Stoney formula for piezoelectric film/elastic substrate system*

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With the trends in miniaturization, and particularly the introduction of micro- and nano-electro-mechanical system, piezoelectric materials used in microelectronic devices are deposited usually in the form of thin film on elastic substrates. In this work, the bending of a bilayer comprising a piezoelectric film deposited on an elastic substrate, due to the mismatch, is investigated. An analytic formula relating the curvature of the bilayer to the mismatch, the electroelastic constants and the film thickness is obtained, and from this formula, a transverse piezoelectric constant d_{31} can be estimated. Meanwhile the influence of electromechanical coupling coefficient on the curvature is discussed.

Keywords: Stoney formula, piezoelectric film, bending, electromechanical coupling coefficient

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1. Introduction

With the trends in miniaturization of electric devices, and particularly the introduction of micro- and nano-electro-mechanical system, piezoelectric materials are widely used in microelectronic devices, such as sensors where an applied stress induces a charge, or actuators where an applied voltage induces strain,[1–6] and a component in a fast, low power transistor.[7] Such applications usually require piezoelectric films deposited on elastic substrates.

Stoney [8] observed 100 years ago that when a system is free of the external loads, a metallic film deposited on a thicker substrate undergoes stretching or compressing, resulting in the strain and bending in the substrate. He presented a simple analysis which is called the Stoney formula relating the stresses in the film to the curvature of the substrate. Estimations of stress in films in modern applications including micro-electronics, photoelectron and surface coating of structure components, etc. are always based on his analytic concept.

Following the initial formulation by Stoney, a number of extensions have been derived by various researchers by relaxing some of the other assumptions made in his analysis. A biaxial form of Stoney, applicable for anisotropic film stresses, including different stress values in two different directions and non-zero, in-plane shear stresses, was derived by relaxing the assumption of curvature equi-biaxiality.[9] Relevant analyses treating discontinuous films in the form of bare periodic lines[10] or composite films with periodic line structures (e.g., bare or encapsulated periodic lines) have also been derived.[11–13] Single, multiple, and graded films and substrates have been treated in various large deformation analyses.[14–17] None of the above-discussed extensions of the Stoney method have relaxed Stoney's original assumption of spatial uniformity which does not allow film stress or curvature components to vary across the plate surface, and the Stoney formula has been extended to non-uniform misfit strain in thin film/substrate systems.[18,19] In addition, modified Stoney formulas have been derived in the presence of interfacial sliding.[20,21]

A piezoelectric thin film deposited on an elastic substrate is bent, due to residual stress induced by mismatches between the film and substrate. It is difficult to accurately measure piezoelectric properties of the bent film. It is well known that the measured longitudinal piezoelectric constant, d_{33}, of a piezoelectric film is smaller than d_{33} of the bulk material.[22,23] The main reason is because of bending of the sample.[24–31] In other words, the occurrence of bending deformation influences piezoelectric properties of piezoelectric devices.

To the best of our knowledge, extension of the Stoney formula to the piezoelectric material has not been done so far. It is very necessary therefore to study the bending deformation of a bilayer comprising a piezoelectric film deposited on an elastic substrate. The main objective of this paper is to extend Stoney's work to the piezoelectric materials, and provide an equation relating to the curvature of the bilayer to mismatch, which may result from the lattice mismatch, or thermal mismatch between the piezoelectric film and elastic substrate, and the electric mismatch induced by an applied voltage, the electroelastic constants and the film thickness, thus the transverse piezoelectric constant d_{31} can be estimated.

