoblasts and osteoclasts. There exist different theories explaining the mechanisms by which the tissues sense the actual state of strains. Among the others, piezoelectric effects were considered by Gjelsvik (1973a,b), microcracks by Carter (1984), Radin (1972) and Prendergast and Huiskes (1995), changes of solubility of hydroxiapatite by Justus and Luft (1970), hydrostatic pressure of extracellular fluid by Pauwels (1960), and others.

Despite the fact that various conditions influence the process of adaptation, the present discussion based on the idea introduced by Lekszycki (1999) is restricted to a simple case of remodeling controlled only by *mechanical* environment of bone – an assumption is made that strain variations within the considered domain result in appropriate local changes of material properties. It should be emphasized that main effort in this paper is directed towards promotin of the approach – variational formulation based on the hypothesis of optimal response of a bone. Which effects are included in the formulation by means of objective functional and constraints and what is selected as "control variables" represents here a secondary question because the method is general and various phenomena can be investigated. In contrast to most of the formulations exploiting the ideas developed in structural optimization, where only optimal solution is searched for, i.e. the final asymptotic state to which the bone tends under constant external conditions but never reaches it, the approach discussed in the present paper enables one to follow in time the changes of bone internal structure and its external shape due to varying "excitations".

In the next section the formulation of adaptation problem is discussed and specific adaptation law is derived to illustrate the general idea. The simplest case – when only material changes are considered and no external shape undergoes variations, and local material parameter is selected to represent the "design variable". The goal of the adaptation is to determine the action ensuring, within the specified constraints and actual mechanical state, maximal velocity of global stiffness increase or – if impossible because of constraints – minimal decrease at each moment of time.

Selected illustrative numerical examples of possible applications of the proposed mathematical description are presented in the following sections. They do not deplete a list of possible applications, e.g. the effects of osteoporosis can be examined in different situations. This and other problems will be discussed in forthcoming papers (e.g. anisotropic characteristics of the material).

2. Hypothesis of optimal response of bone and the associated adaptation law

Most actions which happen in nature can be treated as a result of optimization – this is a very strong statement and is rather a matter of belief than a scientific reasoning. At the moment it can't be proved in general, but on the other hand, there are many examples showing that there exists some "general deep thought" governing the actions and Nature minimizes "efforts" or "costs" of events. Indeed, many phenomena are associated with an extremum of some functional under adequate additional constraints. The main difficulty is probably to realize that the event under consideration is an effect of optimal decision and the determination of the functional and especially of appropriate constraints is in most cases very difficult in practice. But they probably exist, not only for many physical, chemical or biological processes, but also economical, social and others. Of course no random events are considered here, but what is random and what deterministic is again more a philosophical question which is not a subject of present discussion. The approach proposed in this paper is based on the hypothesis of optimal response of a bone and is discussed in detail in the present section.

As was pointed out by Huiskes (1997) there exist numerous mathematical and computational models of bone adaptation; since many of them have never been validated in medical and biological investigations this situation is very confusing. The present work does not fall into the category mentioned above.

This is not the aim of the present paper to present one more, specific model representing the adaptation phenomenon of bone tissues. On the contrary, the goal is to propose a general approach, based on the assumption of optimal response of a bone, which enables one to construct a large variety of models, associated with a specific objective functional and a set of constraints. This selection depends very much on the specific phenomenon that is to be represented by the model. It was mentioned above that the search for an objective functional associated with a specific behavior of a considered system is often a complex and difficult task. On the other hand, such an approach, if successful, puts more light to the problem and allows better understanding of the mechanisms governing the considered process. In addition, such variational approach is often associated with significant practical advantages. One of the examples is the application of variational methods to computational aspects of numerical analysis of the adaptation process.

In the present paper a simple model is derived and used in numerical computations. The reason that this analysis is included here, in spite of the fact that the model was not validated and has no links to the results of medical research, is simple – this is just the illustration of possible application of the general approach proposed in the paper. In future research, the facts obtained from biological investigations can be included in the formulation as constraints or objectives and models derived in this manner can possibly be compared with medical observations. Only then, the model can be used in prediction of specific bone behavior.

