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Characterization of structure and properties of bone by spectral measure method

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A B S T R A C T

Novel mathematical method called spectral measure method (SMM) is developed for characterization of bone structure and indirect estimation of bone properties. The spectral measure method is based on an inverse homogenization technique which allows to derive information about the structure of composite material from measured effective electric or viscoelastic properties. The mechanical properties and ability to withstand fracture depend on the structural organization of bone as a hierarchical composite. Information about the bone structural parameters is contained in the spectral measure in the Stieltjes integral representation of the effective properties. The method is based on constructing the spectral measure either by calculating it directly from micro-CT images or using measurements of electric or viscoelastic properties over a frequency range. In the present paper, we generalize the Stieltjes representation to the viscoelastic case and show how bone microstructure, in particular, bone volume or porosity, can be characterized by the spectral function calculated using measurements of complex permittivity or viscoelastic modulus. For validation purposes, we numerically simulated measured data using micro-CT images of cancellous bone. Recovered values of bone porosity are in excellent agreement with true porosity estimated from the micro-CT images. We also discuss another application of this method, which allows to estimate properties difficult to measure directly. The spectral measure method based on the derived Stieltjes representation for viscoelastic composites, has a potential for non-invasive characterization of bone structure using electric or mechanical measurements. The method is applicable to sea ice, porous rock, and other composite materials.

1. Introduction

Bone is a hierarchical composite whose ability to withstand fracture depends on the bone structural organization. At the micro-scale, cancellous bone is a heterogeneous composite formed of trabeculae with bone marrow filling its porous spaces (see Fig. 1). The macroscale mechanical properties such as bone stiffness and strength depend on bone microstructure, density, and stiffness of the bone tissue (Hollister et al., 1991; Crolet et al., 1993; Aoubiza et al., 1996; Lakes, 2001; Cowin, 2001; Hellmich et al., 2004). To analyze the dependence of the bone properties on its structure, trabecular architectures were idealized as open and close cell high porosity models (Gibson, 1985; Keaveny, 1997; Kabel et al., 1999b). Non-destructive imaging methods such as X-ray and micro-CT, have been developed to predict the mechanical properties of the bone from its structure by correlating measured by X-ray or CT structural parameters with results of mechanical tests or numerical simulations (Kabel et al., 1999a). Bone morphology was related with ultrasound propagation, methods aimed at numerical recovery of bone density and structural parameters from ultrasonic data have been developed (Chaffai et al., 2002; Padilla and Laugier, 2005; Padilla et al., 2008; Fang et al., 2007; Buchanan et al., 2003, 2004; Gilbert et al., 2009).

Mechanical properties of bone are linked with bone volume, fabric tensor, and anisotropy (Cowin, 1985; Hodgskinson and Currey, 1990; Zysset et al., 1998; Goulet et al., 1994; Van Rietbergen et al., 1998; Borah et al., 2000). Relationships between the elasticity tensor, structural density, and the invariants of the fabric tensor were developed in Cowin (1985), Turner et al. (1990) and Kabel et al. (1999a). Statistical correlations of structural and elastic parameters give significant correlation coefficients for particular bone samples; however, in general, they could be not applicable to another bone sample (Van Rietbergen et al., 1998; Van Rietbergen and Huiskies, 2001). Though the trabecular morphology determines the elastic properties of cancellous bone, not many analytical models are available to relate the properties and morphology (Kabel et al., 1999a).

Spectral measure method of characterization of bone structure is a method that provides relations between structural parameters and electric and viscoelastic properties. It is based on results of

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Fig. 1. At the microscale, cancellous bone is a heterogeneous composite material formed of trabeculae and bone marrow. Photograph of trabecular bone is courtesy of Scott C. Miller.

forward and inverse homogenization for materials with microstructure. This method is not site specific, it relies neither on correlation analysis nor on assumptions about a particular morphology of bone. Based on analytical relations and characterization of resonances of the bone structure, spectral measure method provides a basis for relating microstructural parameters to effective electric, elastic, and viscoelastic behavior of bone as well as for modeling and predicting bone structure from electrical, mechanical, and potentially, ultrasound data.

Mechanical behavior of a composite material depends on properties of the components as well as on the microarchitecture. Various approaches to calculation of effective properties from known microstructural information, have been developed using homogenization theory (Sanchez-Palencia, 1980; Hollister et al., 1994; Bergman, 1993; Zoui, 2002; Milton, 2002). One of the methods developed for bounding the effective complex permittivity of a composite formed by two materials with given complex permittivity, used the analytic Stieltjes representation of the effective property (Bergman, 1978, 1980; Milton, 1980; Golden and Papanicolaou, 1983). The Stieljtes representation analytically relates the effective properties to microstructural information through the spectrum of a corresponding linear operator. Specifically, the moments of the spectral measure in this representation are linked to the n-point correlation functions of the microstructure. Another important feature of the Stieltjes representation of the effective properties is that it factors out the dependence on the constituents in the composite from the dependence on the microgeometry. The information about the microstructure is contained in the spectral measure in the Stieltjes representation of the effective properties. This feature of the Stieljtes representation allows us to recover microstructural parameters from effective properties using inverse homogenization. The inverse homogenization is based on the recovery of the spectral measure which contains information about the microgeometry (Cherkaev, 2001). Once the spectral measure is known, it can be used to characterize the bone morphology. The spectral measure can be constructed directly from the images obtained from regular CT or micro-CT, or it can be recovered from non-invasive electric or viscoelastic measurements over a range of frequencies.