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2. Model and assumption

Consider a system comprised of a transversely isotropic piezoelectric film polarized in the z direction with the circular plate shape of uniform thickness $h_{\rm f}$ and radius R, deposited on and perfectly bonded to an elastic substrate of uniform thickness $h_{\rm s}$ and radius R as shown in Fig. 1. The total thickness of the bilayer is given by $h = h_{\rm f} + h_{\rm s} \ll R$. To apply an electrical potential difference across the film, infinitesimally thin electrodes are assumed to be located on the free surface of the piezoelectric film and at the interface between the film and the substrate. Within the electrodes, the electric field is zero, but electric charges may reside at the interfaces between the electrodes and the piezoelectric film, inducing an electric field in the film between the electrodes. The electric field is thus assumed to be zero except in the piezoelectric film, and the electrical potential difference V induces an approximately uniform effective electric field $E_{\rm eff} = V/h_{\rm f}$ in the piezoelectric film, if the film is very thin. The role of the electrodes in the analysis is merely to act as planar locations for the accumulation of charge, and they have no mechanical effect on the deformation of the system. Figure 1 also illustrates the cylindrical coordinate system (r, θ, z), where the origin of the coordinate system is at the center of the mid-plane of the substrate, and the z-axis is perpendicular to the plane, the mid-plane of the substrate is then $z = 0$, and the film is bonded on the plane $z = h_{\rm s}/2$.

Relative to the substrate, an inharmonious elastic mismatch strain $\varepsilon_{\rm m}$ exists in the piezoelectric film. The strain may result from the lattice mismatch, or thermal mismatch between the piezoelectric film and elastic substrate, and the electric mismatch induced by an applied voltage, namely,

$$\varepsilon_{\rm m} = \varepsilon_{\rm m}^{\rm c} + \varepsilon_{\rm m}^{\rm t} + \varepsilon_{\rm m}^{\rm e}. \tag{1}$$

Here, the lattice mismatch $\varepsilon_{\rm m}^{\rm c} = \frac{a_{\rm f} - a_{\rm s}}{a_{\rm s}}$ with $a_{\rm s}$ and $a_{\rm f}$ being the lattice constants of the substrate and the film, respectively; the thermal mismatch $\varepsilon_{\rm m}^{\rm t} = (\alpha_{\rm f} - \alpha_{\rm s})\Delta T$ with $\alpha_{\rm s}$ and $\alpha_{\rm f}$ being the thermal expansion coefficients of the substrate and the film, respectively, ΔT being the change of temperature; the electric mismatch $\varepsilon_{\rm m}^{\rm e} = d_{31}E_{\rm eff}$ with $E_{\rm eff} = V/h_{\rm f}$ being the effective electric field.

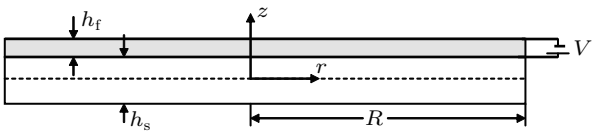


Fig. 1. Schematic diagram of the piezoelectric film/elastic substrate and its electrical connection.

Assume that the deformation of the bilayer, induced by the mismatch strain follows the assumptions on thin plate deformation by Kirchhoff,[32] e.g., the through-thickness stress component $\sigma_{zz} = 0$, a straight line perpendicular to the mid-plane of the substrate before deformation is still maintained after deformation, and thus strains $\varepsilon_{rz} = \varepsilon_{\theta z} = 0$. Deformation is axially symmetric, meaning that all the electroelastic fields are independent of θ. The bending curvature k and the stretching or shrinking strain ε_0 of the mid-plane of the substrate are uniform in the plane. Edge effects may be ignored due to $h = h_{\rm f} + h_{\rm s} \ll R$. Because of the symmetrical and small deformation, and the isotropy in the plane, the bending of the mid-plane has a shape of approximately spherical surface.

3. Stoney formula

Under these assumptions mentioned above, the linear constitutive equations for a transversely isotropic piezoelectric film polarized in the z direction and an elastic substrate are, respectively, written as

