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Fracture Toughness Evaluation of a Cracked Au Thin Film by Applying a Finite Element Analysis and Bulge Test

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Abstract. This paper presents a finite element analysis of a pre-cracked freestanding gold thin film subjected to bulge test. These tests were conducted in order to determine the elasto-plastic properties and fracture toughness of the gold films. For the experimental tests, a pre-crack was introduced in the center of the film by focused ion beam (FIB) milling with a length of 10 μm and a width of 100nm. For the numerical fracture analysis, the problem was divided into two stages; the first stage was the development of the numerical model on the whole film without pre-crack (elasto-plastic analysis) and the second one was performed on a film portion that included the pre-crack (sub-modeling stage). Three different notches (rounded, sharp and V-sharp) were applied to calculate the stress intensity factor around the crack tip using path independent J-integral. The obtained results show that the load-deflection curves for non-cracked and pre-cracked film reproduced the experiments using the calculated elasto-plastic properties. This indicates that the proposed models presented a good correlation and robustness. Additionally, fracture toughness values were calculated between 0.288 and 0.303 $MPa \cdot m^{0.5}$ with J-integral values 1.037 J/m^2 (elastic) and 1.136 J/m^2 (elasto-plastic) which correspond with other calculations available in the literature.

Introduction

Fracture toughness is a material property able to avoid that a crack propagates unstable until the fracture, and it can be determined for bulk materials in plane strain conditions by standard methods [1]. However, for very thin materials, the fracture toughness is not determined by a standardized test since it depends on different factors. For instance, the geometric effects have influence over the mechanical properties of these. Fracture toughness can vary with the thickness as demonstrated by different studies [2-4]. Also, crack-tip stress distribution is assumed in plane stress (free surface) and therefore the normal stresses to the crack front direction dominate to the crack opening. Different experimental tests have been proposed to calculate the fracture toughness of thin films (mode I), such as nanoindentation or bulge testing among others [5-6]. Bulge test is a technique performed on freestanding thin films that are deformed by a pressure load. For a cracked thin film, a biaxial stress condition is achieved with the bulge test [4-5,7], this can be considered an advantage from the theoretical point of view. The interest in the determination of the fracture properties is due to the diversity of functional applications developed for micro-/nano devices.

In this paper, a numerical fracture analysis for freestanding thin films is presented. Finite element simulations were performed to reproduce the bulge tests applying a numerical approach defined by two stages; one on a film without a crack (whole model) and the another one in a film portion that includes a crack (sub-model). The methodology is applied on a gold thin film loaded on the level corresponding to fracture toughness.

Materials and Methods

Load-deflection model for elastic thin films loaded by bulge testing.

Bulge test relates the static (force) and kinematic (displacements) parameters of a thin film in order to determine experimentally some of its mechanical properties; a scheme of a film bulged by a controlled pressure load *P* is shown in Figure 1a. Let's consider a rectangular thin film $2a \times 2b$ being $b \geq a$, which is pre-stressed by residual stress σ_r and its curvature is defined by internal pressure loading *P* and its material properties. In those conditions, [7] proposed a classical analytical solution that correlates the maximum deflection w_0 with *P* as follows

$$P = C_1(a,b)\frac{\sigma_r t w_0}{a^2} + C_2(v)\frac{E t w_0^3}{a^4}, \tag{1}$$

where $C_1(a,b)$ and $C_2(v)$ are constants that depend on the geometry and the material, σ_r represents the residual stress induced by the film manufacturing, t is the thickness and E Young's modulus. In this study, $C_1(a,b)$ is obtained from finite element computations and $C_2(v)$ is computed by the following expression $C_2(v) = (\alpha + \beta v)/(1-v)$, where α and β are constants, v is Poisson's ratio to be determined. Equation (1) is called load-deflection model, it can be used to determine the elastic limit (limit pressure which leads to the first plastification of the film) in the bulging problem, for example, if Equation (1) is divided by w_0, it is possible to obtain the following linear relationship

