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ON A MATHEMATICAL MODEL IN BIOPIEZOELECTRICITY

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The present paper is an attempt to obtain a mathematical model of electromechanical interaction in biomaterials exhibiting piezoelectric behaviour. In the present investigation the modelling has been facilitated by considering the electromechanical interaction in the form of "piezoelectric scattering". The analysis reveals a quicker energy conversion and hence, a greater involvement of the electrical response in the regulations of the cells.

INTRODUCTION

Studies in electromechanical interactions are replete with those on uses of biomaterials exhibiting piezoelectric behaviour, particularly in the area of electromechanical conversion (Bassett 1972). The main purpose is to look for electrical responses corresponding to mechanical stimuli and vice-versa. While one can cite a number of studies in electromechanical interactions in nonbiological materials, (Cady 1946, Tiersten 1969, Mason 1958) along with their mathematical counterparts, there are not many studies, along these directions in mathematical terms for biological materials exhibiting piezoelectricity, to explain the known experiments on the subject (Shamos 1963, Lang 1969, Ramachandran and Kartha 1954, Bassett and Becker 1962, Fukada and Yasuda 1957). It, therefore, seems imperative to obtain a mathematical model of such a biopiezoelectric situation and this is what the present paper seeks to do. The modelling should be reinforced by the experimental findings which attribute piezoelectricity to a kind of protein, namely, collagen (Ramachandran and Kartha 1954, Fukada and Yasuda 1957). A semiconducting dimension of piezoelectric materials inevitably leads to the determination of scattering, called the piezoelectric scattering to be taken as a convenient form of the required response. The mathematical analysis proceeds on the lines of Seeger (1973, pp. 190–92) and Ghosh *et al.* (1978). The scattering yields a mobility along with contribution to it by space charge. Another result stemming from it, is a greater mobility and so a greater conduction than in the case free from space charge. This can be interpreted as indicating a quicker energy conversion essential for purposes and in biological terms, a greater involvement of the electrical response in the regulations of the cells.

PROBLEM AND MATHEMATICAL MODEL

If piezoelectric scattering is to be taken to represent responses in biological materials exhibiting piezoelectric behaviour, one can have its mathematical model by working out an expression for mobility of carriers. The equations which represent the model are:

(i) the constitutive relations of the material,

$$D = \epsilon E + e_{pz} S \quad \text{...(1)}$$

where D is the electric displacement, E the electric field, S the strain, ϵ the dielectric permittivity at constant strain, e_{pz} the piezoelectric constant. [For longitudinal wave travelling in the x-direction the quantities in (1) may be considered as scalars.]

(ii) the Gauss' equation and the equation of continuity of charge flow for unidirectional motion (in the x-direction) given by (Seeger 1973, pp. 277–85).

$$\frac{\partial D}{\partial x} = e n_s \quad \text{...(2)}$$

and

$$e \frac{\partial n_s}{\partial t} + \frac{\partial j}{\partial x} = 0 \quad \text{...(3)}$$

where the current density j is given by (Seeger 1973, pp. 277–85)

$$j = | e | (n_0 + f n_s) \mu_{e_{pz}} E - e D_n \frac{\partial}{\partial x} (n_0 + f n_s) \quad \text{...(4)}$$

n_0 being the mean carrier density, $(n_0 + f n_s)$ the instantaneous local density of carriers, D_n the diffusion constant and $\mu_{e_{pz}}$ the mobility determined on the basis of negligible displacement of carriers relative to ions, as in (Seeger 1973, pp. 190–92). In the above equations $e < 0$ for electrons and the longitudinal wave is taken to be travelling in the x-direction.

Mathematical Analysis

A reduction to a suitable form of the above equations is necessary for analysis of the problem. To do this we differentiate eqn. (2) with respect to t and using (3) and (4), we get

$$\frac{\partial^2 D}{\partial x \partial t} = - \frac{\partial}{\partial x} \left[\left(| e | n_0 \mu_{e_{pz}} - \mu_{e_{pz}} f \frac{\partial D}{\partial x} \right) E \right] + D_n f \frac{\partial^3 D}{\partial x^3}. \quad \text{...(5)}$$

Since piezoelectric scattering is an electrical response due to a mechanical excitation, the excitation can be taken as a longitudinal acoustic wave in the form given by

$$\delta x = \delta x_1 \, e^{i(\omega t - qx)}. \quad \text{...(6)}$$

We also take

$$E = E_1 \, e^{i(\omega t - qx)}. \quad \text{...(7)}$$

The amplitudes in (6) and (7) are considered to be small. Now using (6) and (7) in the equation, we get

$$\{\epsilon(\omega - iq^2 fD_n) - i \mid e \mid n_0\mu_{e_{pz}}\} E_1 = iqe_{pz}(\omega - iq^2 D_n f)\, \delta x_1 \qquad \text{...(8)}$$

where eqn. (1) is applied.