The formulation discussed in the present work combines the two characteristic trends of the research into bone remodeling, i.e., adaptive elasticity introduced by Cowin and Hegedus (1976) and developed in numerous papers, see e.g. Taber (1995), Huiskes (1997), Hart and Davy (1989), Huiskes et al. (1987) and – the application of the optimization theory, see e.g. Pedersen (1993), Bendsøe and Mota Soares (1993), Bendsøe et al. (1994). For more comprehensive discussion of adaptation models see e.g. the review paper by Telega and Lekszycki (in preparation). In the present work the hypothesis of "optimal response of bone" introduced by Lekszycki (1999) and developed by Lekszycki and Sławiński (1998) is used and instead of optimization of bone shape and its internal structure, what is usually made in the works representing application of optimization theory, the optimization of actual response of bone due to variable in time mechanical conditions is performed. Basing on the functional representing the rate of a change of the bone global stiffness, described by the velocity of the potential energy, and – in addition – on the set of equality an inequality constraints the adaptation law is derived. The control variable, or in another words – the design variable, is represented in the case discussed here by the local Young modulus. For the same of simplicity the second material coefficient, the Poisson ratio, is assumed constant. The adaptation law together with constraints and classical formulas for equilibrium state and geometrical relations determine a set of equations describing fully the adaptation process.

The present derivation is made for non-homogeneous, isotropic material, but extension of the formulation is simple. Let us consider a body made of non-homogeneous, isotropic material (Fig.1). To begin the discussion let us assume that the loading and boundary conditions do not change in time and formulate the classical optimization problem. In order to do so the objective functional has to be specified. An arbitrary functional of displacement field, strain or stress can be selected. In the present discussion the global stiffness of the body represented by the total potential energy is chosen. This is the simplest possible case, but since this is not a goal of the present discussion to derive a specific sophisticated model, but rather to illustrate the general

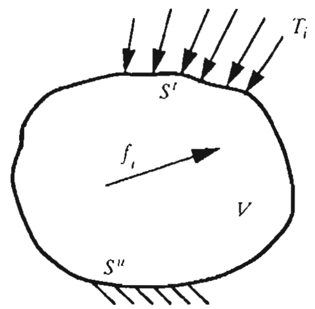

Fig. 1. A body under consideration

procedure such a functional can serve as a good example

$$G = \Pi(u) = \int_V U(e_{ij})\, dV - \int_{S^t} T_i u_i\, dS^t - \int_{S^u} f_i u_i\, dV \tag{2.1}$$

where $U = \sigma_{ij} e_{ij}$ denotes the density of the strain energy. In the optimization problem the design variables (control variables), i.e. the variables that undergo changes due to optimization and have to be selected to satisfy the extremum of the objective functional, should be defined. In the present formulation the local material properties are selected for optimization. In a more sophisticated formulation the micro-structure of the material described by a set of parameters defined in the unit cell can be selected and related by means of homogenization with material constants as e.g. the Young modulus. At present, directly the Young modulus E is selected to control local changes of the material associated with remodeling. To do so Hook's law for linear isotropic elastic material is assumed. To perform an effective optimization a set of constraints for the design variables or/and the state of the considered body should be defined. Let us put the constraints for the maximal and minimal values of the Young modulus. In the normal situation they follow from the assumed micro-structure of the material and can be determined using the geometrical parameters defining this micro-structure. As the material is porous the bounds depend on minimal and maximal porosity admissible. They should be also validated in experimental investigations. Here we simply set the local constraints and state that

$$E(x) \geqslant E_{min} \qquad\qquad E(x) \leqslant E_{max} \tag{2.2}$$

In addition, the global constraint is defined. Assuming that the Young modulus is related to the porosity this equation constraints the total amount of the available material