$$\begin{aligned}
\varepsilon_{rr}^{\rm f} &= s_{11}^{\rm f}\sigma_{rr}^{\rm f} + s_{12}^{\rm f}\sigma_{\theta\theta}^{\rm f} + d_{31}E_z,\\
\varepsilon_{\theta\theta}^{\rm f} &= s_{12}^{\rm f}\sigma_{rr}^{\rm f} + s_{11}^{\rm f}\sigma_{\theta\theta}^{\rm f} + d_{31}E_z,\\
2\varepsilon_{zr}^{\rm f} &= s_{44}^{\rm f}\sigma_{zr}^{\rm f} + d_{15}E_z,\\
D_r &= d_{15}\sigma_{zr}^{\rm f} + \in_{11} E_r,\\
D_z &= d_{31}\sigma_{rr}^{\rm f} + d_{31}\sigma_{\theta\theta}^{\rm f} + \in_{33} E_z,
\end{aligned} \tag{2}$$

and

$$\begin{aligned}
\varepsilon_{rr}^{\rm s} &= s_{11}^{\rm s}\sigma_{rr}^{\rm s} + s_{12}^{\rm s}\sigma_{\theta\theta}^{\rm s},\\
\varepsilon_{\theta\theta}^{\rm s} &= s_{12}^{\rm s}\sigma_{rr}^{\rm s} + s_{11}^{\rm s}\sigma_{\theta\theta}^{\rm s}.
\end{aligned} \tag{3}$$

The equilibrium equations in the absence of body forces or free charges are

$$\begin{aligned}
&\frac{\partial\sigma_{rr}}{\partial r} + \frac{\partial\sigma_{rz}}{\partial z} + \frac{\sigma_{rr} - \sigma_{\theta\theta}}{r} = 0,\\
&\frac{\partial\sigma_{rz}}{\partial r} + \frac{\sigma_{rz}}{r} = 0,\\
&\frac{\partial D_r}{\partial r} + \frac{\partial D_z}{\partial z} + \frac{D_r}{r} = 0.
\end{aligned} \tag{4}$$

The gradient equations are given by

$$\varepsilon_{rr} = \frac{\partial u_r}{\partial r}, \quad \varepsilon_{\theta\theta} = \frac{u_r}{r}, \quad E_r = -\frac{\partial\phi}{\partial r}, \quad E_z = -\frac{\partial\phi}{\partial z}, \tag{5}$$

where σ_{ij}, ε_{ij}, and u_i are the stress, strain, and displacement, respectively; D_i, E_i, and φ are the electric displacement, electric field, and electric potential, respectively; s_{ij}, d_{ij}, and $\in_{ij}$ the elastic constant, piezoelectric constant, and dielectric constant respectively; superscripts f and s denote the quantities in the film and the substrate, respectively.

The radial and normal displacements of the mid-plane of the substrate are chosen as

$$u_r(r,0) = \varepsilon_0 r, \quad u_z(r,0) = \frac{1}{2}kr^2, \tag{6}$$

where ε_0 and k are the stretching or shrinking strain and the mean curvature of the plane, respectively. The strains in the

bilayer then are given as

$$\varepsilon_{rr}=\varepsilon_{\theta\theta}=\begin{cases}\varepsilon_0-kz+\varepsilon_{\rm m}, & \frac{1}{2}h_{\rm s}<z<\frac{1}{2}h_{\rm s}+h_{\rm f},\\ \varepsilon_0-kz, & -\frac{1}{2}h_{\rm s}<z<\frac{1}{2}h_{\rm s}.\end{cases}\tag{7}$$

The equilibrium equations for the piezoelectric film result in

$$\frac{\partial^2\varphi}{\partial r\partial z}=0,\quad \frac{\partial^2\varphi}{\partial r^2}+\frac{1}{r}\frac{\partial\varphi}{\partial r}=0,$$
$$\left(1-k_{\rm p}^2\right)\frac{\partial^2\varphi}{\partial z^2}+\frac{k_{\rm p}^2}{d_{31}}k=0,\tag{8}$$

in which,

$$k_{\rm p}=\frac{\sqrt{2}d_{31}}{\sqrt{\left(s_{11}^{\rm f}+s_{12}^{\rm f}\right)\in_{33}}},$$

known as the electromechanical coupling coefficient or the piezoelectric coupling factor of the thin circular plate piezoelectric film, is a parameter reflecting the electromechanical coupling effect of the film polarized and electrically excited in the thickness direction, and elastically vibrated in the radial direction, and represents the efficiency in the mutual conversion between mechanical energy and electrical energy for piezoelectric vibrator in the process of vibration,[33] $k_{\rm p}^2<1$.

