Analytical Modeling of the Stress-Strain Distribution in a Multilayer Structure with Applied Bending

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November 8, 2010

Abstract

It is presented *FleSS*: a Matlab based Graphical User Interface that provides the tools for a rapid and easy modeling and monitoring of the elastic deformation of multilayer structures due to residual stresses and applied external bending. Several geometric models have been considered and made available.

Keywords: Stress-strain modeling, thin-films, multilayered devices, bending, flexible electronics.

1 Introduction

There is growing interest in flexible electronics, including foldable displays, sensor skins and flexible sensors for medical applications. Functionality and reliability of multilayered systems are strongly influenced by residual stresses. If over a certain limit, these stresses may lead to failure of the device. Bending is one of the main movements in flexible electronics and cracks caused by it are determinant to the malfunction of flexible structures. It is then obvious that the stresses arising during fabrication and during the use under bending of flexible applications must be taken into account in the designing step. Stoney was the first to formulate a simple analytical relationship between the stress in a thin film and the curvature of the substrate. Several authors used this approximation to derive the so called classical model, based on the assumption that the film thickness is much smaller than the substrate [3] [1]. When the film thickness cannot be ignored, higher order terms of film thickness must be included in the analytical solution. Analytical models for different geometries of elastic de-

formation in multilayer structures due to residual stresses and with or without applied bending have already been derived [3] [1][2][4][5]. In this work it is presented the inclusion of all geometries and different origins of bending (thermal strain versus built-in strain versus applied bending) into a single closed-form generalized solution.

1.1 Types of Bending

The bending of devices can happen by a combination of two distinct processes: Applied Bending and Natural Bending. If a bending moment is imposed to a body initially at rest, it will bend until reaching equilibrium with the applied moment. When the applied moment forces the body to bend downwards, the top surface is tensile (positive elastic strain) while the bottom one is compressive, and vice-versa for an opposite applied moment. This means it exists a surface where the strain is null. This surface is called the Bending Axis (h_b). At this location, the surface dimension remains constant throughout the bending action. A device is said to bend with positive curvature, if it bends downward and with negative curvature if otherwise. The elastic strain (ε) profile throughout the body's thickness (y) is:

$$\varepsilon = \frac{y - h_b}{R} \tag{1}$$

where R is the radius of curvature of the structure [3]. A body can suffer stress-free deformations, due to several phenomena: thermal expansion of the materials along a temperature change; epitaxial incompatibility between layers; humidity absorption, etc.. Because these deformation prevail without any applied stress field, the strain associated with it is called residual strain and is denoted by ε^0. In this work, for each layer i, two types of residual strains are considered: the thermal strain (ε^{th}) and the built-in strain (ε^{Btin}). The first represents the variational deformation each layer feels going from its own deposition temperature (T_i) to room temperature (T_{room}):

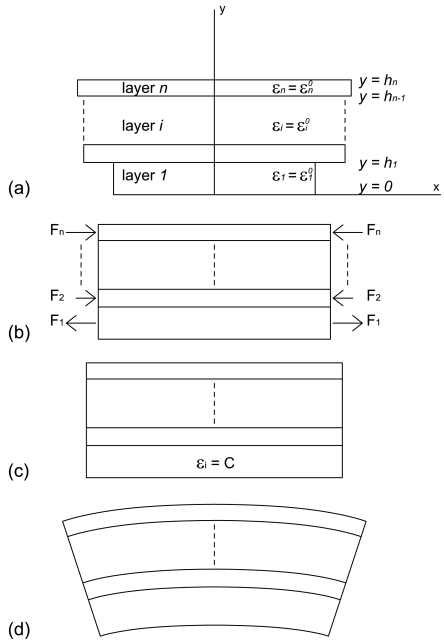
$$\varepsilon_i^{th} = \alpha_i \left(T_{room} - T_i\right) \tag{2}$$

where α_i is the layer's coefficient of thermal expansion. The second one represents all tunned-in initial strains (e.g. growth strains). All residual strains that are not the dimensioned thermal strain can be included in this term:

$$\varepsilon_i^0 = \varepsilon_i^{th} + \varepsilon_i^{Btin} \tag{3}$$

When a device is composed by multiple layers, with different mechanical properties and different residual strains, the elastic accommodation of these differences causes the structure to planarly relax (or contract) and bend, in a process called *Natural Bending*. In fig.1 is presented a scheme of this phenomenon for a 2D conceptual structure, composed of n layers [2]: each layer i possesses different initial residual strains ε_i^0 (a); to accommodate this mismatch, it is necessary to apply external forces on the edges of the layers to constrain them to an equilibrium length while the layers are being bonded together (b); as soon as these external constraints

are released, the layers will tend to oppose it, planarly relaxing (or contracting) until reaching zero net force, with a common strain, constant throughout the device thickness (C - Uniform Strain) (c) and bending until reaching zero net momentum



(d).