$$\int_V E(x)\, dV = E_0 \tag{2.3}$$

To this end the classical problem often considered in structural optimization was defined (except maybe for the choice of the design variable, what is not typical for structure optimization). This formulation is very convenient for the reason of its simplicity – the minimum of the objective functional with respect to the variation of displacement field is associated with the equilibrium equations (after application of geometric relation between strain and displacement fields). The condition for maximum of the objective with respect to design variables deliver the optimality criteria. But until now no adaptation phenomenon has been modeled. To do so let us extend the previous formulation and assume that the external loading can vary in time. Accordingly, the displacement, strain and stress fields are also time-dependent. Moreover, we also let the local Young modulus to change its values $E(x,t)$ during the process. So now, the variations of mechanical state of the body under consideration, caused by variable external conditions and, in addition, modifications of control variables are examined. This point of the discussion is crucial. Actually, no more the final state of the body is considered (what was the goal of the classical formulation). Instead, the reaction of the material to variable loading and resulting displacements, strains and stresses is the subject of interest. Let us assume the hypothesis that the material reacts in optimal way according to the available information concerning:

- Objective functional
- Actual mechanical state
- Present constraints.

Since the primary goal is to ensure the objective maximization within possible bounds, and the material does not know anything about the future, the actual change of the control variables should result in associated maximal growth of the objective functional. But the control variable is assumed to be continuous, so no instantaneous jump is admissible. Therefore, instead of control variables (in this formulation – the Young modulus $E(x,t)$) their velocities are taken now to be modified and represent new control variables. It means that velocity of Young modulus is to be determined in order to maximize the velocity of the objective, or (if impossible due to existing constraints) minimization of its loss. To perform this the previous formulation has to be modified.

Instead of the objective functional its velocity is considered and undergoes maximization. The design variables, as was argued above, are represented now by the velocities of Young modulus. In addition to the constraints already defined the new ones should be considered. First, let us impose inequality constraints for the admissible velocities of Young modulus. These constraints have grounds in biological observations which confirm that velocity changes can not exceed some given values. In the present model the limiting values can be "tuned" according to the phenomenon modeled and the results of biological investigations

$$\dot{E}(x,t) \geqslant \dot{E}_{min}(t) \qquad\qquad \dot{E}(x,t) \leqslant \dot{E}_{max}(t) \tag{2.4}$$

Let us also define the two global constraints, one defining the total velocity of changes, and other – the "power" of changes. As before the Poisson ratio does not undergo modifications

$$\int\limits_V \dot{E}(x,t)\, dV = E_1(t) \qquad\qquad \int\limits_V \dot{E}^2(x,t)\, dV = E_2(t) \tag{2.5}$$

These two constraints are crucial and to great extent determine the form of adaptation law following from the stationarity condition of the objective functional. The first of the constraints is responsible indirectly for the amount of material. So, for $E_1(t) = 0$ the remodeling with a given amount of mass can be modeled. For negative values of $E_1(t)$ the decrease of total mass, e.g. osteoporosis effect can be observed. For positive values the process with production of mass is described. The second constraint defines the total ability of the considered system to perform changes. In fact, if this equality constraint is replaced by the inequality constraint defining the maximum efficiency of the system the situation is more reasonable and very interesting cases occur. Then there exist more then one adaptation law, or to say more precisely, the adaptation law switches from one to the other according to the distance of actual material configuration from the optimal one. But this case requires detailed discussion which will be postponed to the subsequent paper.

The defined above constraints can be attached to the objective functional by means of Lagrange multipliers and slack variables (used for inequality constraints)

$$\begin{aligned} G^* &= \dot{\Pi} + \mu_1\Big(\int\limits_V \dot{E}\, dV - E_1\Big) + \mu_2\Big(\int\limits_V \dot{E}^2\, dV - E_2\Big) + \\ &+ \int\limits_V \eta_1(\dot{E} - \dot{E}_{min} - a_1^2)\, dV + \int\limits_V \eta_2(\dot{E}_{max} - \dot{E} - a_2^2)\, dV \end{aligned} \tag{2.6}$$

The variation in the extended functional G^* with respect to the variation of the displacement field and its velocity vanishes because the equilibrium equation and rate equilibrium equation have to be satisfied. Variation with respect to the Lagrange multipliers and slack variables provides a set of constraints and the triggers necessary to switch the control variables from intermediate values to the assumed extremal values. Finally, from the vanishing variation requirement of the objective functional with respect to the variation of $\dot{E}$ the adaptation law follows

$$\frac{\partial \dot{U}}{\partial \dot{E}} + \mu_1(t) + 2\mu_2(t)\dot{E}(x,t) + \eta_1(x,t) - \eta_2(x,t) = 0 \tag{2.7}$$

