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MODIFIED CONTINUUM DAMAGE-REPAIR THEORY APPLIED TO BONE REMODELING

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Abstract. Internal bone remodeling models have been proposed in order to address behavior under everyday loading of hard tissues. Models, in general, are not general as to apply to all bones in human body. Also trauma cases are not covered by many of the models. Here, one such a model, Doblare's model of damage-repair is revisited, and modified in some aspects to address specific internal bone remodeling problems. In the model, elastic constitutive parameters are formulated in terms of the bone density and the fabric tensor, both dependent upon the amount of mechanical stimulus and the local present state of structure. Bone material is taken as inherently anisotropic. Density, instead of an intermediate tensor, configures the pseudo-damage variable, with a different undamaged state mapping. Strain energy equivalence is kept, however. Different elasto-damage surfaces are discussed in order to describe update of internal variables. Resorption and apposition are treated with similar, but different, surfaces. Evolution equations set the rate of change of density and constitutive components. Loading direction is directly related to the evolution of these components, as discussed here. Model is coded in a Fortran routine to use with Abaqus program. Comparison with some other available models is performed in some problems. Some experimental validation is also undertaken.

Keywords: hard tissue, damage-repair, remodeling, finite element model

1. INTRODUCTION

Process of generation of bone by means of use of a drawing force is known as osteogenesis by distraction. In the present case applied to a facial bone, the mandibula. The procedure was introduced by Codivilla in 1905. In the following 35 years, Ilizarov applied the technique to hundreds of patients, having lots of reports on the subject in the literature. However, these reports show little modeling of the process. Here an attempt in this direction is pursued.

In synthesis the experimental program supposes mapping the structure of a human mandibula, from a skeleton, through x-rays. Constructed the 3D image, from several takes, it is assembled into a wire form in a computer program, where it is converted into a solid from mesh. It is on this model that loads will be applied, and simulated the response obtained from application of constitutive model presented ahead, and due to Doblare, but here included with some modifications.

In order to gather the parameters required to generate results from the model, parameters present in it will have to be measured. Testing of the human mandibula will provide the input parameters for the model. Traditional techniques and equipment for this testing will be used, as available. For the parameters where measurements are not possible, literature values will be employed.

In parallel to this procedure, a patient submitted to mandibular distraction will be accompanied, with variables of the procedure generated from experimental evidence, practice and estimations from the model. This will serve the purpose of verifying the adequacy of dead mandibula test parameters for the model. It will bring attention to some specifics of the process not brought into the model, and possibly construct a tool for automatic integration between practice and finite element estimation parameters as a guide to a better medical procedure.

2. FORMULATION

Since Wolf (Wolff, 1892) first observed the relationship between bone structure and applied loads, several models have been constructed to try to establish the behavior of bone, the evolution under mechanical stimulus. Many variables have been considered in the modeling. The apparent density of bone is a essential one. It is affected by bone porosity and its anisotropy. Therefore construction of a constitutive model for bones, requires use of concepts considered in the description of porous materials, which are encompassed by the damage mechanics concepts. Though there is a continuous change of size, and orientation of porous inside the bone structure, with few cases of fracture, yet the equations of continuous damage mechanics CDM may be applied. In this case the treatment receives the name of continuum damage-repair theory. Here one such a description will be analyzed, modified in some aspects, and considered in the case of bone distraction

2.1. Modified Doblare's model

Internal structure of bone tissue is similar to that of an elastic-porous material, with continuous evolution of constitutive elements. In it, stresses and strains are related by means of a linear relationship:

$$\boldsymbol{\sigma} = \tilde{\mathbf{C}} : \boldsymbol{\varepsilon} \tag{1}$$

where $\tilde{\mathbf{C}} = \hat{\tilde{\mathbf{C}}}(\boldsymbol{\Phi})$ is the constitutive tensor, function of porosity $\tilde{\rho}$ and fabric tensor being $\tilde{\mathbf{H}}$, being $\boldsymbol{\Phi}^2 = \sqrt{\tilde{\mathrm{d}}}\tilde{\mathbf{H}}$, with $\tilde{d} = (\frac{\tilde{\rho}}{\hat{\rho}})^{\beta} A$. Here $\hat{\rho}$ is the full density of bone, β and A material parameters, particular to each bone. The constitutive tensor $\tilde{\mathbf{C}}$ depends upon elastic moduli $< \tilde{E}_1 \quad \tilde{E}_2 \quad \tilde{E}_3 >$ and shear moduli $< \tilde{G}_{12} \quad \tilde{G}_{23} \quad \tilde{G}_{31} >$, all functions of porosity and direction. Here reference coordinate natural axes are identified as $< 1,2,3 >$.

