Mechanical Parameter Extraction of Thin-Film Coated Materials

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ABSTRACT

Materials coated with thin-films have become popular in many advanced applications. The thin layer of high-strength coating can improve the performance of the material. However, challenges arise when characterizing or extracting mechanical parameters for this class of material due to the presence of one or multiple layers of coating. Experimental methods such as nanoindentation and scratch test can be used to determine the mechanical properties for a given specimen. This paper presents a modeling framework for predicting the mechanical property of thin-film coated materials based on the image method. Analytical closed-form expressions for the stress distribution on a coated material subjected to a distributed loading on the surface of the coating material are derived in recursive forms. These recursive equations are implemented numerically to calculate the solutions of the problem. Theses solutions can be used to validate the experimental results of nanoindentation and scratch tests.

Keywords: nanoindentation, thin-film, image method, interface, distributed force

1 INTRODUCTION

Materials coated with thin-films have become popular in many advanced applications including semiconductors and optical storage devices for modern computers. The thin layer of high-strength coating improves the overall mechanical and electro-mechanical performance of the material. However, challenges arise when characterizing or extracting mechanical parameters for this class of material due to the presence of one or multiple layers of coating. Experimental methods involving contact probes such as nanoindentation and scratch test can be used to determine the mechanical properties for a given specimen. This can be used to calibrate a characterization and parameter extraction framework comprising a combination of analytical formulations and numerical algorithms. Such a modeling framework will provide a useful tool for predicting the mechanical property of thin-film coated materials. This paper will present a modeling framework for predicting the mechanical property of thin-film coated materials based on the image point method. Analytical close-form expressions for the stress distribution on a thin-film coated material subjected to a distributed loading on the surface of the coating material are derived in recursive forms. These recursive equations are implemented numerically to calculate the solutions of the problem. These solutions can be used to validate the experimental results of nanoindentation and scratch tests.

2 FOUNDAMENTAL SOLUTION

Consider a semi-infinite plane substrate deposited by a thin film, shown as Fig. 1, subjected to a concentrated force. A concentrated point force applies on the free surface. The upper thin layer is denoted by material 'I' and is with the thickness 'h', shear modulus μ_1, and Poisson's ratio ν_1. The substrate, denoted by material 'II', is a half-infinite plane, of which the shear modulus is μ_2 and Poisson's ratio ν_2. The x-axis is set to lie along the interface. Image points upon the free surface (including surface) are denoted by O_i, and the corresponding local coordinates are expressed by the complex form as $z_k = x + iy_{k1}$. The image points underneath the interface are denoted by C_i with the corresponding local coordinates: $\varsigma_k = x + iy_{k2}$. The relationship between the local coordinates and the global coordinates are:

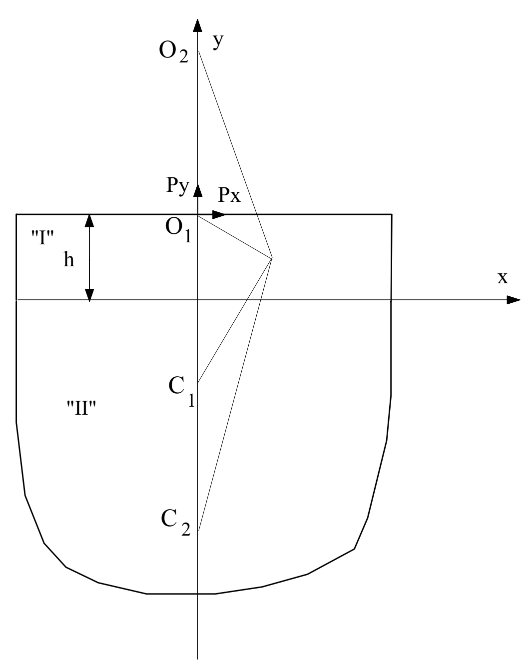


Fig. 1 Analysis model

$$
\begin{aligned}
&z = x + iy, \quad \bar{z} = x - iy, \quad i = \sqrt{-1} \\
&z_k = z - 2(k-1)hi \\
&\varsigma_k = z + (2k-1)hi
\end{aligned} \tag{1}
$$