$$Y = C_1\frac{\sigma_r t}{a^2} + C_2(v)\frac{Et}{a^4}X, \tag{2}$$

where $Y = P/w_0$ and $X = w_0^2$. If there is deviation respect to the linear part, it indicates that nonlinear material effects are introduced on the film as sketched in Figure 2b. Taking as reference $Y_l = mX_l$ (m obtained with the first part of experimental data) and comparing it with all experimental data X_{exp} and Y_{exp}; a deviation model between Y_l and Y_{exp} can be determined through an error function as follows $e_Y = (Y_{exp} - Y_l)/Y_{exp}$. It is established that for $e_Y \geq 0.6\%$, plasticity effects are assumed in the bulged film, and at this point, an elastic limit should be demarked.

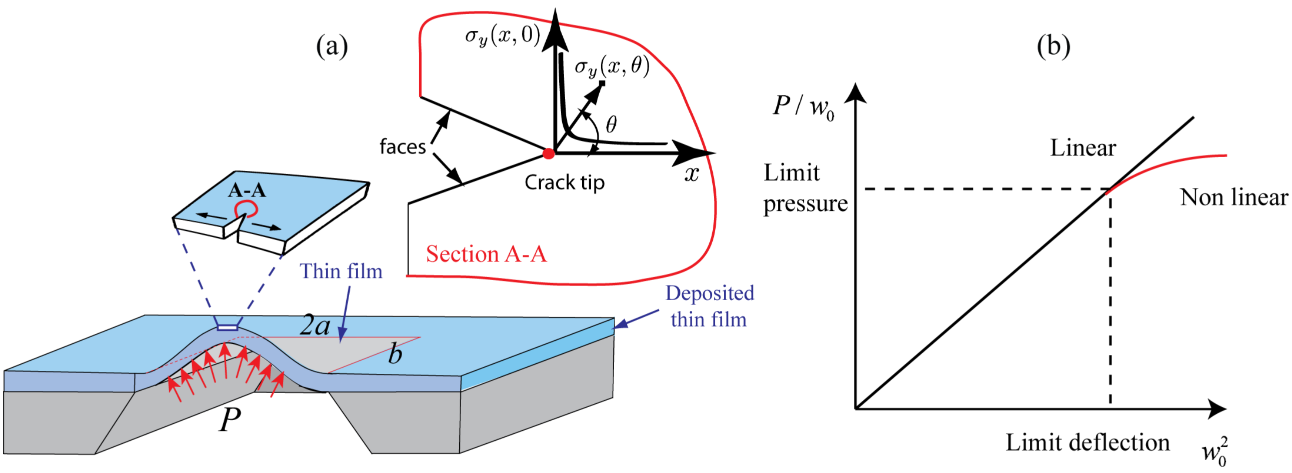

Figure 1. a) Bulge test on a cracked thin film (half model). b) Linear relation to establish limit points with the load-deflection parameters.

Stress intensity factor K_I and $J-$integral

The stress field $\sigma_y(r,\theta)$ in the vicinity of an infinitely sharp crack tip is described mathematically by the following expression [8]

$$\sigma_y(x,\theta)=\frac{K_I}{\sqrt{2\pi x}}\cos\left(\frac{\theta}{2}\right)\left(1-\sin\left(\frac{\theta}{2}\right)\sin\left(\frac{3\theta}{2}\right)\right), \tag{3}$$

where K_I is the stress intensity factor (SIF), θ and x are the direction and position of the stress field $\sigma_y(x,\theta)$. In the crack tip ($x=0$), K_I can be estimated for a sharp notch as $K_I(x)=\sigma_y(x,0)\sqrt{2\pi x}$. This above expression shows that stress values should be known to compute K_I. For instance, the direct method is based on finite element solutions obtained for $\sigma_y(x,\theta),\forall x\in(x_1,x_2)$. The idea is to choose an interval (x_1,x_2) where stress values are used to compute K_I. The cut domain defined in $(0,x_1)$ is an uncertainty domain because stress values are not defined properly by the numerical singularity that represents the crack front. To calculate K_I in $x=0$, an extrapolation is proposed to project the value of K_I using stress values obtained by finite element solutions. However, this method is very sensitive in the vicinity of the crack tip since there is a dependence with the meshing as well as with the shape of the crack root. Therefore, in this study elastic part of J- integral was used. J-integral value is determined by the strain energy release rate close to the crack tip. For plane stress state, the relation between K_I (stress intensity factor) and J_e (elastic part [11]) is given by

