Dynamic characterization and remodelling of interfaces with microstructure

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SUMMARY. The paper presents a mechanical model which allows to characterize the dynamics of interfaces with microstructure. With reference to interfaces in biological tissues, it is then employed the proposed model for analyzing remodelling processes, from the theoretical point of view.

1 INTRODUCTION

From the geometrical point of view, interfaces are ideal common boundary surfaces between two different material regions. Physically speaking, they represent two-dimensional mathematical models derived from three-dimensional interfacial material volumes, making vanishing the thickness and preserving information about microstructure and local mechanical properties by means of homogenization techniques. The mechanical modelling of interfaces represents a very important problem because they may become crucial in many different situations, such as in the analysis of delamination phenomena in composite, crack propagation, localized damage and remodelling of bone tissue around prostheses.

Bertoldi, Bigoni and Drugan [1] already proposed a new model of structural interface, by introducing a true structure in the transition zone joining continuous bodies able to take into account features directly obtained by the geometrical and microstructural properties of the interfacial material. The model captures effects absent in all previous interface models, including the stress/deformation field effects due to the discrete structure and the great stress concentration reduction due to non-locality, and it is aimed to investigate the influence of a selected interface microstructure on the mechanical interaction of an infinite matrix with a possible inclusions. Successively, Bertoldi, Bigoni and Drugan [2] also explored the role of the microstructure on the mechanical properties of composite (fiber- and particulate-reinforced) materials, in the framework of two-dimensional linear elasticity. However, as mentioned above, the analysis of interfaces constitute a very important topic also in the description of the mechanical behaviour of orthopaedic devices, i.e. hip prostheses, when one needs to estimate durability, mechanical performance and bone remodelling around an implant for predicting aseptic mobilization phenomena.

In literature, within this realm, Moreo, Pérez, Garcia-Aznar and Doblaré [3] developed a failure model for the cement–bone interface in cemented hip prostheses. Other authors (Netti et al. [4]) explored the effect of inserting biomaterials between bone and prosthesis, as well as research efforts have been produced on the effect of surface roughness on bone remodelling due to a hip implant, by verifying the formation of particular kind of structures, *trabecular hubs* and *spokes*, at the interface bone-implant (see Figure 1).

2 THE MODEL

By starting from the geometry, the present paper makes a proposal of a new model of interface, constituted by an arrangement of one-dimensional beam elements – in both axial strain and bending regimes – responsible of the structural connection between two idealized circular surfaces, representing the boundaries of matrix and inclusion, respectively. In a certain sense, the proposed approach can be considered complementary respect to that by Bertoldi, Bigoni and Drugan, being our model mainly interested to follow the overall mechanical response of the interface and its reconfiguration, under prescribed load and displacement conditions at the matrix and inclusion boundary levels. This complementary focus is obviously motivated by biomechanical applications which can consider compact bulk bone and implant as significantly stiffer than interfacial bone tissue. As a consequence, the goal is here to analyse the mechanical character of the joint region with reference to possible remodelling phenomena induced by mechanical stimuli.

2.1 *Micromechanical characterization of interfaces*

By using a classical homogenization technique, we firstly focused the attention on the elastic and ultra-elastic characterization of the interface, determining its homogenized Young's and Lamè moduli and evaluating gross yield stress and buckling load due to local plastic and stability phenomena. Therefore, in order to complete the characterization of the structural interface, we analysed its overall dynamic behaviour, especially in terms of frequency eigenvalues and viscosity. All these properties at the macroscopic level are derived as functions of both the mechanical features of the constituents and a set of three micro-geometrical parameters, that is the beam volumetric fraction, γ, the number of elements, n, and their averaged inclination, α.

2.2 *Interface Remodelling*

Because living tissues are able during the entire lifetime to adapt their internal microstructure – and consequently the associated mechanical properties – to the specific physical and physiological environment through a process called remodeling, after the micromechanical characterization, we considered interfaces evolution phenomena, evaluating the way in which elements reorganize themselves in terms of inclination and volumetric fraction.

Solving the *remodeling problem* means here to be able of following the evolution of the interface and therefore to describe the relationships between the internal tissue's microstructure and the mechanical load that it supports. This reduces to find how the variation in time of the density and inclination of the beam elements obeys to the mechanical stimuli, related to prescribed boundary data given in terms of displacements/velocities or forces. This part of the work invokes a few biomechanical researches that consider the mechanical stimulus as the main activator of the remodelling process. In accord with experimental observations, different suggestions about the choice of the mechanical stimulus are proposed. In particular, it is defined as function of the strain (Cowin *et al.*, [5]), the rate of deformation (Cowin,[6]), the stress (Rodriguez, [7]), the effective stress (Beaupré *et al.*, [8]) or the strain energy (Huiskes *et al.*,[9). In more recent proposals, the microdamage is also considered as an activator of the remodeling process (Ramtani *et al.*,[10]; Doblaré *et al.*, [11]). Indeed, experiments suggest that the presence and formation of microcracks seem to stimulate the bone remodeling sequence and tests show that the magnitude, the frequency and the duration of the loading also affect bone remodeling.