The problem of extraction of structural information from measured transport properties of composite materials was introduced in McPhedran et al. (1982) for estimating volume fractions of constituents in the composite. In Cherkaev (2001), identification of structural information from measured effective property was formulated as an inverse problem for the spectral measure in the Stieltjes analytic representation. It was shown that the spectral measure can be uniquely recovered from the measurements of the effective property over a range of frequencies (Cherkaev, 2001). Uniqueness of reconstruction of the spectral measure gives the basis for the theory of inverse homogenization and the spectral measure method (SMM). The term SMM was coined in Bonifasi-Lista and Cherkaev (2009), where the method was used to estimate bone porosity from data of complex conductivity of bone samples numerically simulated using micro-CT images.

The analytic Stieljtes representation was extended to the effective elastic properties of a composite material in Kantor and Bergman (1982, 1984), Bergman (1985), Dell'Antonio et al. (1986), Bruno and Leo (1993), Milton (2002) and Ou and Cherkaev (2006). Stieltjes representation for the effective viscoelastic shear modulus obtained from torsion of a viscoelastic cylinder whose microstructure does not depend on the axial direction, was derived in Tokarzewski et al. (2001), Bonifasi-Lista and Cherkaev (2006a, b, 2008), assuming St.Venant principle and using mathematical equivalency between conductivity problem and elastic torsion of such cylinder. In Tokarzewski et al. (2001), this representation was used to bound the effective shear modulus of cancellous bone filled with bone marrow. Based on this representation, the inverse homogenization approach was applied in Bonifasi-Lista and Cherkaev (2006a, b, 2008), and Bonifasi-Lista et al. (2009) to successfully recover porosity of cancellous and compact bone from simulated measurements of the viscoelastic shear modulus for the simplified model of bone viewed as a cylinder, filled with viscoelastic composite of trabecular tissue and bone marrow, realistic data were simulated using micro-CT images of cancellous bone.

2. Mathematical methods

2.1. Spectral measure method

We consider bone as a two component composite formed by trabecular tissues and bone marrow and introduce a characteristic function χ of the subdomains occupied by one of the materials. In bioelectrical applications, low frequency electric fields are used in practice, the appropriate parameter characterizing properties of the medium, is complex conductivity σ. The complex conductivity σ of the medium is modeled by a function $\sigma(\mathbf{x}) = \sigma_1\chi(\mathbf{x}) + \sigma_2(1-\chi(\mathbf{x}))$, where $\sigma_i, i = 1,2$, is complex conductivity of the i-th material, bone marrow or trabecular tissue, and the characteristic function $\chi = \chi(\mathbf{x})$ takes values 1 if $\mathbf{x}$ is in the region of first material, bone marrow, and zero if $\mathbf{x}$ is in the region occupied by the second material. The effective tensor $\boldsymbol{\sigma}^*$ is a coefficient of proportionality between the averaged electric and displacement fields: $\langle J \rangle = \sigma^* \langle E \rangle$, and the electric field is governed by equation: $\nabla \cdot (\sigma_1\chi(\mathbf{x}) + \sigma_2(1-\chi(\mathbf{x})))E = 0$. Introducing $s = 1/(1-\sigma_1/\sigma_2)$, the derivation of the Stieltjes representation uses a spectral decomposition of an operator $\Gamma\chi = \nabla(-\Delta)^{-1}(\nabla\cdot)\chi$, and results in the integral representation for a function $F(s) = 1 - \sigma^*/\sigma_2$ as an analytic function off [0, 1)-interval in the complex s-plane:

$$F(s) = \int_0^1 \frac{d\eta(z)}{s-z} \tag{1}$$

Here the function η is the spectral measure of the self-adjoint operator $\Gamma\chi$, which contains information about the structural parameters. The spectral function η can be uniquely reconstructed if measurements of the effective properties of the composite are known along some arc in the complex s-plane (Cherkaev, 2001). Such data can be obtained from effective measurements in an interval of frequency provided the properties of the constituents are dependent on frequency. The spectral moments η_n of the spectral measure η,

$$\eta_n = \int_0^1 z^n \, d\eta(z), \quad \eta_0 = \int_0^1 d\eta(t) = p_1 \tag{2}$$