The strain being equal to $\partial(\delta x)/\partial x = -iq\delta x_1\, e^{i(\omega t - qx)}$, eqn. (8) can be written as

$$\{\epsilon(\omega - iq^2 f D_n) - i \mid e \mid n_0\mu_{e_{pz}}\} E = -(\omega - iq^2 D_n f)\, S. \qquad \text{...(9)}$$

The potential energy $\delta\epsilon_1$ is computed to be

$$\delta\epsilon_1 = \mid e \mid \int E\, dx$$

$$= -\frac{i \mid e \mid e_{pz}}{q\epsilon} \cdot \frac{(\omega - iq^2 D_n f)}{\{\epsilon(\omega - iq^2 f D_n) - i \mid e \mid n_0\mu_{e_{pz}}\}} S \qquad \text{...(10)}$$

where $\quad q = \mid \mathbf{k}' - \mathbf{k} \mid \approx 2 \mid \mathbf{k} \mid \sin \tfrac{1}{2}\theta$

$\mathbf{k}$, $\mathbf{k}'$ being respectively the wave vectors of carrier before and after scattering and θ the scattering angle.

Then the absolute magnitude of Hamiltonian matrix element $H_{k'k}$ is given by (Seeger 1973, pp. 190–92)

$$\mid H_{k'k} \mid = \frac{\mid e \mid e_{pz}}{q\epsilon}\left(\frac{k_B T}{2Vc_1}\right)^{1/2}\left[\left(\omega^2 + q^4 D_n^2 f^2 + \frac{\mid e \mid n_0}{\epsilon}\mu_{e_{pz}} D_n f q^2\right)^2 + \frac{\omega^2 e^2 n_0^2\mu_{e_{pz}}^2}{\epsilon^2}\right]^{1/2} \Bigg/ \left[\omega^2 + \left(q^2 f D_n + \frac{\mid e \mid n_0\mu_{e_{pz}}}{\epsilon}\right)^2\right]$$

$$= \left[\frac{e^2 K^2 k_B T}{2V\epsilon q^2} \cdot \frac{\left(\omega^2 + q^4 D_n^2 f^2 + \frac{\mid e \mid n_0}{\epsilon}\mu_{e_{pz}} D_n f q^2\right)^2 + \frac{\omega^2 e^2 n_0^2 \mu_{e_{pz}}^2}{\epsilon^2}}{\left\{\omega^2 + \left(q^2 f D_n + \frac{\mid e \mid n_0 e_{pz}}{\epsilon}\right)^2\right\}}\right]^{1/2} \qquad \text{...(11)}$$

where the electromechanical coupling coefficient K is given by $K^2 \approx e_{pz}^2/\epsilon c_1$.

The expression for momentum relaxation time τ_m is given by (Seeger 1973, pp. 190–92)

$$\frac{1}{\tau_m} = V(2\pi)^{-2} \int k'\, dk' \int_0^\pi S(\mathbf{k}, \mathbf{k}')\,(1 - \cos\theta)\sin\theta\, d\theta \qquad \text{...(12)}$$

where the scattering probability $S(\mathbf{k}, \mathbf{k}')$ in (12) is given by

$$S(\mathbf{k}, \mathbf{k}') \approx 2.\frac{2\pi}{\hbar} \mid H_{k'k} \mid^2 \delta\{\epsilon_1(\mathbf{k}) - \epsilon_1(\mathbf{k})\} \qquad \text{...(13)}$$

Since q^2 is approximately given by $4k^2 \sin^2(\theta/2)$ and $dk = \hbar(m/2\epsilon)^{1/2} d\epsilon_1$, we get from (12)

$$\tau_m = \frac{2^{3/2} \pi\hbar\epsilon}{m^{1/2}e^2K^2k_BT}\left(1 + \frac{e^2n_0^2\mu_{e_{pz}}^2}{\omega^2\epsilon^2}\right)\epsilon_1^{1/2}. \qquad ...(14)$$