Figure 1: Natural bending scheme

The total strain profile of the structure is then:

$$\varepsilon = \frac{y - hb}{R} + C \tag{4}$$

In this 2D configuration, the normal stresses in each layer are related to strains by:

$$\sigma = Y_i \left(\varepsilon - \varepsilon_i^0\right) \tag{5}$$

where Y_i is the Young modulus of layer i, which represents the proportionality constant between the elastic strain and stress in this configuration.

Essentially a device can bend in two different ways: with biaxial geometry - which considers that the device bends in both orthogonal directions, forming a spherical shape or with uniaxial geometry - which considers that the device bends in just one direction, rolling. The first, normally occurs when both length and width of the structure are comparable, the latter when one of the planar dimensions of the layers (length or width) is much bigger than the other, or when there is an applied constraint or residual strain anisotropy.

1.2 Models

The 2D conceptual scheme can be generalized for a 3D problem. Different geometries where considered and summarized into a single closed-form solution, which describes the stress and strain distribution, in an longitudinal section, relative to the (one of the) bending axis. The models that can be retrieved from this generalization are called 'flexible models'. Using the assumption that a substrate is much thicker and stiff than the thin films placed on top of it, the 'classical model' was derived from the biaxial flexible approach. All models were implemented in FleSS. Next, it is presented the generalized flexible model. Consider a device operating at room temperature, with each layer i having the following constant physical properties: Y_i - Young modulus, ν_i - Poisson ratio, α_i - coefficient of thermal expansion, D_i - Thickness, T_i - Deposition temperature; ε_i^{Btin} - Built-in Strain. For a device composed of n layers, $i = 1, ..., n$, aligning its (one of) bending axis(es) with xx and the thickness with yy, the generalized flexible model of its

stress-strain distribution is (6):

$$\begin{cases} \varepsilon_{xi}(y) = \dfrac{y - h_b}{R} + C \\ \\ \sigma_{xi}(y) = \bar{Y}_i \left[\dfrac{y - h_b}{R} + C + \nu_i A - \eta_i \varepsilon_i^0 \right] \\ h_b = \dfrac{\sum_{i=1}^{n} \bar{Y}_i D_i h_{mi}}{\sum_{i=1}^{n} \bar{Y}_i D_i} \\ C = \dfrac{\sum_{i=1}^{n} \bar{Y}_i D_i \left[\eta_i \varepsilon_i^0 - \nu_i A \right]}{\sum_{i=1}^{n} \bar{Y}_i D_i} \\ \dfrac{1}{R} = \dfrac{\sum_{i=1}^{n} \bar{Y}_i D_i \left[h_{mi} - h_b \right] \left(\eta_i \varepsilon_i^0 - C - \nu_i A \right)}{\sum_{i=1}^{n} \bar{Y}_i D_i \left[h_i^2 + \dfrac{D_i^2}{3} - h_i D_i + h_b \left(h_b - 2h_{mi} \right) \right]} \end{cases} \tag{6}$$

where h_i is the layer's height coordinate and h_{mi} is the layer's mid point. For every layer i: $h_{i-1} \leqslant y \leqslant h_{i-1}$. A, $\bar{Y}_i$ and η_i are parameters that depend on the geometry at study. A is the Axial constant strain of the structures; $\bar{Y}_i$ is the Elastic modulus of layer i and η_i is the transformed Possion ratio of layer i. For the user to determine which geometry better represents the real structure at study, five models were implemented:

1. **Classical biaxial model**: based on the approximation 'thin-films on thick substrate' with biaxial geometry [3] [1];

2. **Flexible biaxial model**: follows (6) with $\bar{Y}_i = \frac{Y_i}{1-\nu_i}$, $\eta_i = 1$, $A = 0$ [3] [1];

3. **Flexible model with *plane-stress* condition**: model with uniaxial geometry, which considers the width of the device so much smaller than the length that no stress develops in the width direction. Follows (6) with: $\bar{Y}_i = Y_i$, $\eta_i = 1$, $A = 0$ [2];

4. **Flexible model with *plane-strain* condition**: model with uniaxial geometry, which considers the width much bigger than the length so that the strain in the width direction is considered null. Follows (6) with: $\bar{Y}_i = \frac{Y_i}{1-\nu_i^2}$, $\eta_i = 1 + \nu_i$, $A = 0$ [4];

5. **Flexible model with *generalized plane-strain* condition**: correction to the previous model, where the strain in the width direction is not considered null but a constant value that represents an axial strain compensation of the deformation in the bending direction. Follows (6) with: $\bar{Y}_i = \frac{Y_i}{1-\nu_i^2}$, $\eta_i = 1 + \nu_i$, $A = \text{constant} \neq 0$ [5].