We obtain from Eq. (8) that

$$\varphi(z,r)=f(r)+g(z),\quad f''(r)+\frac{1}{r}f'(r)=0,$$
$$g''(z)=\frac{k_{\rm p}^2}{\left(k_{\rm p}^2-1\right)d_{31}}k,\tag{9}$$

where $f(r)$ and $g(z)$ are the functions to be determined. Equation (9) gives

$$E_r=-\frac{\partial\varphi}{\partial r}=-f'(r)=\frac{C}{r},\quad C\ \text{is a constant.}\tag{10}$$

The finiteness of the electric field at $r=0$ gives $C=0$. Namely, the electric field in the radial direction is

$$E_r=0,\tag{11}$$

and the electric field in the Z direction is

$$E_z=-\frac{\partial\varphi}{\partial z}=-g'(z)=-\frac{k_{\rm p}^2}{\left(k_{\rm p}^2-1\right)d_{31}}kz+D,$$
$$D\ \text{is a constant,}\tag{12}$$

where $D=V/h_{\rm f}$ with V being the electrical potential difference across the film. Namely, the electric field in the thickness direction

$$E_z=\frac{k_{\rm p}^2}{\left(1-k_{\rm p}^2\right)d_{31}}k\left(z-\frac{h}{2}\right)+\frac{V}{h_{\rm f}}.\tag{13}$$

The equilibrium equations for the substrate are satisfied automatically. From Eqs. (2), (3), (7), (11), and (13), the stress components and electric displacement components can be derived.

The density of internal energy of the bilayer is given by

$$\begin{aligned}&U(r,z)\\ &=\frac{1}{2}\sigma_{rr}\varepsilon_{rr}+\frac{1}{2}\sigma_{\theta\theta}\varepsilon_{\theta\theta}+\frac{1}{2}D_zE_z\\ &=\begin{cases}\dfrac{\left(\varepsilon_{rr}^{\rm f}\right)^2}{s_{11}^{\rm f}+s_{12}^{\rm f}}+\dfrac{1}{2}\in_{33}\left(1-k_{\rm p}^2\right)E_z^2, & \frac{1}{2}h_{\rm s}<z<\frac{1}{2}h_{\rm s}+h_{\rm f},\\ \dfrac{\left(\varepsilon_{rr}^{\rm s}\right)^2}{s_{11}^{\rm s}+s_{12}^{\rm s}}, & -\frac{1}{2}h_{\rm s}<z<\frac{1}{2}h_{\rm s}.\end{cases}\end{aligned}\tag{14}$$

The total potential energy of the bilayer is

$$V(\varepsilon_0,k)=2\pi\int_0^R\int_{-\frac{h_{\rm s}}{2}}^{\frac{h_{\rm s}}{2}+h_{\rm f}}U(r,z)\,rdzdr.\tag{15}$$

In the allowable deformation, the deformation of the midplane of the substrate makes the total potential energy minimal for the stretching strain ε_0 and the mean curvature k, i.e., $\frac{\partial V}{\partial\varepsilon_0}=0$ and $\frac{\partial V}{\partial k}=0$, it follows that

$$\begin{aligned}\frac{k}{k_{\rm st}}&=\left[1+\frac{h_{\rm f}}{h_{\rm s}}\right]\left\{1+4\frac{M_{\rm f}}{M_{\rm s}}\frac{h_{\rm f}}{h_{\rm s}}+6\frac{M_{\rm f}}{M_{\rm s}}\left(\frac{h_{\rm f}}{h_{\rm s}}\right)^2\right.\\ &\quad+\left(4+\frac{k_{\rm p}^2}{1-k_{\rm p}^2}\right)\frac{M_{\rm f}}{M_{\rm s}}\left(\frac{h_{\rm f}}{h_{\rm s}}\right)^3\\ &\quad\left.+\left(1+\frac{k_{\rm p}^2}{1-k_{\rm p}^2}\right)\left(\frac{M_{\rm f}}{M_{\rm s}}\right)^2\left(\frac{h_{\rm f}}{h_{\rm s}}\right)^4\right\}^{-1},\end{aligned}\tag{16}$$