In derivation of this law an assumption was made that no body forces are present. It does not restrict the consideration performed, the appropriate term can be easily included if necessary. In Eq (2.6) μ_1, μ_2, η_1, η_2 denote the Lagrange multipliers and a_1, a_2 are slack variables. The adaptation law derived here is similar to the relations discussed in the works originating from the theory of adaptive elasticity. In the present approach the variational formulation has been applied as it brings significant advantages. Besides the fact that such a formulation, if successful and validated in biological tests, enables better understanding of the problem under consideration, it also makes possible to use well established computational methods of structural optimization in analysis of the adaptation process. In the next section this adaptation law is used in two-dimensional numerical examples in order to illustrate selected applications.

3. Numerical examples

In this section four numerical examples are shortly discussed. The choice was determined by the will of presentation of selected applications. Since the applied model of adaptation have never been validated in medical investigations these examples can not have practical importance. On the other hand, the results of calculations show great similarity to the natural solutions, i.e., what really happens with bones. Therefore one can expect that after more profound investigations and after validation of this or similar model in clinical observations it could possibly be used in future to predict bone remodeling.

The general relations discussed in the previous section are applied to the specific case of two-dimensional "structures". A simple model of trabecular bone material composed of beams is selected in order to examine the effect of adaptation process for the evolution of internal bone structure.

3.1. Example 1: Sample of material under variable loading – shear test followed by tension

This example is selected to show how the sample of material changes its internal structure under variable in time external conditions. The square sample of material is considered.

The initial material was assumed to have homogeneous trabecular microstructure. First the shear forces were applied at the four edges of the sample, see Fig.2a. After some period of time the loading was changed. The horizontal tension was applied, Fig.2b and the same period of time considered. The adaptation process of the sample, with constant mass, according to the law discussed in the previous section can be observed and the successive steps of adaptation in equal time intervals are presented in Fig.2.

3.2. Example 2: Growth of bone internal structure under external constant loads

No external remodeling is considered in this example despite the fact that it also plays important role in total rebuilding of bone. Simple trabecular microstructure of the material is assumed. In the initial situation, on the macro scale the material is homogeneous (see Fig.3 the topmost figure). The bone presented in Fig.3 is clamped at the left end and subject to distributed surface loads on the parts of the right-hand end. After adequate long period of time the material is transported from some subdomains into another regions resulting in a growth of bone total stiffness (the time scale depends of the applied constraints and can be "tuned" according to clinical observations). The total mass is assumed to keep a constant value during the process. The intermediate result of this adaptation process – the bone internal structure - is displayed in the middle picture in Fig.1. The final result, i.e., the effect of adaptation after a long period of time, is shown in the lowest picture. As can be observed, the investigated process results in strong non-homogeneity and anisotropy. The comparison of the obtained scheme with the internal structure of real bone indicates close similarity. The results of another computation shows that the internal structure is very sensitive to the applied loads. This is confirmed by medical observations.