It is relevant to state that these models are valid only away from the edges of the structures and apply only to elastic deformations.

2 Software

FleSS (Flexible StressStrain) was implemented using MATLAB2008b. With this tool the user can create multilayer devices and obtain the stress or strain distributions along the thickness of the structure, either due to the natural bending caused by its fabrication or to an imposed bending. These

distributions are of the outmost importance in the design of flexible thin-films devices, because they allow the determination of the best location for the critical components of a device (e.g. sensors active parts), ideally at points of lowest stress. It is composed of two main Graphics User Interfaces (GUI): 'Inputs Interface' and 'Graphics Interface'.

2.1 Inputs Interface

This GUI is composed of four main parts where the user can visualize, create, edit and delete materials and devices and where he can choose which models and devices to plot . In the panel 'Library of Materials' the mechanical properties (Young modulus, coefficient of thermal expansion, Poisson ratio) of several materials used in MEMS technology are listed. They can be edited by the user and new materials can be added. In the panel 'Library of Devices' the user can create the desired multilayer structure (device), by selecting the materials from the 'Library of Materials' and defining the thickness, deposition temperature, built-in strain and possible annealing temperature of each layer. Once a device is selected from the 'Library of Devices' panel, the position of the bending axis, the radius of curvature, the uniform and the axial strains values calculated using each model are instantaneously displayed in the 'Library of Models' panel. It is also possible to analyze whether the classical model is accurate enough or if one of the four flexible models have to be used (this method is denoted as ClvsFl). Finally, the panel 'Plots' allows the user to choose which model to use when plotting a device. Several models and devices can be plotted simultaneously. An example of *ClvsFl: 'Classical versus Flexible' analysis*, where a curvature comparison between classical and flexible models is generated, is presented in fig.2.

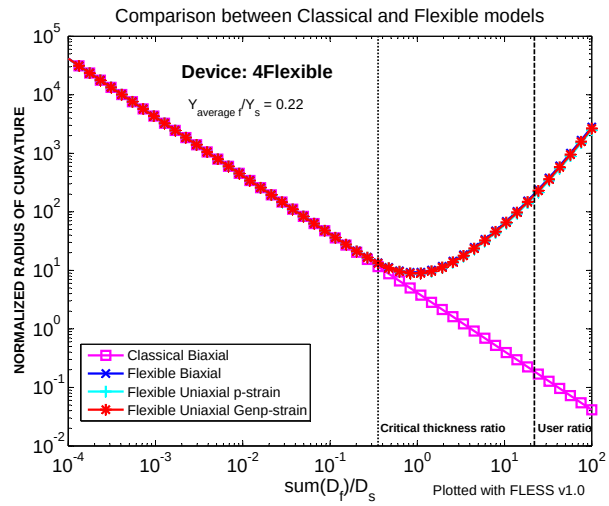


Figure 2: Example of 'ClvsFl' analysis

To correctly perform this analysis on devices with several thin films, their thicknesses are summed and all the other relevant quantities are weighted averaged (with the thickness). The difference between classical and flexible models average is calculated, and a 'critical thickness ratio' (10% deviation between models) is obtained. Above this ratio the classical model is not considered as accurate anymore and a flexible approach is mandatory.

2.2 Graphics Interface

This GUI is composed of three main parts. The main panel displays the stress or strain distribution throughout the thickness, for each devices and models chosen. The user is able to impose curva-

tures and can monitorize the stress-strains distribution of the layers while the structure is being fabricated. All graphs can be saved to editable plots or CSV (comma separated values) files.

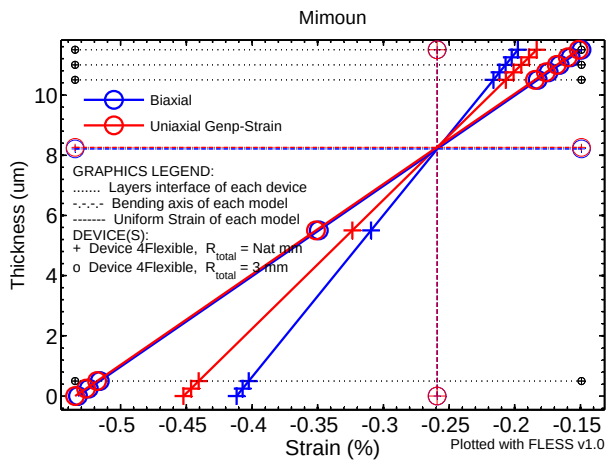


Figure 3: Example of the strain distribution for 2 different curvatures, and 2 different models

In the panel Final Total Curvature a radius of curvature can be applied to the devices at study individually, changing their stress-strain distributions. The values can be either positive (bending downwards); negative (bending upwards); infinite (if the user wants to flatten the device); or natural (if the user wishes to study the natural bending radius), (cf.fig.3). The program applies a spherical curvature if the chosen model is biaxial and a cylindrical curvature if the model is uniaxial, matching the geometry of the natural bending.