Were the material supposed dense, therefore in an undamaged state, relationship between stresses and strains would be much simpler, as the coefficients in the constitutive equation would become constant. Therefore if a mapping into this state is considered, then:

$$\tilde{\boldsymbol{\sigma}} = \mathbf{C} : \tilde{\boldsymbol{\varepsilon}} \tag{2}$$

where:

$$\tilde{\boldsymbol{\sigma}} = \boldsymbol{\Phi}^{-1}.\boldsymbol{\sigma}.\boldsymbol{\Phi}^{-1} \tag{3}$$

are the stresses in the undamaged space and:

$$\tilde{\boldsymbol{\varepsilon}} = \boldsymbol{\Phi}.\boldsymbol{\varepsilon}.\boldsymbol{\Phi} \tag{4}$$

are the corresponding strains. Here $\boldsymbol{\Phi}$ is a diagonal tensor, in the principal natural system, representing the damage effects. It depends upon $\tilde{\mathrm{d}}$ and the fabric tensor $\tilde{\mathbf{H}}$ with components $< \tilde{H}_1 \quad \tilde{H}_2 \quad \tilde{H}_3 >$, such that $\det \tilde{\mathbf{H}} = 1$. Tensor $\boldsymbol{\Phi}$ is also called the remodeling tensor (Doblare, 2002).

The constitutive tensor $\mathbf{C}$ should not, though, be isotropic, as the mapping should discount the porosities, but not the anisotropic character of the fabric itself. It only changes its distribution. The three elastic moduli as well as the three shear moduli should be constant, and obtained from the $< \hat{E}, \hat{\nu} >$ by considering $\tilde{\mathbf{H}}$ (Cordebois and Sideroff, 1982). For first direction, it reads:

$$\frac{1}{\tilde{E}_1} = \frac{1}{\hat{E}\tilde{H}_1^4} \tag{5}$$

$$-\frac{\tilde{\nu}_{12}}{\hat{E}_2} = -\frac{\tilde{\nu}_{21}}{\hat{E}_1} = -\frac{\hat{\nu}}{\hat{E}}\frac{1}{\tilde{H}_1^2\tilde{H}_2^2} \tag{6}$$

$$\frac{1}{2\tilde{G}_{12}} = \frac{1+\hat{\nu}}{\hat{E}}\frac{1}{\tilde{H}_1^2\tilde{H}_2^2} \tag{7}$$

what differs from Doblare's model. Other two directions follow likewise.

Mapping, the most important point here, is constructed from the principle of equivalence of elastic strain energy in both domains, porous or damaged, and dense, or undamaged domain. In the present scenario it is termed the daily tissue stress level. Hence, if:

$$\tilde{\psi}_e = \psi_e \tag{8}$$

being $\tilde{\psi}_e = \hat{\tilde{\psi}}(\tilde{\boldsymbol{\varepsilon}})$ and $\psi_e = \hat{\psi}(\boldsymbol{\varepsilon}, \boldsymbol{\Phi})$:

$$\tilde{\psi}_e = \frac{1}{2}\boldsymbol{\sigma} : \boldsymbol{\varepsilon} = \frac{1}{2}\tilde{\mathbf{C}} : \boldsymbol{\varepsilon} : \boldsymbol{\varepsilon} \tag{9}$$

$$\psi_e = \frac{1}{2}\tilde{\boldsymbol{\sigma}} : \tilde{\boldsymbol{\varepsilon}} = \frac{1}{2}\mathbf{C} : \tilde{\boldsymbol{\varepsilon}} : \tilde{\boldsymbol{\varepsilon}} \tag{10}$$

