Stoney Equation limits for samples deformed as a cylindrical surface

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In a previous work, Pureza et al [1] proposed an approach for the evaluation of the stress in thin films deposited on substrates much thicker than itself. This problem is a relevant issue for several areas of science [2-9], being the theme of a recent review [10] in commemoration of 100 years of the first description of the problem, proposed by Stoney in 1909 [11] who considered the sample as an one-dimensional plate. The Stoney equation indicates a linear relationship between the film stress (σ) and its bending, being straightforwardly modified for two-dimensional systems with small deformation by including the substrate Poisson ratio (ν_s) [12], as seen in equation (1).

$$\sigma = \frac{E_s \cdot t_s^2}{6 \cdot (1-\nu_s)\, t_f} K \qquad (1)$$

where E_s is the substrate Young modulus, t_s e t_f are the substrate and film thickness, respectively, and K is the film curvature. It has become the standard expression for the analysis of this problem with reasonable agreement with experimental results. However, Stoney equation does not take into account relevant aspects like the non-uniformity of the stresses as well as the tri-dimensionality and the boundary conditions of the samples. Such aspects gave rise to semi-empirical modifications, with little experimental agreement [12-14] and more elaborated models (see e.g. [15] and references therein, [1,16-18]), as well as finite-element simulations that present local dependence to stress distribution [3,19].

Finot et al [3] using a finite element analysis identified three distinct regimes for the evolution of curvature, which are dependent on the quantity $A = \sigma\, t_f\, l_s^2\, t_s^{-3}$, where l_s is the characteristic size of the sample: (I) for lower values of A, the deformation has a spherical shape and Stoney equation is satisfied considering 10% of error as acceptable; (II) as the parameter A increases, deformation maintains the spherical shape but Stoney equation looses validity and (III) for even larger values of A, Stoney equation is no longer valid and the sample undergoes two abrupt changes, initially to an ellipsoidal shape and finally to a cylindrical shape.

In the previous work [1], by means of the minimization of the deformation energy, we derived an expression for the thin film stress when the deformation maintains the spherical shape (regimes I and II in Finot et al [3]). We considered samples with thickness ratio t_f/t_s<<1, a assumption that allows the simplification of the deformation energy of the sample and consider that the substrate thickness change is a lower order term. So, the stress of the film is written in terms of the curvature K of the sample, as seen in equation (2)

$$\sigma_\theta = \sigma_\varphi = \frac{E_s}{6} \frac{1}{1-\nu_s - 2\nu_s^2} \frac{t_s^2}{t_f} K \qquad (2)$$

which is quite similar to Stoney's. Figure 1 shows agreement between this equation and Stoney's at regime I but, at regime II, results stay in between the finite element (obtained by Finot et al [3]) and the other formulations [12,14-16]. However, the analysis of the values obtained by Finot [3] using finite element simulation, see Figure 1, indicate a important change on the dependence between the curvature and the stress at regime III.

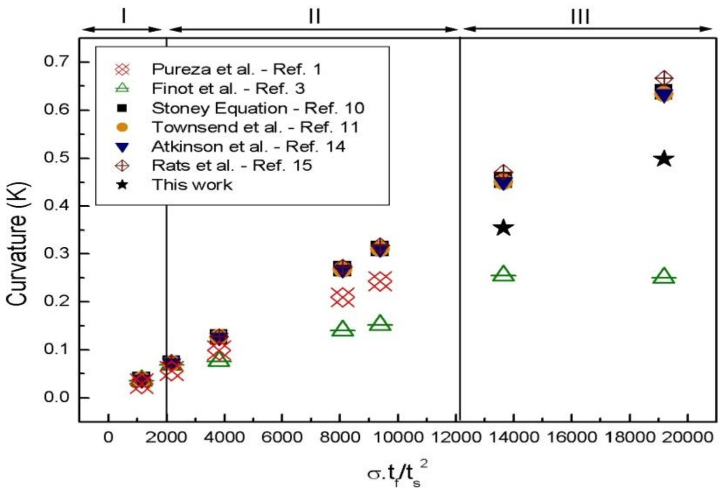

Figure 1: Sample curvature for different models.