The idea of the present work is based on an energetic approach, but the activator of the remodeling process doesn't merely the strain energy, but a functional that we called *Metabolic Cost Function*.

This functional is defined as the sum of two terms. The first one is still the strain energy of the structure in the final configuration, written in a regime of large displacements. The second one is represented by the energy that the structure spends to pass from the initial to the final configuration and it decides if the remodeling of the microstructure is convenient or not. This gets over some limits of literature approaches. In fact, if one assumes that the sole strain energy governs the remodeling, this process has to begin and to go on toward the same optimum, independently from the initial microstructural organization. On the contrary, by following the new way, the problem of remodeling becomes a problem of optimization, that consists in the minimization of the Metabolic Cost Function upon the parameters that describe the density distribution and the material directionality. With the bone interface in mind, the strategy is then applied to the structural interface previously characterized, setting a finite number of beam elements that deform in extensional and bending fashion and establishing a selected initial configuration, showing then how the mathematical model allows to predict optimal interface microstructure as explicit function of both the micro-geometrical parameters and the type of boundary data.

3 NUMERICAL RESULTS

3.1 Micromechanical analysis of interfaces

The interface normalized Young and shear modulus are evaluated through an homogenization technique as functions of both the mechanical features of the constituents and a set of three micro-geometrical parameters, that is the beam volumetric fraction, γ, the number of elements, n, and their averaged inclination, α.

$$\eta = 1.072 \cdot \frac{n^2 A}{8\gamma\left(R+r\right)\pi r}\left\{\cos^2\beta + \frac{12}{l^2}\left[\frac{t\gamma\left(R+r\right)}{nl}\right]^2 sen^2\beta\right\} \tag{1}$$

$$\mu = 0.385 \cdot \frac{n^2 A}{8\gamma\left(R+r\right)\pi r}\left(sen^2\beta + \frac{12}{l^2}\left[\frac{t\gamma\left(R+r\right)}{nl}\right]^2 \cos^2\beta\right) \tag{2}$$

The buckling load for the interface is evaluated as the average among the buckling loads of all beams and it results a function of the same parameters introduced above.

$$\bar{\sigma}_{cr} = \frac{16\pi E t^4 \gamma^4 \left(R+r\right)^4}{n^4\left(r^2 + R^2 - 2r\cos\alpha\sqrt{R^2 - r^2 sen^2\alpha} + 2r^2 sen^2\alpha\right)^3} \tag{3}$$

3.2 Interface Remodelling: Numerical Applications

We have investigated the way in which an interface can modify its internal microstructure when a mechanical load is applied on its internal surface. The problem has been approached by an energetic point of view through the minimization of the Metabolic Cost Function, a functional that is composed of two terms; the first is an elastic strain energy, the second the energy that the structure needs to pass from the initial to the final configuration.

Thus, the remodeling occurs if $\int_0^1 U_0(u(t))dt - C_{opt} \geq 0$, that means that the process is really advantageous for the structure, as described before.

The optimization parameters are the volume fractions ρ_i and the final inclinations β_i of the n elements that connect the two circular surfaces of the structure.

The interface has been loaded by a uniform displacement field and a uniform force field. We have chosen two laws, the first constant and the other linear with the same average value, that produce displacements compatible with the geometry of the interface.

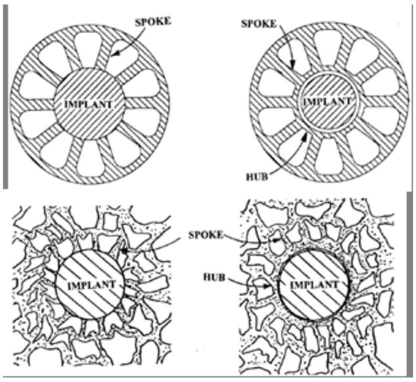

Figure 1

4 CONCLUSIONS

The model captures effects absent in all previous interface models, such as the dependence of Young’s and shear moduli and of buckling load not only from the volumetric fraction, but also from the numbers of elements, *n*, and their inclination, *α*. The moduli sensibly vary with the geometric features of the structure, so, not only density plays a decisive role in the description of the structure. It’s important, for this reason, to characterise the structure with all these parameters.

The mechanical interface properties are very important for the prevision of the structural evolution of biological interfaces. A new formulation is proposed to explore the answer of the structure to two different stimuli. In the first case, when a displacement field is imposed on the internal surface, to minimize C is equivalent to minimize the stiffness, while, in the second case, to maximize the stiffness.

This work has many possibilities of development. First of all, the extension of this model to the 3D- case. This discrete well-representative model of interfaces could be introduced in a structural computation program to model the interaction between two surfaces or volumes. In biomechanics, there are different areas of application of this model, such as bone-prosthesis interface modelling in order to predict possible causes of failure (linked to the implant mobilization), which request a new surgery, or in the mechanical characterization of the cell, where cytoskeleton could be depicted as a structural interface which connects the nucleus to the cell membrane.

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