The Role of Gradient Effects in the Piezoelectricity of Bone

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Abstract—**Stress-gradient effects in piezoelectricity are obtained from general nonlocality considerations. A nonlocal continuum representation of bone is appropriate, in view of bone's structure.**

INTRODUCTION

Bone generates an electrical polarization when subjected to mechanical stress [1]-[3]. The linearity of this response, as well as the presence of the appropriate converse effect, i.e., the development of strain in response to an imposed electric field, suggested to some workers that bone is a piezoelectric material in the classic sense [4]. The constitutive equations for such a material are

$$D_i = d_{ijk}\sigma_{jk} + K_{ij}E_j \tag{1}$$

$$\epsilon_{ij} = S_{ijkl}\sigma_{kl} + d_{kij}E_k \tag{2}$$

in which D is the electric displacement, E is the electric field, d is the piezoelectric tensor, K is the dielectric tensor, S is the compliance tensor, ϵ is the strain tensor, and σ is the stress tensor. Several investigators have assumed these constitutive equations to be valid and have determined elements of the tensor d [5]; others have assumed that the material coefficients are complex and frequency dependent, and have performed experiments to determine the d's and the k's [6], [7]. Recently, evidence has been found that (1) and (2) may be inadequate to describe the electromechanical behavior of bone. For example, the results of studies in bending indicate that polarization may result from the stress gradient as well as the stress itself [8], [9]. The constitutive equation in this case can be written

$$D_i = d_{ijk}\sigma_{jk} + f_{ijkn}\sigma_{jk,n} + K_{ij}E_j \tag{3}$$

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in which f is a fourth rank tensor relating electric displacement to the stress gradient and the comma denotes differentiation with respect to the coordinate specified by the index n. It has been suggested that this theory is *ad hoc*, and other explanations have been advanced to explain the results in bending. Indeed, it has been suggested that the postulated fourth rank gradient tensor f, providing a polarization comparable to that resulting from the third rank tensor d, has no counterpart for other materials in nature, and must be regarded in a tentative manner [10]. In addition, the lack of an explicit relationship between the phenomenology of the stress-gradient hypothesis and the known structure of bone is seen as a drawback. The purpose of the present communication is to examine the role of the stress gradient theory among continuum theories and to explore possible relationships between this theory and the structure of bone.

NONLOCAL THEORY

Nonlocal theories are continuum models in which the effect at a point depends not only on a cause at that point, but on the causal variable at all points in the solid [11]. Nonlocal theories of piezoelectricity and dielectric response have been proposed, particularly in relation to ferroelectrics [12]. For example, consider

$$D_i(X_p) = \int \Delta_{ijk}(X_p - X_p')\,\sigma_{jk}(X_p')\,dX_p' \tag{4}$$

in which Δ is a function which expresses the nonlocal coupling between stress and electric displacement; the electric field E is assumed to be zero for simplicity. In this expression, the electric displacement D at a point specified by the position vector X_p depends on the stress at points, specified by the vectors X_p', in a neighborhood of X_p. To illustrate how this expression can be specialized, we follow a procedure similar to that used in [13]. Expand the stress in a power series about the point X_p

$$\sigma_{jk}(X_p') = \sigma_{jk}(X_p) + \frac{\partial\sigma_{jk}(X_p)}{\partial X_n}(X_n - X_n') + \cdots. \tag{5}$$

Substitute this in (4).

$$D_i(X_p) = \int \Delta_{ijk}(X_p - X_p')\,\sigma_{jk}(X_p)\,dX_p' + \int \Delta_{ijk}(X_p - X_p')\,\frac{\partial\sigma_{jk}(X_p)}{\partial X_n}(X_n - X_n')\,dX_p'. \tag{6}$$

If we define

$$d_{ijk} \equiv \int \Delta_{ijk}(X_p - X_p')\,dX_p',$$

$$f_{ijkn} \equiv \int \Delta_{ijk}(X_p - X_p')(X_n - X_n')\,dX_p' \tag{7}$$

then (6) can be written

$$D_i(X_p) = d_{ijk}\sigma_{jk}(X_p) + f_{ijkn}\sigma_{jk,n}(X_p) + \cdots. \tag{8}$$

The first term in this last expression represents the classical (local) theory of linear piezoelectricity: the electric displacement at a point depends on the stress at that point. The second term is the stress-gradient effect term discussed above; it has emerged in a natural fashion from considerations of nonlocality and should not be regarded as ad hoc. The higher order terms contain higher spatial derivations of the stress and represent a closer approximation to the general nonlocal theory.

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Properties of Real Materials

Both the nonlocal and classical theories of piezoelectricity are continuum representations and as such make no reference to structure. Lattice theory, which considers the atomic structure of crystals, can be used to derive classical piezoelectricity and elasticity in a zeroth-order or long wave limit approximation. Lattice theory can also be used to derive nonlocal representations, if higher order terms are retained. For most macroscopic applications of ionic crystals, e.g., quartz, the classical (local) theories are entirely adequate, since effects due to nonlocality are neither predicted [14] nor observed to be significant at wavelengths many orders of magnitude longer than the atomic spacing. In ferroelectric materials, however, there is a long range interaction from which a nonlocal piezoelectric effect can be predicted [12]; this is related to phase transitions and is unlikely to constitute a dominant mechanism for such effects in bone. Experimental evidence for nonlocality in ferroelectric materials has been found [15], therefore bone is not the only material for which gradient effects have been reported.

Compact bone has a complex structure which is a significant impediment to the development of rigorous theoretical connections between structure and properties. Theoretical studies have been performed, however, on simple laminated and lattice structures: a continuum representation of the elastic behavior of such structures contains a dependence on elements of the strain gradient [16], [17]. The characteristic length which appears in these theories is of the order of the size of the structural elements; significant deviations from classical theory are expected for specimens ten times the characteristic length or less. The largest structural elements in human compact bone are osteons, which have a diameter of about 0.25 mm. Since specimens of bone used in studies of electrical effects are typically only a few millimeters thick, it is conceivable that effects of microstructure will contribute to the total effect, and that extended continuum theories could be used in a description of such effects.

Gradient effects in the elastic properties could enter a piezoelectric constitutive equation as follows. In the linear local theory, piezoelectric coupling may be represented by any one of four tensors, depending on the choice of field variables [18]. The equations which interrelate pairs of these tensors contain the elastic tensor or the dielectric tensor. So if the elastic properties are perturbed by a gradient effect and one piezoelectric tensor represents a purely local effect, then at least one of the other piezoelectric representations will suffer a perturbation. Unfortunately, no data concerning elastic gradient effects in bone are presently available.

Discussion

Stress gradient effects in piezoelectricity arise in a natural way from the nonlocal relationship between stress and electric displacement. Nonlocal continuum representations can be derived from microstructural considerations. Since the microstructural features of bone are not negligibly small compared with typical specimen dimensions, a nonlocal representation, to which the stress-gradient theory is an approximation, may be appropriate. It has yet to be established that all observations of stress-generated potentials in bone can be modeled by a continuum theory. To the extent that such modeling is possible, investigation of nonlocal representations is likely to be fruitful.

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