This situation motivated us to apply the same approach to a thin film deposited on a thick substrate that is deformed as a cylindrical surface. In this situation, Figure 2 shows a three-dimensional sample that is subjected to linear and angular deformation components, given by equations (3),

$$\varepsilon_r^s = \frac{(a+b)-t_s}{t_s} = \tau - 1 \qquad \varepsilon_\theta^s(r) = \frac{(r-R)\Omega}{l_s}$$

$$\varepsilon_z^s(r) = -\frac{(r-R)\beta}{l_s} \qquad \gamma_{rz}^s(r) = \frac{\beta z}{S_s - \beta(r-R)}$$

$$\varepsilon_z^f(r) = \frac{(R-a)\beta - l_f}{l_f} \qquad \varepsilon_\theta^f(r) = \frac{(R-a)\Omega - l_f}{l_f} \qquad \gamma_{ij}^f = 0 \tag{3}$$

where $i,j = r,\ \theta,$ z. In the elastic regime, the film and substrate stress states are described by equations (4)

$$\sigma_i^\alpha = \frac{E_\alpha}{1-\nu_\alpha - 2\nu_\alpha^2}\left[(1-\nu_\alpha)\varepsilon_i^\alpha + \nu_\alpha(\varepsilon_j^\alpha + \varepsilon_k^\alpha)\right] \qquad \tau_{ij}^\alpha = \frac{E_\alpha}{2(1+\nu_\alpha)}\gamma_{ij}^\alpha \tag{4}$$

where $\alpha = s,f$. The deformation energy is simplified by the fact that the film is very thin and is given by the integrals in equation (5)

$$U = U_s + U_f = \frac{1}{2}\int(\sigma_i\varepsilon_i + \tau_{ij}\gamma_{ij})dz\cdot dr + t_f\frac{1}{2}\int(\sigma_i\varepsilon_i + \tau_{ij}\gamma_{ij})dz \tag{5}$$

with the limits:

$$z \in \left(-\frac{S_s}{2} + \frac{\beta}{2}(r-R), \frac{S_s}{2} - \frac{\beta}{2}(r-R)\right) \text{ and } r \in \left[R-a, R+b\right]$$

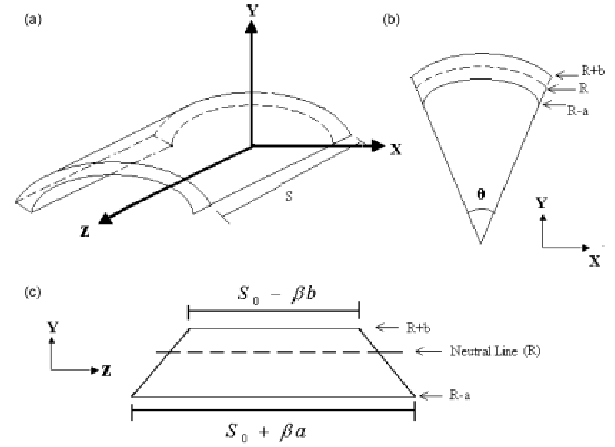

Figure 2: Projections of deformed sample as a cylindrical surface.

Finally, taking into account that changes in the substrate thickness ($t - t_s$) is a lower order term and making use of dimensionless variables, the energy (U) is written in the form of equations (6)