$$J_e=K_I^2/E, \tag{4}$$

where E is Young's modulus. For plane strain conditions *J*-integral is calculated by $J=K_I^2(1-v^2)/E$.

Determination of elastic properties for freestanding thin films loaded by bulge testing

In this section, a sequential numerical procedure to determine Young's modulus and Poisson's ratio is presented. It consists of a set of 10 steps that permit to obtain both parameters combining finite element analysis with the classical analytical solution (see Equation 1). For the finite element analysis, it is important to take into account large deformations since the thicknesses are very thin (nanometric scale). The first three steps deal with the estimation of C_1 and σ_r parameters from the finite element model and experimental data. Given that C_1 is dependent on the residual stress σ_r, a set of output data m is created with input parameters known ($E_j,\sigma_{rj},v_j\forall j=1,2,..m$), therefore, C_1 is calculated fitting these in Equation 1. Posteriorly, C_1 is used to compute the residual stress σ_r using the experimental data for any Young's modulus chosen in Equation 1. We suggest choosing a value close to materials with similar mechanical characteristics since for the true solution it is an initial value. In steps 4, 5 and 6; the main objective is to establish a model to calculate $C_2(v)$ from the simulations. Then, there are proposed numerical estimations to calculate a set of two parameters (E_1,v_1) and (E_2,v_2) that satisfy the load-deflection curve obtained experimentally. Using all determined parameters (E_i,σ_r,C_1) and experimental data, $C_{2(i)}$ is computed with both Poisson's ratio found. So, parameters α,β are calculated as follows

$$\alpha=\frac{v_2C_{2(1)}(1-v_1)-v_1C_{2(2)}(1-v_2)}{v_2-v_1},\beta=\frac{C_{2(2)}(1-v_2)-C_{2(1)}(1-v_1)}{v_2-v_1}. \tag{5}$$

Using α and β values, we can calculate any value of $C_2(v)$ with values of v known; as explained in [9]. With all parameters calculated until step 7, the following error function can be mapped such as

$$e_{p(k)}(E,v)=\sum_{j=1}^{n}\left|\frac{P_{\exp(j)}-P(C_{2k}(v_k),E_k,w_{\exp(j)})}{P_{\exp(j)}}\right|/n, \tag{6}$$

where subscript k means a set of parameters E_k and v_k determined for each load-deflection curve with n data. Equation 6 represents an error surface in which the minimum errors should be in the places where a set of E and v satisfy the experimental measurements. The minimum value $\min\left|e_{c(k)}\right|, \forall k = 1,2...,p$ indicates that the elastic parameters (E^* and v^*) are the best approximations for the load-deflection curves obtained experimentally. Detailed information about the procedure is shown in [9-10].

Fracture analysis for a pre-cracked and non-cracked gold thin film

In Figure 2, a brief scheme of a numerical approach proposed to simulate a bulged film with a pre-crack that passes through the thickness is described. The approach is based on two solution stages; the first stage is developed on a film without crack and the second one on a film portion that includes the pre-crack (sub-model). A geometric division of the membrane is carried out with the aim to control the meshing parameters around the crack. The film is divided into two geometric sections that are composed by a scaled section (sub-region of 1% of the size film – sub-model) located in the center of the film and the second one part is the complement of it, as illustrated in Figure 2. It is very important to point out that the sub-section contains the crack, further, three notch types were considered for the fracture analysis; rounded, V-sharp and sharp.