The elastic fields should satisfy the Goursat formula:

$$
\begin{aligned}
&\sigma_y + i\tau_{xy} = \varphi' + \overline{\varphi}' + \bar{z}\varphi'' + \psi', \qquad \sigma_x + \sigma_y = 4\,\mathrm{Re}(\varphi') \\
&2\mu(u + iv) = \kappa\varphi - z\overline{\varphi}' - \overline{\psi}
\end{aligned} \tag{2}
$$

where

$$
\begin{cases}
\kappa = 3 - 4\nu & \text{for plane strain} \\
\kappa = (3-\nu)/(1+\nu) & \text{for plane stress}
\end{cases} \tag{3}
$$

Assuming stress functions take the following form:

$$
\begin{cases}
\varphi_I = \sum_{k=1}^{\infty}[A_k(z_k) + \Phi_k(\zeta_k)] \ , \varphi_{II} = \sum_{k=1}^{\infty} a_k(z_k) \\
\psi_I = \sum_{k=1}^{\infty}[B_k(z_k) + \Psi_k(\zeta_k)] \ , \ \psi_{II} = \sum_{k=1}^{\infty} b_k(z_k)
\end{cases} \tag{4}
$$

Substituting Eq. (4) into Eq. (2) yields the following set of equations for the stresses in the problem:

$$
\begin{aligned}
\sigma_{yI} + i\tau_{xyI} &= \varphi_I' + \overline{\varphi}_I' + \bar{z}\varphi_I'' + \psi_I' \\
&= \sum_{k=1}^{\infty}\left[A_k'(z_k) + \Phi_k'(\varsigma_k)\right] + \sum_{k=1}^{\infty}\left[\overline{A_k'}(z_k) + \overline{\Phi_k'}(\varsigma_k)\right] \\
&+ \bar{z}\sum_{k=1}^{\infty}\left[A_k''(z_k) + \Phi_k''(\varsigma_k)\right] + \sum_{k=1}^{\infty}\left[B_k'(z_k) + \Psi_k'(\varsigma_k)\right]
\end{aligned} \tag{5a}
$$

$$
\sigma_{xI} + \sigma_{yI} = 4\,\mathrm{Re}(\varphi_I') = 4\,\mathrm{Re}\left(\sum_{k=1}^{\infty}\left[A_k'(z_k) + \Phi_k'(\varsigma_k)\right]\right) \tag{5b}
$$

$$
\begin{aligned}
2\mu_I(u_I + iv_I) &= \kappa_I\varphi_I - z\overline{\varphi}_I' - \overline{\psi_I} \\
&= \kappa_I\sum_{k=1}^{\infty}\left[A_k(z_k) + \Phi_k(\varsigma_k)\right] - z\sum_{k=1}^{\infty}\left[\overline{A_k'}(z_k) + \overline{\Phi_k'}(\varsigma_k)\right] \\
&- \sum_{k=1}^{\infty}\left[\overline{B}_k(z_k) + \overline{\Psi}_k(\varsigma_k)\right]
\end{aligned} \tag{5c}
$$

$$
\begin{aligned}
\sigma_{yII} + i\tau_{xyII} &= \varphi_{II}' + \overline{\varphi}_{II}' + \bar{z}\varphi_{II}'' + \psi_{II}' \\
&= \sum_{k=1}^{\infty} a_k'(z_k) + \sum_{k=1}^{\infty}\overline{a_k'}(z_k) + \bar{z}\left[\sum_{k=1}^{\infty} a_k''(z_k)\right] + \sum_{k=1}^{\infty} b_k'(z_k)
\end{aligned} \tag{6a}
$$