Upon equating these expressions, the relationship between the constitutive tensors $\mathbf{C}$ and $\tilde{\mathbf{C}}$ is drawn. The quantity $\tilde{\psi} = \hat{\tilde{\psi}}(\boldsymbol{\varepsilon}, \boldsymbol{\Phi})$ identifies an amount of strain energy packed in each elementar volume of material, whose rate of change depends upon the level of strain, porosity and fabric directions, last two encompassed in the $\boldsymbol{\Phi}$ tensor. Rate of change of ψ_e with respect to $\boldsymbol{\Phi}$ is termed the stimulus $\mathbf{Y} = \partial_{,\boldsymbol{\Phi}}\psi_e$:

$$\mathbf{Y} = \mathbf{C} : (\boldsymbol{\Phi}.\boldsymbol{\varepsilon}.\boldsymbol{\Phi}).(\boldsymbol{\varepsilon}.\boldsymbol{\Phi} + \boldsymbol{\Phi}.\boldsymbol{\varepsilon}) \tag{11}$$

The stimulus $\mathbf{Y}$ is a tensorial quantity, with principal values $< Y_1 \quad Y_2 \quad Y_3 >$, dependent upon the strains, the porosity and the fabric tensor. The stimulus may be separated into a hydrostatic $\mathbf{Y}_h$ plus a deviatoric $\mathbf{Y}'$ part. The first relates to a volumetric effect whereas the second relates to a distortional effect of the load on the local fabric. Hence:

$$\mathbf{Y} = \mathrm{Y_h}\mathbf{I} + \mathbf{Y}'; \quad \mathrm{Y_h} = \frac{1}{3}\mathrm{tr}\mathbf{Y} \quad \mathrm{tr}\mathbf{Y} = \mathrm{Y_I} + \mathrm{Y_{II}} + \mathrm{Y_{III}} \tag{12}$$

being $\mathbf{I}$ the unit second order tensor. Participation of each component, dependent on the character of the loading, static or alternate, and its resulting effect possibly affected by projection of the load onto the natural fabric system, may be measured by means of the tensor:

$$\mathbf{J} = (1 - 2\omega)\mathrm{Y_h}\mathbf{I} + \omega\mathbf{Y}' \tag{13}$$

that includes parameter ω to check out these factors.

Present state of the bone structure under load stays fixed, until the amount of energy accumulated, after several load cycles gets to a level, where evolution of $\boldsymbol{\Phi}$ takes place. Locus, referent to bone formation, is set by function:

$$g^f = A^f - R^f \tag{14}$$

where, as proposed by Dobrare:

$$A^f = 2\alpha^f A^{\frac{1}{8}} \frac{1}{\sqrt{1-\omega}}\mathbf{J} : \mathbf{J}; \qquad R^f = (\psi_t^* + w)\rho^{2-\frac{5\beta}{8}} \tag{15}$$

being ψ_t^* the reference stimulus, w the half-width of the dead-zone, where equilibrium prevails and no changes occur. Internal tensorial product is denoted by : symbol. Expression of coefficient α^f is:

$$\alpha^f = \frac{\sqrt{2}}{4} n^{\frac{1}{m}} \sqrt{B}\hat{\rho}^{2-\frac{\beta}{8}} 3^{\frac{1}{4}} (\mathbf{J} : \mathbf{J})^{-\frac{3}{4}} \tag{16}$$

with n the number of loading cycles, $\hat{\rho}$ a reference density, β and B experimental coefficients. Fig. 1 shows a plot of this surface in a plane stress case, as affected by ω values. Fig 2 considers the different ratios $\mathrm{H_1}/\mathrm{H_2}$ values.

Evolution of $\mathbf{\Phi}$ takes place whenever $\mu^f \geq 0, g^f \leq 0 \;\wedge \dot{g}^f = 0$ (Koiter, 1953). From the first condition:

$$A^f = R^f \tag{17}$$

whereas from the second:

$$\Delta g^f = \frac{\partial g^f}{\partial \mathbf{Y}} : \Delta \mathbf{Y} + \frac{\partial g^f}{\partial \tilde{\rho}} \Delta \tilde{\rho} \tag{18}$$

with the first increment as:

$$\Delta \mathbf{Y} = \frac{\partial \mathbf{Y}}{\partial \boldsymbol{\varepsilon}} : \Delta \boldsymbol{\varepsilon} + \frac{\partial \mathbf{Y}}{\partial \mathbf{\Phi}} : \Delta \mathbf{\Phi} \tag{19}$$

and the secondas:

$$\Delta \mathbf{\Phi} = \frac{\partial \mathbf{\Phi}}{\partial \tilde{\mathbf{H}}} : \Delta \tilde{\mathbf{H}} + \frac{\partial \mathbf{\Phi}}{\partial \tilde{\rho}} \Delta \tilde{\rho} \tag{20}$$