$$\begin{aligned}\frac{\varepsilon_0}{\varepsilon_{0,\rm st}}&=\left[1+\frac{1}{1-k_{\rm p}^2}\frac{M_{\rm f}}{M_{\rm s}}\left(\frac{h_{\rm f}}{h_{\rm s}}\right)^3\right]\left\{1+4\frac{M_{\rm f}}{M_{\rm s}}\frac{h_{\rm f}}{h_{\rm s}}+6\frac{M_{\rm f}}{M_{\rm s}}\left(\frac{h_{\rm f}}{h_{\rm s}}\right)^2\right.\\ &\quad+\left(4+\frac{k_{\rm p}^2}{1-k_{\rm p}^2}\right)\frac{M_{\rm f}}{M_{\rm s}}\left(\frac{h_{\rm f}}{h_{\rm s}}\right)^3\\ &\quad\left.+\left(1+\frac{k_{\rm p}^2}{1-k_{\rm p}^2}\right)\left(\frac{M_{\rm f}}{M_{\rm s}}\right)^2\left(\frac{h_{\rm f}}{h_{\rm s}}\right)^4\right\}^{-1},\end{aligned}\tag{17}$$

where $M_{\rm f}=(s_{11}^{\rm f}+s_{12}^{\rm f})^{-1}$ and $M_{\rm s}=(s_{11}^{\rm s}+s_{12}^{\rm s})^{-1}$ are the equibiaxial elastic moduli for the film and the substrate respectively.

$$k_{\rm st}=\frac{6\varepsilon_{\rm m}}{h_{\rm s}}\frac{M_{\rm f}}{M_{\rm s}}\frac{h_{\rm f}}{h_{\rm s}},\quad \varepsilon_{0,\rm st}=-\varepsilon_{\rm m}\frac{M_{\rm f}}{M_{\rm s}}\frac{h_{\rm f}}{h_{\rm s}}.\tag{18}$$

Equations (16)–(18) are called the extended Stoney formulas. From Eqs. (16)–(18), it can be seen that the deformation of the system is closely related to the mismatch, the relative rigidity and the relative thickness between the film and the substrate, and the electromechanical coupling coefficient of the piezoelectric film.

4. Discussion

Equations (16)–(18) are reduced into the following Stoney formulas[8,9] if the film has no piezoelectric effect:

$$\frac{k}{k_{\rm st}} = \left[1+\frac{h_{\rm f}}{h_{\rm s}}\right]\left\{1+4\frac{M_{\rm f}}{M_{\rm s}}\frac{h_{\rm f}}{h_{\rm s}}+6\frac{M_{\rm f}}{M_{\rm s}}\left(\frac{h_{\rm f}}{h_{\rm s}}\right)^2 +4\frac{M_{\rm f}}{M_{\rm s}}\left(\frac{h_{\rm f}}{h_{\rm s}}\right)^3+\left(\frac{M_{\rm f}}{M_{\rm s}}\right)^2\left(\frac{h_{\rm f}}{h_{\rm s}}\right)^4\right\}^{-1}, \tag{19}$$

$$\frac{\varepsilon_0}{\varepsilon_{0,\rm st}} = \left[1+\frac{M_{\rm f}}{M_{\rm s}}\left(\frac{h_{\rm f}}{h_{\rm s}}\right)^3\right]\left\{1+4\frac{M_{\rm f}}{M_{\rm s}}\frac{h_{\rm f}}{h_{\rm s}}+6\frac{M_{\rm f}}{M_{\rm s}}\left(\frac{h_{\rm f}}{h_{\rm s}}\right)^2 +4\frac{M_{\rm f}}{M_{\rm s}}\left(\frac{h_{\rm f}}{h_{\rm s}}\right)^3+\left(\frac{M_{\rm f}}{M_{\rm s}}\right)^2\left(\frac{h_{\rm f}}{h_{\rm s}}\right)^4\right\}^{-1}, \tag{20}$$

