CHARACTERIZATION OF THE COMPLETE STRESS STATE IN THIN-FILM CMOS LAYERED MATERIALS

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ABSTRACT

We present a new methodology for characterizing the complete stress state (effective mean compressive and gradient stresses) in CMOS layered materials that also assesses non-ideality of clamped boundaries. The approach uses a closed-form solution for the nonlinear post-buckling of micromachined beams also including non-ideal boundaries, and experimental measurements of deflected beams. For the CMOS materials examined here, the accuracy was $\pm 2\text{MPa}$ for mean compressive stress and $\pm 3\text{MPa}/\mu\text{m}$ for gradients, limited by measurement errors and uncertainty on material properties. Boundary non-ideality is found to be $\sim 90\%$ of perfectly clamped for the CMOS-released structures and has a significant effect on the extracted stresses such that it must be modeled appropriately. The method is transferrable from test structures to device level, and can be used to measure packaging stress as well.

INTRODUCTION

Characterization of thin-film layered materials is critical to the development of many MEMS devices. Residual stresses from production determine both the final shape and the performance of microdevices, and should therefore be accurately assessed if possible. Mean residual stress determination is especially relevant for many microbridge-type devices, as large compressive stresses may cause the device to buckle (Figure 1a) and, in some instances, to fail. On the other hand, stress gradients become particularly acute as the films become thinner [1], which may lead to (undesired) large out-of-plane deformation (Figure 1b). To date, a variety of approaches to characterize the stress state of thin materials have been developed, most of which are based on the information obtainable by studying the post-release deformation (e.g., bending, buckling, twisting) of simple micromechanical components. As an example, mean compressive stress is typically determined using arrays of clamped-clamped beams of different lengths [2], whereas tensile stress is extracted using more complicated geometries such as crossbar rings and "T"- or "H"-like structures or on wafer/cantilever beam measurements utilizing the well-known Stoney's relation [1, 3]. Curvature of released microcantilevers is instead measured to estimate the gradient stress in thin-films, as first demonstrated by Chu and Mehregany [4]. Although well-established, these approaches to material characterization have two major limitations. First, their accuracy is directly proportional to their cost. This is especially true for mean compressive stress, where more accurate estimates require a larger number of different test structures. Second, they oversimplify the test-structure boundary conditions by assuming them to be ideal (e.g., perfectly clamped in the case of buckled beams for mean compressive stress determination [1]). A first attempt to resolve these issues was performed by Fang and Wickert in 1995. In their paper [6], the authors discuss the effect of boundary condition on the deformation of single material micromachined cantilevers, and propose a new way of estimating residual stresses by measuring cantilever curvature and boundary rotation. Based on a numerically-derived description of the deformation of micromachined structures, this approach requires the field to be made of the same material combination as the

cantilevers, and therefore cannot be generalized to the analysis of general test structures (or, more broadly, of actual devices). Furthermore, the extant techniques cannot provide information regarding the effect of packaging on the final stress state of the device, as packaging does not affect fully released cantilevered structures.

Figure 1: Post-release out-of-plane deformation of (a) doubly-clamped microbridge and (b) microcantilever

Here we introduce a new approach to the characterization of the complete stress state in multi-layered thin-film materials which addresses the issues above, and demonstrate it for CMOS layered films. The technique is based on a closed-form solution of the buckling problem of micromachined beams including non-ideal boundaries (see detail in Figure 1a), and allows for extraction of the effective mean and gradient stresses using as few as two different sets of test structures (namely, one set of cantilevers, and one set of doubly-clamped beams per layered material combination). Non-ideality of the boundary is considered by introducing a flexible boundary with spring constant κ_T , determined experimentally concomitant with the residual stresses. In the CMOS examples herein, the method provides stress estimates accurate up to $\pm 2\text{MPa}$ for mean stresses and $\pm 3\text{MPa}$ for gradients, significantly better than what standard critical-length buckling approaches can provide. The accuracy is largely due to proper quantification of the boundary-condition, a main determinant of extracted stress values. For the structures analyzed here, the results point to non-ideal boundaries having approximately 10% less fixity than the perfectly-clamped boundary. The accuracy in the results is limited by displacement profile error (non-contact profilometry) and uncertainty in material properties of the films comprising the layers. The approach is

applicable to both micromachining and CMOS processing, and can be extended to packaging and processing stress characterization at a device level.