In this, we have neglected the effect of diffusion i.e., $D_n \approx 0$ and we can afford to do so if frequencies are taken to be small (White 1962). Now the mobility (μ) of non-degenerate carriers satisfying the power law $\tau_m = \tau_0\epsilon_1^p$ is given by (Kireev 1975)

$$\mu = \frac{e\tau_0(k_BT)^p}{m} \cdot \frac{\Gamma(5/2+p)}{\Gamma(5/2)}. \qquad ...(15)$$

Hence from (14) we get a modified expression for mobility of carriers as

$$\mu = \frac{16\sqrt{2\pi}}{3}\frac{\hbar^2\epsilon}{m^{3/2}eK^2(k_BT)^{1/2}}\left(1 + \frac{e^2n_0^2\mu_{e_{pz}}^2}{\omega^2\epsilon^2}\right)$$

$$= \mu_{e_{pz}}\left(1 + \frac{e^2n_0^2\mu_{e_{pz}}}{\omega^2\epsilon^2}\right). \qquad ...(16)$$

As already mentioned, $\mu_{e_{pz}}$ being the mobility when the spatial displacement of carriers is negligible compared to the spatial displacement of ions, we see from (16) that space charge contribution can result in an increase in mobility and further the modified mobility (μ) which is also a more generalized expression is greater than $\mu_{e_{pz}}$.

Conclusions

Let us now attempt to interpret the above analysis in the light of biopiezoelectric situations. A greater mobility of carriers, as established earlier leads to a greater flow of current which, of course, originates on account of acousto-electric effect. This obviously implies a greater net energy transfer from mechanical to electrical (Seeger 1973, pp. 277–85) than their counterparts without the reckoning space charge in mobility (Seeger 1973, pp. 190–92). This conclusion is also re-inforced by the findings of (Bassett 1971) in his attempt to identify and to relate electromechanical factors to responses of connective tissues. This fact taken along with that established by (Bassett 1971) ought to imply a greater involvement of the electrical response in the regulation of the cells than what it ought to be if there be no contribution of space-charge (to mobility). Summing up, the model presented above has relevance to the design and fabrication which make use of solid-state characteristics responsible for piezoelectric responses and thereby involved in cell nutrition and energy conservation (Bassett 1971).

REFERENCES

Bassett, C. A. L. (1971). Effect of force on skeleton tissue — Applied Physiology. W. B. Saunders Co., pp. 283–16.

——— ——— (1972). A biophysical approach to craniofacial morphogenesis. *Acta Morphol. Nederl-Scad.* Votto, pp. 71–86.

Bassett, C. A. L., and Becker, R. C. (1962). Generation of electric potentials by bone in response to mechanical stress. *Science*, **137**, 1063-64.

Cady, W. G. (1946). Piezoelectricity. McGraw-Hill Book Co., Inc., New York.

Fukada, E., and Yasuda, I. (1957). On the piezoelectric effect of bone. *J. phys. Soc. Japan*, **12**, 1158–62.

Ghosh, S., Gupta, M., and Sinha, D. K. (1978). A note on an analytical model of a thermopiezo-semiconducting medium with biological attributes — Trends in Biomedical Engineering. *Proc. Int. Sym. & Workshop on Biomedical Engng*, New Delhi, pp. 173–78.

Kireev, P. S. (1975). Semiconductor Physics. MIR Moscow, p. 429.

Lang, S. B. (1969). Thermal expansion coefficients and the primary and secondary pyroelectric coefficients of animal bone. *Nature*, **174**, 269.

Mason, W. P. (1958). Physical Acoustics and Properties of Solids. D. Van Nostrand & Co., Amsterdam.

Ramachandran, G. N., and Kartha, (1954). Structure of collagen. *Nature*, **174**, 269.

Seeger, K. (1973). Semiconductor Physics, Springer-Verlag Wein, New York, pp. 190–92, 277–85.

Shamos, S. (1963). Piezoelectric effect in bone. *Nature*, **197**, 81.

Tiersten, H. F. (1969). Linear Piezoelectric Theory : Piezoelectric Plate Vibrations. Plenum Press, New York.

White, D. L. (1962). Amplification of ultrasonic wave in piezoelectric semiconductors. *J. appl. Phys.*, **33**, 2547–54.