$$k_{\rm st} = \frac{6\varepsilon_{\rm m}}{h_{\rm s}}\frac{M_{\rm f}}{M_{\rm s}}\frac{h_{\rm f}}{h_{\rm s}}, \quad \varepsilon_{0,\rm st} = -\varepsilon_{\rm m}\frac{M_{\rm f}}{M_{\rm s}}\frac{h_{\rm f}}{h_{\rm s}}, \quad \varepsilon_{\rm m} = \varepsilon_{\rm m}^{\rm c}+\varepsilon_{\rm m}^{\rm t}. \tag{21}$$

Comparing Eqs. (16)–(18) with Eqs. (19)–(21), it is easy to find that piezoelectric effect can reduce the curvature for given modulus ratio $M_{\rm f}/M_{\rm s}$, thickness ratio $h_{\rm f}/h_{\rm s}$ and mismatch $\varepsilon_{\rm m}$, with choosing voltage V to be zero for piezoelectric film, and because of $\frac{\partial k}{\partial k_{\rm p}^2} < 0$, the larger the electromechanical coupling coefficient $k_{\rm p}$, the smaller the curvature k is. In particular, the curvature $k \to 0$ for $k_{\rm p}^2 \to 1$, i.e., when the efficiency in mutual conversion between mechanical energy and electrical energy $k_{\rm p}$ takes maximum value 1 (so far the piezoelectric materials have not been found), there is no bending, and only stretching strain ε_0 exists, thus

$$\varepsilon_0 = -\varepsilon_{\rm m}\frac{M_{\rm f}}{M_{\rm s}}\frac{h_{\rm f}}{h_{\rm s}}\left(1+\frac{M_{\rm f}}{M_{\rm s}}\frac{h_{\rm f}}{h_{\rm s}}\right)^{-1}. \tag{22}$$

If the thickness of the film relative to the substrate is very thin, equation (16) is expanded to the first order in $h_{\rm f}/h_{\rm s}$, one obtains

$$\frac{k}{k_{\rm st}} = 1+\left(1-4\frac{M_{\rm f}}{M_{\rm s}}\right)\frac{h_{\rm f}}{h_{\rm s}}, \tag{23}$$

which shows that the bending is influenced by the elastic rigidity of the system, but is almost not influenced by the electromechanical coupling coefficient of the film if the film is very thin. The thicker the film, the more obvious the influence of piezoelectric effect on the system bending is.

If an applied electric potential difference is adjusted so that the curvature $k = 0$ (i.e., there is no bending, the corresponding voltage $V_{\rm C}$ is called the critical voltage), this shows $\varepsilon_{\rm m} = \varepsilon_{\rm m}^{\rm c}+\varepsilon_{\rm m}^{\rm t}+d_{31}E_{\rm eff} = 0$, then

$$d_{31} = -\frac{\varepsilon_{\rm m}^{\rm c}+\varepsilon_{\rm m}^{\rm t}}{E_{\rm eff}} = -\frac{\varepsilon_{\rm m}^{\rm c}+\varepsilon_{\rm m}^{\rm t}}{V_{\rm C}}h_{\rm f}, \tag{24}$$

which is consistent with the result by McCartney *et al.*,[28] but the derivation procedure is simpler. In other words, the transverse piezoelectric constant d_{31} can be estimated by monitoring the deformation of the bilayer experimentally.

5. Conclusions

We report an analytical model to represent the deformation result from a voltage applied across a piezoelectric film bonded to an elastic substrate. The model, which accounts for the relation among the bending effect, the piezoelectric effect, the elastic rigidity, the film thickness and the mismatch, is shown to provide a method of estimating a bending curvature, or a transverse piezoelectric constant. Meanwhile, the influence of electromechanical coupling coefficient on the curvature is discussed.

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