THEORY

In our analytical method we model a microfabricated layered beam as a homogenized structure characterized by effective weighted-properties in bending and extension [7], and constrained at both ends by torsional springs allowing a range of boundary conditions from simply-supported to clamped (Figure 2). The layered beam has length L , width b , and thickness h . The torsional spring constant (κ_T) represents the boundary bending stiffness, and is determined experimentally along with the mean and gradient stresses. The in-plane boundary condition is assumed to be completely fixed (no in-plane sliding). The released layered beam structure is subjected to residual stresses ($\sigma_{\text{intrinsic}} = \sigma_{\text{mean}} + \sigma_{\text{gradient}}$) which may cause bending and buckling.

Figure 2: Schematic representation of a micromachined beam subjected to residual stresses (σ_{mean} , σ_{gradient}), with non-ideally clamped boundary modeled by torsional springs (κ_T). Deflections w do not require buckling.

Using a linear through-thickness variation to approximate the distribution of stresses gives rise to an effective σ_{gradient} [1]. Linear-elastic Euler-Bernoulli beam-column theory is utilized to obtain the governing equations for the system of Figure 2:

$$\frac{EI}{L^4} \frac{d^4 w}{dx^4} + \frac{EA}{2L} \int_0^L \left(\frac{dw}{dx} \right)^2 dx \frac{d^2 w}{dx^2} = -P_0 \quad (1)$$

$$M = M_0 + EI \frac{d^2 w}{dx^2} \quad (2)$$

where w is the vertical (z -axis) displacement along the beam, A is the cross-sectional area, E is the layered beam effective bending modulus, EA is the layered beam effective axial modulus, P is the thrust developed inside the structure, and $P_0 (= \sigma_{\text{mean}} A)$ and $M_0 (= \sigma_{\text{gradient}} A h^2 / 6)$ are the thrust and the moment due to residual stresses, where A is the total cross-sectional area of the layered beam, and h is the total beam thickness. The boundary conditions are:

$$w(0) = 0 \quad , \quad M(0) = +\kappa_T w' \quad (3)$$

$$w(L) = 0 \quad , \quad M(L) = -\kappa_T w' \quad (4)$$

where the effect of boundary flexibility becomes apparent. Using a sinusoidal post-buckling deformation mode for the structure:

$$w(x) = C_1 \sin(\lambda x) + C_2 \cos(\lambda x) + C_3 \frac{x}{L} + C_4 \quad (5)$$

with C_1 , C_2 , C_3 , and C_4 being constants, the following formula for the critical buckling load (P_{cr}) of doubly-hinged columns can be obtained [8]:

$$P_{\text{cr}} = \frac{\pi^2 EI}{L^2} \left(\frac{0.4 + \varphi}{0.2 + \varphi} \right)^2 = P_{\text{Euler}} \left(\frac{0.4 + \varphi}{0.2 + \varphi} \right)^2 \quad , \quad \varphi = \frac{EI}{\kappa_T L} \quad (6)$$

Equation 6 is plotted in Figure 3 for a typical CMOS polysilicon beam ($400\mu\text{m} \times 40\mu\text{m} \times 3.3\mu\text{m}$), where we show the dependence of the non-dimensional critical load ($\bar{P}_{\text{cr}} = P_{\text{cr}}/P_{\text{Euler}}$) on the boundary stiffness (κ_T). The non-dimensional critical load ranges from 1 for simply-supported beams, to 4 for clamped structures. Importantly, the results show the presence of two different boundary flexibility values ($\kappa_{T,ss}$ and $\kappa_{T,clamped}$) below/above which the microbridge can be effectively considered simply-supported/clamped (no variation in buckling load). Whereas most structural models assume $\kappa_{T,ss}=0$ and $\kappa_{T,clamped}=\infty$, the results of Figure 3 show the existence of large ranges of finite κ_T where, from a buckling load perspective, the beam response behaves like one of the ideal boundary conditions, with an intermediate range that is between these behaviors. $\kappa_{T,ss}$ and $\kappa_{T,clamped}$ depend on the beam's material and geometrical properties, and their quantification is fundamental for proper characterization of microfabricated structures.

Figure 3: Effect of boundary flexibility on the critical buckling load of a doubly-hinged polysilicon beam ($400\mu\text{m} \times 40\mu\text{m} \times 3.3\mu\text{m}$, $E=129\text{ GPa}$)