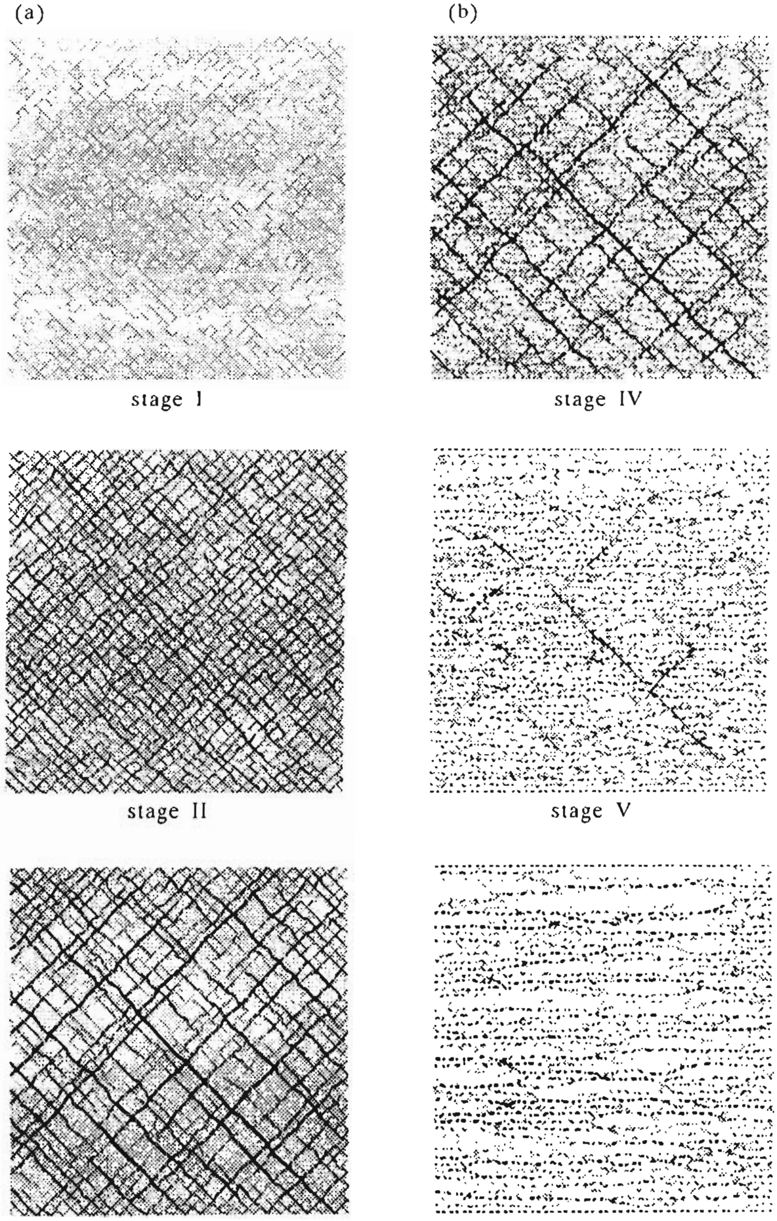

Fig. 2. Sample of material under shear followed by tension test – successive steps in equal time intervals; (a) internal remodeling due to shear, (b) internal remodeling due to tension

Fig. 3. The growth of bone internal structure due to physiological constant load – successive steps in equal time intervals

3.3. Example 3: Remodeling of material in a cantilever beam after application of rigid inclusion

A non-homogeneous cantilever beam, clamped at the left end, displayed in Fig.4 (topmost picture) in tension and bending state was analyzed. The analysis of adaptation process starts after application of a rigid inclusion at the left end (gray region). The intention of this example was the observation of the remodeling process resulting in the a loosening of the prosthesis, what is sometimes observed in reality. It seems that even such a simple model of the adaptation phenomenon can reflect the characteristic changes in bone. Of course, in order to analyze the real situations much additional research is required, e.g., the tuning of a system in order to express reasonably the amount of changes in time (this depends on the extremal values defined in the constraints). More investigations are planned in order to include more realistic description of a connection between the inclusion and bone material (here the rigid connection was assumed), as well as more realistic modeling of bone geometry (2 and 3-dimensional models).

3.4. Example 4: Remodeling in the vicinity of crack and healing process

In the last example a very simple model of a healing process in the vicinity of a crack is considered. No biological effects are taken into consideration and only mechanical remodeling effects the "healing" of the bone.

The cantilever beam clamped at the left end and subject to the vertical force applied at the right-hand end is considered. The initial crack at the distance of one-fourth of the length of the beam from the clamped edge is introduced. We also assume that some initial time is needed to activate the growth of a new tissue in a crack and enable it to bear the load. In Fig.5 the subsequent stages of remodeling are presented. In the first three figures the growth of reinforcement passing by the crack can be observed. The next three figures show the situation when the growth of new tissue in the crack was initiated and then this tissue is able to bear the load. Finally the crack vanishes.