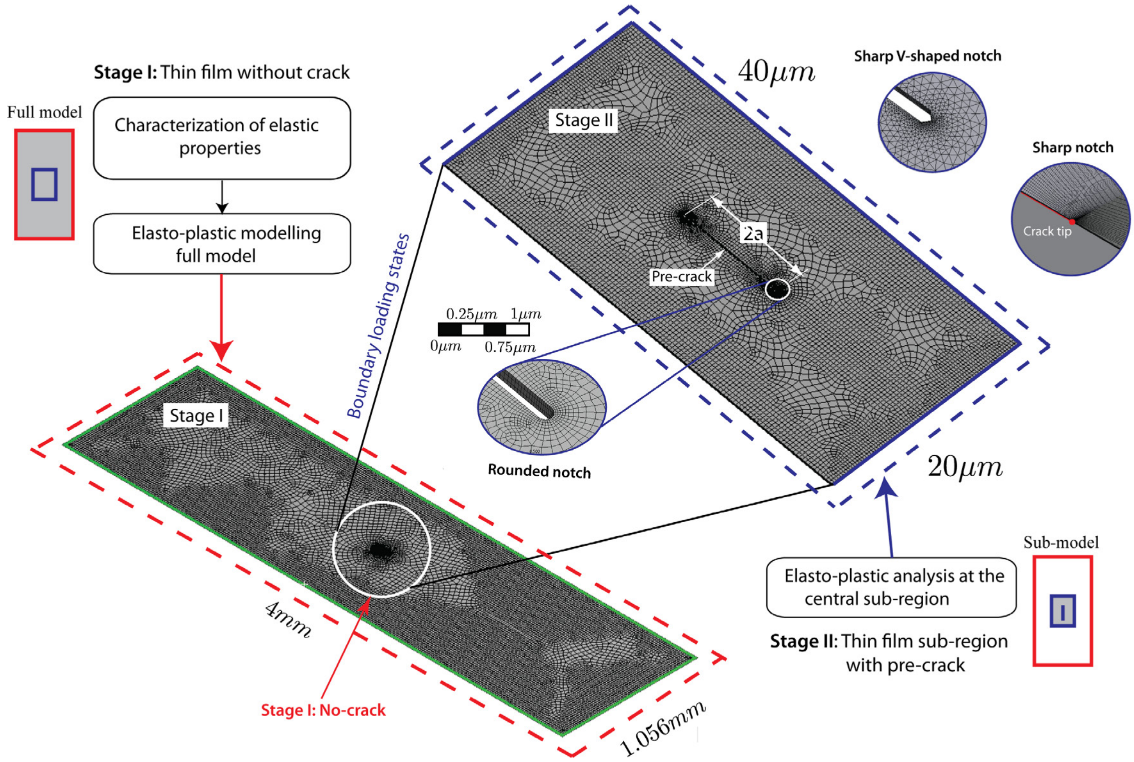

Figure 2. Scheme of the solution process by finite element analysis

In the solution stage I, the model without pre-crack is used to characterize the elasto-plastic properties with the aim to approximate the load-deflection curve measured experimentally. For the stage II, the loading states (those obtained in the stage I) are applied at the boundaries of the sub-region that includes the pre-crack. It means that the solution is computed only for the chosen sub-region. This process is called sub-modelling and the advantage is given by the reduction of computations in the whole geometry. The application of the sub-modelling obeys to Saint-Venant's principle that guarantees the same load state at the boundaries of the sub-regions in both problems. This technique has been applied in different studies. For the analysis, a gold thin film is considered since experimental data of bulge tests were available for this purpose [4]. In Figure 2, the overall views of both finite element models are shown, the whole model (stage I) and sub-region (stage II). The size of the thin film is 1.056x4*mm* with 198.6 *nm* of thickness. A crack of 10μm of length and 100*nm* of width is included in the sub-model(sub-region) with dimensions of 20x40μm as the figure describes it.