Defining the non-dimensional boundary flexibility (K)

$$\begin{cases} K = 0 & , \quad \kappa_T < \kappa_{T,ss} \\ K = \kappa_T / \kappa_{T,clamped} & , \quad \kappa_{T,ss} \leq \kappa_T \leq \kappa_{T,clamped} \\ K = 1 & , \quad \kappa_T > \kappa_{T,clamped} \end{cases} \quad (7)$$

where $K=0$ and $K=1$ respectively indicate simply-supported and clamped boundaries, and noticing that:

$$\frac{P}{P_{\text{Euler}}} = \left(\frac{\lambda L}{\pi} \right)^2 \quad (8)$$

Eqs. 3-4 can be re-written into a non-dimensional form that, given

the intrinsic stresses (σ_{mean} , σ_{grad}) and the boundary condition (κ_T), depend on the deformation wavelength (λ) only. The resulting system of non-dimensional equations can be solved using any numerical method (e.g., Newton-Raphson), providing a full description of the post-buckling of micromachined beams. For a layered beam with known geometry and effective axial (EA) and bending ($\bar{EI}$) stiffness, the solution can be expressed as:

$$w(x) = f(x, \sigma_{\text{mean}}, \sigma_{\text{gradient}}, K) \quad (9)$$

where we note that the post-buckling deflection along the beam's axis (x) is a function of σ_{mean} , σ_{grad} and K only. Eq. 9 is plotted in Figure 4, where we show the effect of boundary flexibility and mean stress on the stress-center displacement ($w_c = w(L/2)$) relation of a CMOS polysilicon beam subjected to a +37 MPa/ μm gradient stress. Here, the effect of boundary condition (K) on the beam's structural response is apparent: microbridges with flexible boundaries buckle at lower loads (lower σ_{mean}) and deform more (larger center deflection for the same mean stress) than more effectively clamped structures. Also, the effect of gradient stresses (σ_{gradient}) on center deflection vanishes as K reaches unity, which can be noticed from the reduction in "0-load" displacement (i.e., the center deflection associated with $\sigma_{\text{mean}}=0$) as K increases.

METHOD FOR EXTRACTING STRESSES AND BOUNDARY FLEXIBILITY

When combined with experimental data, the analytical model presented in the previous section can be used to characterize the intrinsic stress state and the effective boundary condition of microbridges. Taking the inverse of Eq. 9, we can now express intrinsic stresses and boundary flexibility as a function of experimental measurements of w_c :

$$(\sigma_{\text{mean}}, \sigma_{\text{gradient}}, K) = f^{-1}(w_{c,\text{experimental}}) \quad (10)$$

Equation 10 is key in the analytical-experimental method, as it allows one to characterize microstructures by using experimental data on center deflection of buckled beams. If three or more w_c measurements are available, a least squares approach can be applied using Eq. 10 to find the intrinsic stresses and boundary condition that correspond to the experimentally measured deflections. The minimum number of measurements required is three (one per unknown: σ_{mean} , σ_{grad} and K), with higher accuracies associated with larger sample populations. Distinct from critical buckling-length approaches, our technique does not require the beams to be of different lengths, thus significantly reducing costs and characterization complexity. The method's accuracy depends on the total number of w_c measurements, independent of whether they are associated with beams of different/same length. The only requirement on test structures is that they should allow for some deformation to occur at release, thus making slender designs (i.e., $L \gg b, h$) preferable. The method relies on knowledge of material and geometrical properties for the structures, and on accurately measuring the post-buckled deformation of microstructures.

Given the fast decay of gradient effects as boundary stiffness increases (see Figure 4), and the relative ease of characterizing gradient stresses using cantilevered test structures [4], an alternative characterization approach exists in which cantilever curvature measurements are used to extract gradient stresses ($\sigma_{\text{gradient,experimental}}$, Figure 1b), while mean stresses and boundary condition are characterized using a reduced version of the analytical model:

$$(\sigma_{\text{mean}}, K) = f^{-1}(w_{c,\text{experimental}}, \sigma_{\text{gradient,experimental}}) \quad (11)$$

This alternative approach requires two sets of test structures (one set of clamped microbridges and one set of cantilevers), but it does overcome the possible numerical difficulties associated with characterizing structures with very stiff boundaries. Expecting our structures to be characterized by a 'close-to-clamped' boundary condition, both approaches were utilized in this work. An application example of Eq. 11 is presented in Figure 4 for a CMOS polysilicon beam. Here analytical results, deflection measurements ($w_{c,\text{experimental}}$), and gradient stress measurements ($\sigma_{\text{gradient,experimental}}$) are combined to obtain the σ_{mean} - K relation that, using a least-squares approach, provides the mean stress and boundary condition for the structure (Table 1).

Figure 4: Effect of boundary condition on the stress-displacement relation of CMOS polysilicon beams

RESULTS

Four sets of CMOS layered structures were designed and fabricated using standard CMOS techniques, each set having a different material composition (Table 1). All sets consisted of three groups (200-, 400-, and 600 μm -long) of twenty clamped beams, and one group of twenty 300 μm -long cantilevers. The material properties for each of four layered films (A, B, C, D in Table 1) comprising the structures were provided by the foundry, and resulted in the effective moduli of Table 1. Effective bending stiffness ($\bar{EI}$) for the layered structure was computed from the layer thickness (Table 1). All structures were packaged in house, and successively measured using non-contact profilometry (Zygo white-light interferometer, Figure 5). The center deflection of each clamped beam and the curvature of each cantilever were recorded.