$$\overline{U} = D(1+\frac{\sigma\beta}{2}+\omega)\left\{(1-\nu_f)\left[(\delta l+\frac{\sigma}{2}\beta+\omega)^2+(\delta l+\frac{\sigma-2\Sigma}{2}\beta+\omega)^2\right]+2\nu_f(\delta l+\frac{\sigma}{2}\beta+\omega)(\delta l+\frac{\sigma-2\Sigma}{2}\beta+\omega)\right\}+$$
$$+\left(\frac{\beta^2}{4}+\frac{1-\nu_s}{1-2\nu_s}\Sigma^2\Omega^2\right)+\omega\left(\frac{\beta^2}{4}-2\frac{1-\nu_s}{1-2\nu_s}\Sigma\frac{\Omega^2}{\beta}+\frac{1-\nu_s}{1-2\nu_s}\Sigma^2\Omega^2+\frac{2\nu_s}{1-2\nu_s}\Sigma^2\Omega\right)+$$
$$+\left(\frac{\sigma^2}{12}+\frac{\omega^2}{\beta^2}\right)\left(\frac{1-\nu_s}{1-2\nu_s}\Omega^2-2\frac{1-\nu_s}{1-2\nu_s}\Sigma\Omega^2\beta^2+\frac{1-\nu_s}{1-2\nu_s}\beta^2-\frac{2\nu_s}{1-2\nu_s}\Omega\beta+\frac{2\nu_s}{1-2\nu_s}\Sigma\Omega\beta^2\right)+$$
$$+\left(\frac{\sigma^2\omega}{4}+\frac{\omega^3}{\beta^2}\right)\left(\frac{1-\nu_s}{1-2\nu_s}\Omega^2+\frac{1-\nu_s}{1-2\nu_s}\beta^2-\frac{2\nu_s}{1-2\nu_s}\Omega\beta\right)$$

(6)

$$D=\frac{E_f}{E_s}\frac{1+\nu_s}{1-\nu_f-2\nu_f^2}\frac{t_f}{t_s};\qquad \sigma=\frac{t_s}{l_s};\qquad \omega=2\beta\frac{a-b}{l_s};\qquad \delta l=\frac{l_f-l_s}{l_s}$$

The minimum energy configuration of the system (τ, ω e Ω)$_{min}$ is obtained by the following Lagrangean equations:

$$\frac{\partial\overline{U}}{\partial\beta}=\frac{\partial\overline{U}}{\partial\omega}=\frac{\partial\overline{U}}{\partial\Omega}=0 \qquad (7)$$

An exact solution of this system is extremely difficult to obtain. However, it is possible to obtain an approximate solution after the identification of dominant terms in each Lagrangean equation, showed as equation (8)

$$\Omega\cong\frac{\nu_s}{1-\nu_s}\left(\beta-\frac{12\omega^2}{\sigma^2\beta}\right);\qquad \omega\cong-(1-\nu_s)\left[\frac{\beta^2}{8}+D(\delta l+\sigma\beta)\right]\qquad \delta l=-\frac{1}{6D}\frac{\sigma\beta}{1-2\nu_s}$$

(8)

In such a way that the stress of the film is given by equation (9)

$$\sigma_\theta\cong\sigma_r\cong\frac{E_s}{6}\frac{1}{1-\nu_s-2\nu_s^2}\frac{t_s^2}{t_f}K\left(1+\frac{t_sK}{2}\right)^{-1} \qquad (9)$$

with no relevant difference to the results obtained in Ref. 1 (see equation 2). The linear relationship between the stress and the curvature of the sample, as proposed by Stoney, is preserved , but the ($2\nu_s$)-term plays a relevant role for substrates with $\nu_s \geq 0.25$, which includes most of metals and ceramic-like materials and the formula indicates a divergence of the stress when $\nu_s = 0.5$, a critical value corresponding to a truly incompressible (theoretical) material [20].

However, although the results stay in between the values obtained by other formulations and by finite element simulation (see Figure 1, for regime III), this approach was not able to identify a change in the behaviour of the curve at the transition from regime II to regime III. This situation could be better understood by analysing a sample that is deformed as a ellipsoidal surface, in such a way that the spherical and cylindrical surfaces would correspond to eccentricity limits of the figure and maybe the transitions would arise from the relationship with the stress of the film.

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A complete version of this manuscript was published in Applied Surface Science 256 (2010) 4408.