4. Conclusions

In the present work selected preliminary results concerning application of a new approach to the problem of modeling of bone adaptation process are presented. It follows from the initial investigations that the proposed approach

(a)

(b)

(c)

(d)

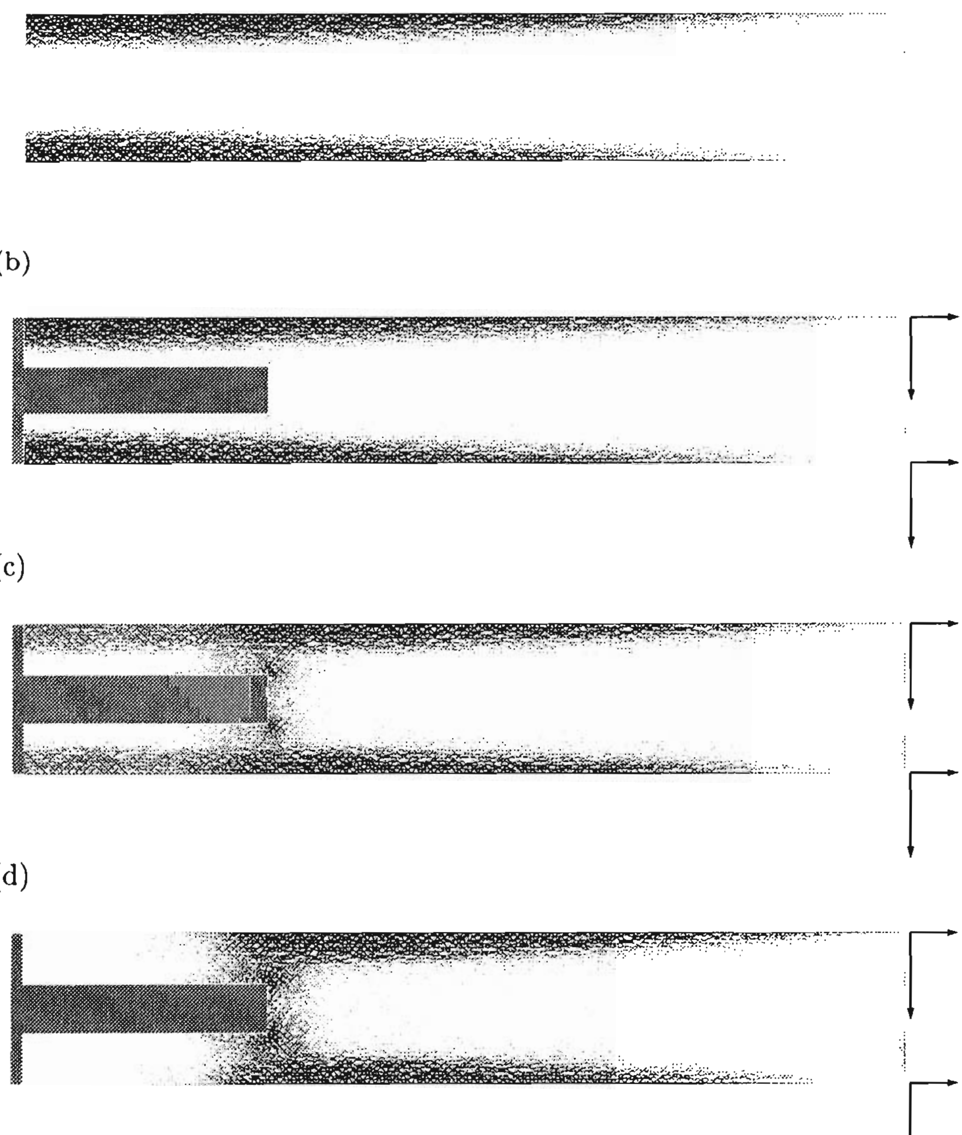

Fig. 4. Internal remodeling in the vicinity of rigid inclusion: (a) initial beam, (b), (c), (d) successive steps of remodeling in equal time intervals