Cantilever curvature measurements were used for gradient stress extraction [4], showing that three out of four material combinations were characterized by positive gradients (Table 1). The extracted gradients were then utilized as input in a numerical implementation of Eq. 11, whose solution was computed using a least-squares approach. The results for the CMOS materials tested show mean stresses ranging between 15 and 105 MPa, thus demonstrating the method's capability to characterize structures subjected to both large and small compressive stresses. This is in contrast with traditional critical length methods that encounter difficulties in quantifying small compressive stresses due to their inability to distinguish between mean stress and gradient stress effects.

5-a) Intensity map

5-b) Surface map

5-c) Surface profile
(section C-C in Figure 5-b)

Figure 5: Profilometric images of an array of 400 μm long buckled CMOS beams (beam A: PolySi/dielectric composite; beam B: dielectric composite)

The extracted values show a standard deviation of $\pm 3\text{MPa}$ for gradients and $\pm 2\text{MPa}$ for mean stresses (Table 1), significantly lower than critical length approaches can provide using the same number of test structures. Critical length and analytical approaches are compared in Table 2 for CMOS polysilicon beams, showing a 41MPa reduction in standard deviation when analytical approaches are utilized. The higher accuracy is largely due to proper quantification of the boundary condition, a main determinant of extracted stress values. Given the non-linear dependence of buckling load on edge flexibility (Figure 3), boundary estimation is paramount to ensure accurate stress extraction. For the CMOS layered structures analyzed here, the results point to a non-perfectly clamped boundary with $K=0.9$, i.e. 90% as stiff in bending as a perfectly-clamped boundary.

Finally, Table 2 contains a comparison between the fully-analytical (Eq. 10) and the semi-analytical (Eq. 11) methods for the same CMOS polysilicon beams. The results show that for the structures analyzed here, which are characterized by relatively stiff boundaries ($K \sim 0.9$), the semi-analytical model provides more accurate estimates. This finding agrees with what we discussed in the previous section, which pointed to the numerical complexity associated with solving Eq. 10 when characterizing structures with very stiff boundaries.

Table 1: Characterization of thin-film CMOS layered materials

Beam composition	Effective Young's modulus ¹ [GPa]	Effective thickness ¹ [μm]	Effective mean (compressive) stress [MPa]	Effective gradient stress [MPa/ μm]	Effective boundary condition [-]
A: PolySi/Dielectric Composite	129	2.9	105 ± 2.1	37 ± 2.9	0.89 ± 0.01
B: Dielectric Composite/ILD/Oxide	111	2.86	90.35 ± 2.3	42 ± 3.1	0.9 ± 0.01
C: Al/Poly/Dielectric Composite	132	2.92	37.1 ± 1.5	25.9 ± 2.8	0.91 ± 0.01
D: Al/Dielectric Composite	113	2.91	15 ± 1.8	-2.7 ± 2.1	0.9 ± 0.01

¹ With these effective Young's modulus and thickness, $\overline{EA}$ and $\overline{EI}$ may be calculated. $\overline{EA}$ and $\overline{EI}$ are derived from actual layer moduli and thicknesses via equivalent weighted properties [7].

Table 2: Characterization of thin-film CMOS polysilicon beams ($L=200, 400, 600\mu\text{m}$ x $w=40\mu\text{m}$ x $h=3.3\mu\text{m}$, $E=129\text{ GPa}$) using critical length and analytical approaches

Extraction method	Effective mean (compressive) stress [MPa]	Effective gradient stress [MPa/ μm]	Effective boundary condition [-]
Critical length ($P_{cr}=4EI\pi^2/L_{crit}^2$)	71.5 ± 43.5	37 ± 2.9	1
Semi-analytical (Eq. 11)	105 ± 2.1	37 ± 2.9	0.89 ± 0.01
Fully-analytical (Eq. 10)	101 ± 11.2	45 ± 14	0.91 ± 0.04

CONCLUSIONS AND RECOMMENDATIONS

We present a new versatile approach to the characterization of stresses (compressive mean and gradient) in thin-film CMOS layered materials using analytical solutions. The method takes into account boundary non-ideality, and it provides significantly higher accuracy compared to critical length approaches. The technique is applicable to the estimation of both very large and very small mean compressive stresses, and it can be extended to packaging stress estimation as well. The method also ensures significant savings in characterization costs and complexity by requiring fewer structures than other traditional approaches. Future work includes packaging characterization, device design and performance prediction using the developed analytical methods.

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