Admitting normality of $\mathbf{\Phi}$ to g^f surface implies, additionally, that::

$$\Delta \mathbf{\Phi} = \Delta \mu^f \frac{\partial g^f}{\partial \mathbf{Y}} \tag{21}$$

However as $\mathbf{\Phi} = \sqrt{d}\,\hat{\mathbf{H}}$, having $\tilde{\mathbf{H}}$ an unitary determinant:

$$\det \mathbf{\Phi}^2 = \left(\frac{\tilde{\rho}}{\hat{\rho}}\right)^{\frac{3\beta}{2}} A^{\frac{3}{2}} \det \tilde{\mathbf{H}} \tag{22}$$

so that:

$$\begin{gathered} \Delta\{\det(\mathbf{\Phi}^2)\} = \frac{3}{2}\frac{\Delta\tilde{\rho}}{\tilde{\rho}} \beta \det(\mathbf{\Phi}^2) \\ \Delta\{\det(\mathbf{\Phi}^2)\} = \det(\mathbf{\Phi}^2).\mathrm{tr}(2\mathbf{\Phi}.\Delta\mathbf{\Phi}.\mathbf{\Phi}^{-2}) \end{gathered} \tag{23}$$

or, in considering Eq. (21):

$$\Delta \mu^f = \frac{3}{4}\frac{\beta}{\tilde{\rho}} \frac{1}{\mathrm{tr}(\mathbf{\Phi}.\frac{\partial g^f}{\partial \mathbf{Y}}.\mathbf{\Phi}^{-2})} \Delta \tilde{\rho} \tag{24}$$

Introduction of these expressions into Eq. (18), will produce:

$$\Delta \tilde{\rho} = -\frac{\frac{\partial g^f}{\partial \boldsymbol{\varepsilon}} : \frac{\partial \mathbf{Y}}{\partial \boldsymbol{\varepsilon}} : \Delta \boldsymbol{\varepsilon}}{\frac{\partial g^f}{\partial \mathbf{Y}} : \frac{\partial \mathbf{Y}}{\partial \mathbf{\Phi}} : \frac{\partial g^f}{\partial \mathbf{Y}} . \frac{3\beta}{4\tilde{\rho}} \frac{1}{tr(\mathbf{\Phi}.\frac{\partial g^f}{\partial \mathbf{Y}}.\mathbf{\Phi}^{-2})} + \frac{\partial R^f}{\partial \rho}} \tag{25}$$

Once the increment in density $\Delta\tilde{\rho}$ is computed, increments in the directional coefficients in the fabric tensor, $\Delta\hat{\mathbf{H}}$ are obtained from the increments computed in Eq. (21). Once defined the increment in density, the increment in the amount of surface remodeled Δr follows from:

$$\Delta r = \frac{\Delta\tilde{\rho}}{\kappa S_v \hat{\rho}}; \quad \Delta r = c_f\,[\psi - (\psi_t^* + w)] \tag{26}$$

being S_v the internal surface per unit volume, called specific surface (Martin, 1984) where bone is added, in completely mineralized form, maximum density $\hat{\rho}$. Fig. 3 shows this form of idealized behavior around the dead zone, equilibrium. Velocities in each regime are denoted by c_a and c_f.

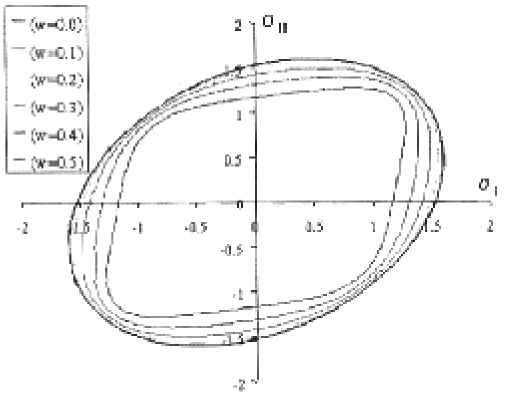


Fig. 1. Locus for apposition as a function of parameter ω.