The user can further analyze a device in the panel 'Process of Fabrication'. Three different operations are possible: i) The 'print to command window' button displays the evolution of the different parameters, such as the position of the bending axis, the radius of curvature, the stress/strain distribution throughout all the fabrication process steps. ii) It is also possible to obtain the stress-strain distribution of a specific *subdevice-j* (structure composed of the first j layers of the total device) at three possible temperatures: room temperature, (optional) annealing temperature and deposition temperature of the next layer $(j+1)$ (cf.fig.4). iii) The user can finally choose to visualize the stress-strain distribution of a specific layer throughout all the fabrication steps (cf.fig.5).

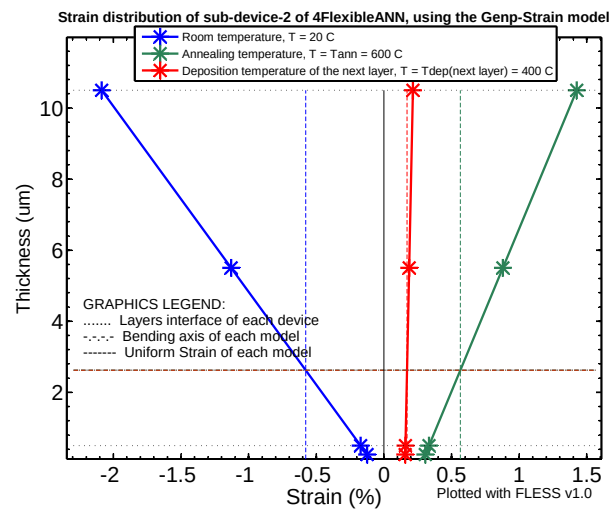


Figure 4: Example of the temperatures states

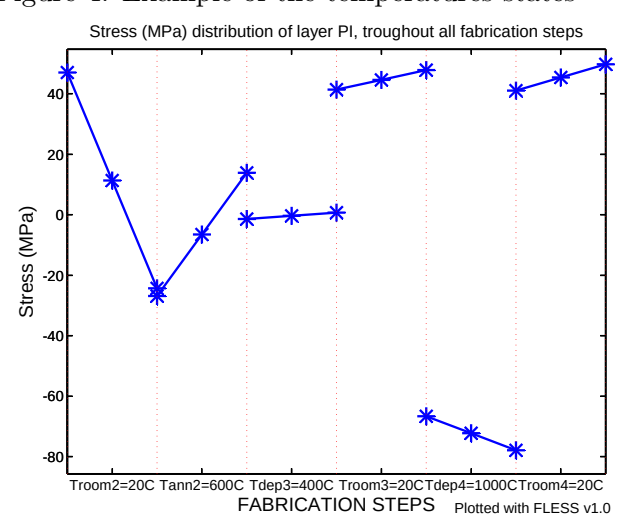


Figure 5: Example of a layer's processline

3 Validation

The implementation of the models in FleSS was validated by modeling two structures already described in the literature. The first one is a double-heterojunction laser diode structure, where the plane-stress condition is compared with the 'thin films on thick substrate' approximation [2]. The second device is a self-positioning hinged mirror structure, where the plane-strain and generalized plane-strain conditions where compared to finite element simulation [5]. The exact same results as those already published where found.

4 Future Work

The ultimate goal is to have a model that can predict when the layers crack. The next step for this project is to apply crack theory to the implemented models, in order to obtain a complete description of the stress-strain distribution variation with residual stresses and applied bending, until the active layers crack, and the devices become unusable.

5 Conclusion

FleSS is a very useful tool to provide information about the stress/strain distribution of multilayer devices during their fabrication and with possibility of applying an external bending. FleSS allows the user to compare different devices; to apply different external bendings to the same device and/or compare different bending geometries in order to understand which one represents more accurately the real device. Ultimately, this software appears to be of great interest during the designing step of a device. The user can indeed determine the maximum stress/strain values each and every layer of the device will go through. Also, studying the effect of different Built-in strains in different layers is of great help in the optimization of a device's design.

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