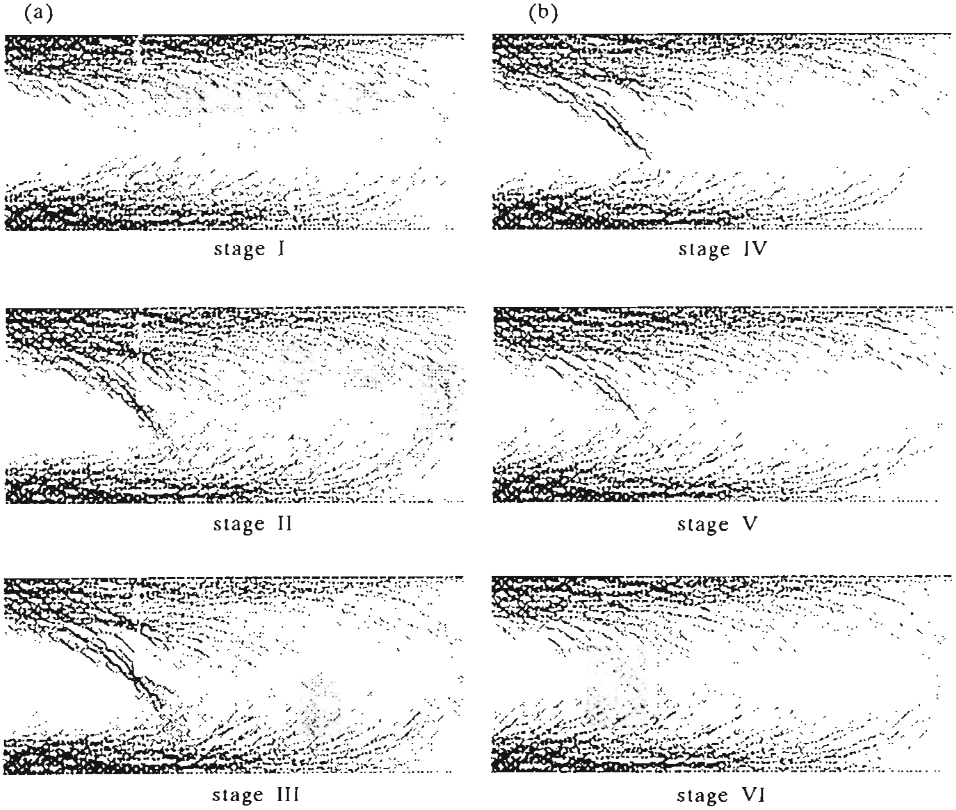

Fig. 5. Remodeling of material in the vicinity of crack – successive stages in equal time intervals; (a) stages I-III – reinforcement around the crack grows, (b) stages IV-VI – healing process predominate and the crack vanishes

can be possibly used to model the phenomenon of bone remodeling due to the adaptation process. More research is planned to examine different objective functions and constraints, and resulting adaptation laws. The validation of theoretical results in medical tests would also be necessary. There are many possible applications of the method discussed here, for instance the analysis of interaction of bone and prosthesis and their optimization, the effects of osteoporosis and possible methods of their reduction, the process of healing after surgery or bone damage and its possible optimization.

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Zastosowanie warunków optymalności w modelowaniu zjawiska adaptacji kości

Streszczenie

Na przebudowę kości mają zasadniczy wpływ dwa procesy: resorpcja tkanek oraz synteza nowej matrycy. W stanie ustalonym są one w równowadze, lecz gdy na skutek zmiennych warunków zewnętrznych któryś z nich zaczyna przeważać może nastąpić nawet znaczna zmiana struktury wewnętrznej i zewnętrznego kształtu kości. W literaturze poświęconej problemowi modelowania zjawiska adaptacji kości można wyróżnić dwa charakterystyczne podejścia, jedno oparte na teorii adaptacyjnej sprężystości i drugie wykorzystujące matematyczne metody optymalizacji. W niniejszej pracy zaproponowano nowe sformułowanie wykorzystujące hipotezę optymalnej reakcji układu. Łączy ono w sobie wiele zalet obu wspomnianych metod. W celu zilustrowania ogólnej idei wyprowadzono konkretne, proste prawo adaptacji. Przedstawiono też kilka przykładów numerycznych ilustrujących niektóre z możliwych zastosowań omawianych związków teoretycznych.

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