Results and Discussion

For the application of the proposed methodology, an experimental bulge test was conducted for a gold film with a surface of $1.056\times 4mm^2$ and thickness $198nm$. Given that the experimental data represent a nonlinear material behavior, it is necessary to establish a limit point to define the elastic behavior of the film. Therefore, applying $Y_l = mX_l$ to experimental data, the load-deflection curve was reduced until 2.75 kPa.

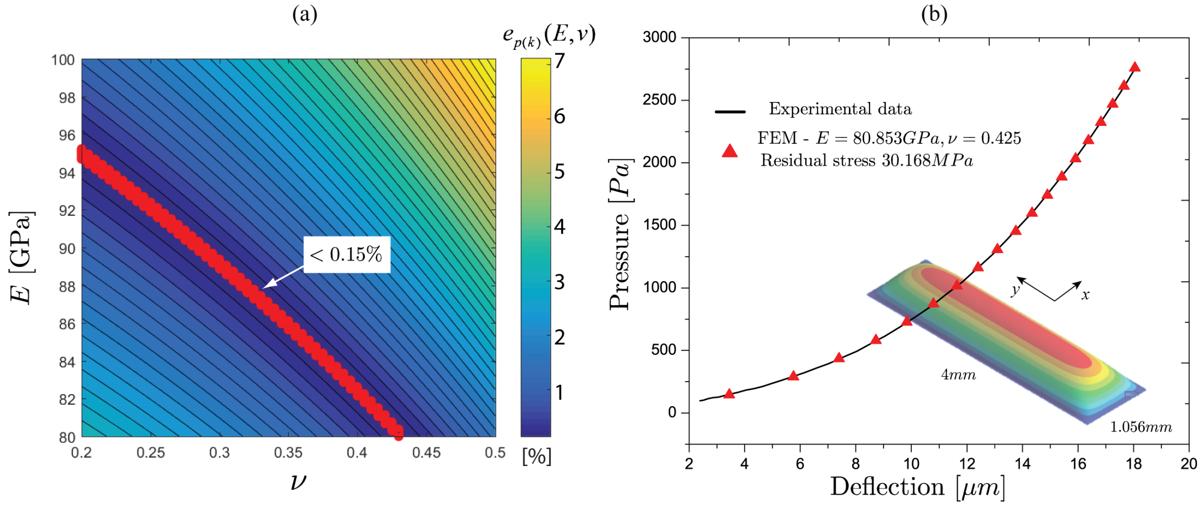

Figure 3. a) $e_p(E,\nu)$ error function. b) Experimental and numerical load-deflection curves (Elastic thin film).

As described in this study and applying the proposed procedures by [10], the following constants were determined for the gold film; $\sigma_r = 30.168MPa$, $C_1 = 1.834$, $\alpha = 1.2809$ and $\beta = -0.7647$. Figure 3a shows the error function $e_p(E,\nu)$ established in Equation (3) which in turn was computed with the parameters anteriorly expressed for the domains $E \in (80,100)GPa$ and $\nu \in (0.2,0.5)$. It is observed that there is a region in which the elastic values (E,ν) minimize the function $e_p(E,\nu)$. These are extracted establishing an error threshold in 0.15%. Figure 3a shows these demarked by a red color. The values indicate that all pairs (E,ν) (within the red line) satisfy load-deflection curve with good accuracy which shows an elastic coupling (dependency between E and ν) in the bulging problem.