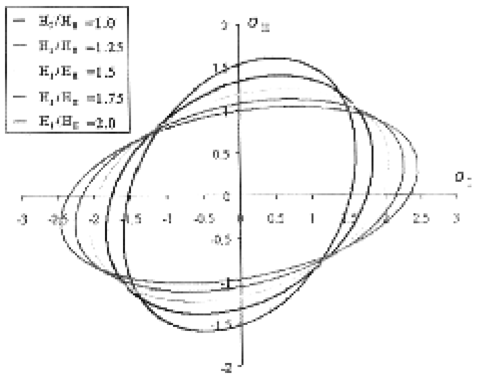
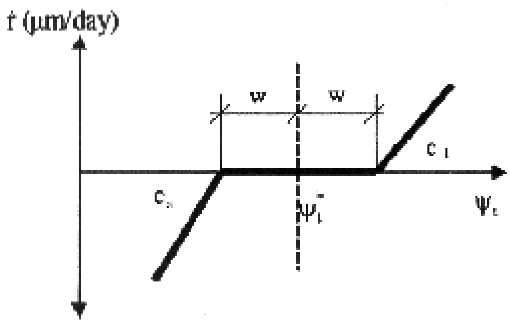


Fig. 2 Locus of apposition as a function of anisotropy ratio.



Fig,.3 Rate of remodeling function versus stimulus in a simplified form

2.2 Numerical Implementation

Constitutive model developed above was coded in a Fortran routines to be used as an user routines inside finite element program Abaqus (Abaqus, 2005). The user material routine, UMAT, given the initial state at a point

$< \boldsymbol{\sigma}_n ; \boldsymbol{\varepsilon}_n ; \Delta\boldsymbol{\varepsilon}; \tilde{\rho}_n ; \tilde{\mathbf{H}}_n >$ plus material data $< \hat{E}, \hat{\nu} >$ computes the elastic energy corresponding to each load step, represented by an load amplitude affected by a time window. This loading itself is handled in a loading routine, ULOAD, where a given a sequence of load steps, associated to a specified load-program is prescribed. Summed energy corresponding to the number of cycles associated to the complete cycling is then considered in a failure routine, UFAILURE, using as input results coming from both routines above. It uses the locus of bone formation/apposition, where the new values of density and anisotropy are decided.

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2.3. Some Characteristics

Human mandibula has some special characteristics that have to be measure, as several of its mechanical properties are not published in the open literature. Presently the set of variables required to implement the model presented above are being measured. They are summarized in Table 1.

Table 1. Listing of parameters required in the definition of apposition surface

Parameter
Reference stimulus ψ^*
Half-width size, w
Exponent, m
Percentage of active surface, κ
Remodelling velocity, c

A part these parameters, the set of anisotropy coefficients included in tensor $\tilde{\mathbf{H}}$, in the beginning and end of the experiments have to be measured. The same is true about the elastic properties of the material, whose general dependence uses to be presented as (Jacobs, 1994):

$$\hat{E} = B\rho^{\beta}; \quad B = \hat{B}(\rho); \quad \beta = \hat{\beta}(\rho); \qquad \nu = \hat{\nu}(\rho) \tag{27}$$

where these functions have to be defined in the experimental program, possibly using numerical fitting.

2.4 Discussion

From what has been analyzed so forth, the most difficult parameter to gather has been the reference stimulus. It's evolution with time and medical conditions of the patient vary. A part from this, lack of homogeneity of bone structure is important, and it possibly may also require different models for different regions of bones. In particular adequacy of the functions describing apposition and resorption locuses have to be analyzed.

The character of the loading is also important. Is seems that static loads require the apposition locus to depend most on the hydrostatic part of the stimulus, whereas variable loads make it more dependent on the deviatoric part. Moreover, directionality of loading plays a factor on the evolution of bone, what would require a kinematic approach to deal with the evolution of the damage surfaces, thing not contemplated so forth. In such a case, besides formatting the evolution of the damage surfaces, loading would reposition of the center of the surfaces itself.

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