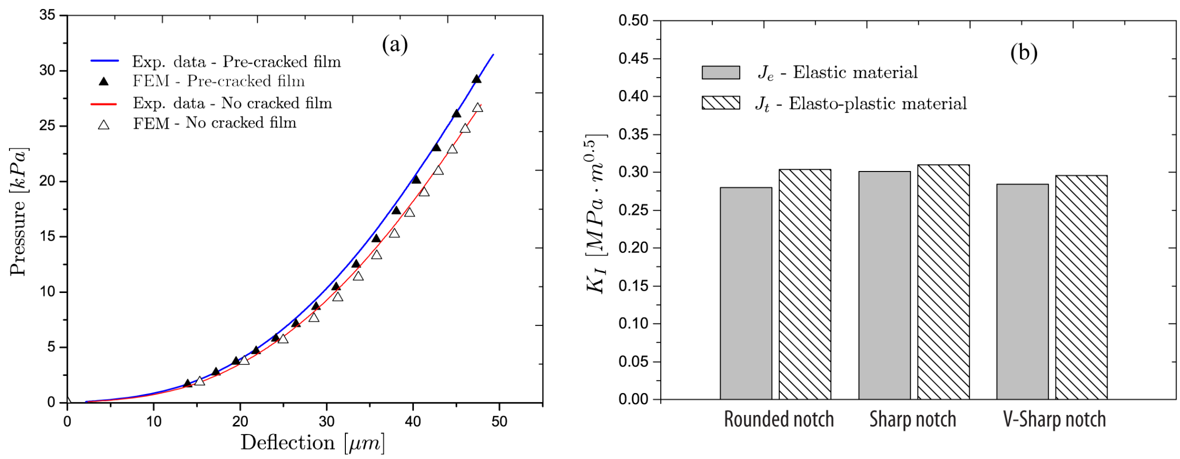

Figure 4. a) Comparisons in load-deflection curves for a non-cracked and cracked film with the experimental data. b) K_{IC} values obtained fro different notches from J-integral.

To determine which pair (E,ν) approximates better the experimental data of load-deflection, finite element simulations were running with the newly extracted data set shown in Figure 3a. All load-deflection curves (for each $(E_i,\nu_i)\forall i = 1,..,20$) obtained by FEA were compared using an error function over the delimited sub-region. From the minimum errors, the following elastic properties were extracted for the gold film: $E = 80.853 GPa$ and $v = 0.425$. The final results are compared and shown in Figure 3b. It is important to point out that the identified elastic properties are necessary for the fracture analysis. Figure 4a shows the numerical results determined for both pre-cracked and non-cracked films which are compared with those obtained by bulge tests, in which the pressure of 31.4 *kPa* corresponds with the broken film. In the figure, there are observed some differences between the simulations and the experimental data. It is primarily identified that the stiffness in the film is higher when there is a presence of the pre-crack and as a consequence, the displacements are lower. Both experiments were approximated with the same nonlinear material model that was initially calculated from analytical equations described by [4] and corrected by finite element analysis. The results indicate that the numerical computations likely approximated both bulge tests. For the fracture analysis; J_t was computed with ANSYS 16.1 and estimations were performed for K_{IC} using different notches at the crack-tip. Figure 4b shows the values calculated for the fracture toughness with *J*-integral and Equation (4). The mean values were determined between 0.288 and 0.303 $MPa \cdot m^{0.5}$ from elastic (1.03 J/m^2) and elasto-plastic (1.136 J/m^2) *J*-integrals. These results agree with the values reported by [2] that determined $0.45 MPa \cdot m^{0.5}$ for gold thin films with thicknesses between 200 and 300 *nm*. It is observed that the plasticity effects have influence at the crack-tip since *J*-integral values obtained from elastic problem were very close to those computed with plasticity.

Conclusions

In this study, an elasto-plastic analysis was conducted for a non-cracked and pre-cracked gold thin film applying finite element analysis and a numerical methodology. For a non-cracked film, both elastic properties, Young's modulus, and Poisson's ratio were determined using experimental data of bulge tests. The load-deflection curve showed a good agreement with the experimental data in the elastic regime. For the analysis of a pre-cracked film, a numerical solution of two stages was proposed with the aim to determine the fracture parameters at the crack tip. Elasto-plastic results correlated the load-deflection curves for non-cracked and pre-cracked films with the same material law, it indicated that the proposed models presented a good correlation and robustness. There were found values of fracture toughness (between 0.288 and 0.303 $MPa \cdot m^{0.5}$) for different notches; rounded, sharp and v-sharp. The calculated values correspond with other values reported in the literature.

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