$$
\sigma_{xII} + \sigma_{yII} = 4\,\mathrm{Re}(\varphi_{II}') = 4\,\mathrm{Re}\left(\sum_{k=1}^{\infty}\overline{a_k'}(z_k)\right) \tag{6b}
$$

$$
\begin{aligned}
2\mu_{II}(u_{II} + iv_{II}) &= \kappa_{II}\varphi_{II} - z\overline{\varphi}_{II}' - \overline{\psi_{II}} \\
&= \kappa_{II}\left[\sum_{k=1}^{\infty} a_k(z_k)\right] - z\left[\sum_{k=1}^{\infty}\overline{a_k'}(z_k)\right] - \sum_{k=1}^{\infty}\overline{b}_k(z_k)
\end{aligned} \tag{6c}
$$

The continuity conditions at the interface are:

$$
\begin{aligned}
&\sigma_{yI} + i\tau_{xyI} = \sigma_{yII} + i\tau_{xyII} \\
&u_I + iv_I = u_{II} + iv_{II}
\end{aligned} \qquad \text{at} \quad y = 0 \tag{7}
$$

Tractions free condition at the free surface is:

$$
\sigma_{yI} + i\tau_{xyI} = 0 \qquad \text{at} \quad y = h \tag{8}
$$

Substituting Eqs. (5a)−(6c) into Eqs. (7) and (8), one can obtain the recurrence relationships of the stress functions:

$$
\begin{cases}
\Phi_k = m_1\left[(\varsigma_k - (2k-1)hi)\overline{A_k'} + \overline{B}_k\right] \\
\Psi_k = -m_2\overline{A}_k - m_1\begin{Bmatrix}(\varsigma_k - (2k-1)hi)^2\,\overline{A_k''} \\ + \left[\varsigma_k - (2k-1)hi\right]\left(\overline{A_k'} + \overline{B_k'}\right)\end{Bmatrix}
\end{cases} \tag{9}
$$

$$
\begin{cases}
a_k = (1 - m_2)A_k \\
b_k = (m_1 + m_2)(z_k + (2k-1)hi)A_k' + (m_1 + 1)B_k
\end{cases} \tag{10}
$$

$$
\begin{cases}
A_{k+1} = -\left[z_{k+1} + (2k+1)ih\right]\overline{\Phi_k'} - \overline{\Psi}_k \\
B_{k+1} = (z_{k+1} + (2k-1)hi)\left(\overline{\Phi_k'} + \overline{\Psi_k'}\right) - \overline{\Phi}_k \\
+ (z_{k+1} + (2k+1)hi)\left[z_{k+1} + (2k-1)ih\right]\overline{\Phi_k''}
\end{cases} \tag{11}
$$

where:

$$
m_1 = \frac{\beta - \alpha}{1 - \beta}\ , \qquad m_2 = \frac{\alpha + \beta}{1 + \beta} \tag{12}
$$

Here α and β are Dundur's parameters[2]:

$$
\alpha = \frac{\mu_1(\kappa_2 + 1) - \mu_2(\kappa_1 + 1)}{\mu_1(\kappa_2 + 1) + \mu_2(\kappa_1 + 1)}, \beta = \frac{\mu_1(\kappa_2 - 1) - \mu_2(\kappa_1 - 1)}{\mu_1(\kappa_2 + 1) + \mu_2(\kappa_1 + 1)} \tag{13}
$$

For a homogenous semi-infinite plane subjected to a concentrated force on the surface, the stress functions are:

$$
A_1 = C\log z_1\ ,\ B_1 = -\overline{C}\log z_1 + \frac{ihC}{z_1} \tag{14}
$$

where

$$
C = -\frac{P_x + iP_y}{2\pi} \tag{15}
$$

Starting from the stress functions in Eq. (14), the other functions can be derived using the recurrence relationships in Eqs. (9), (10), and (11). The symbolic computation software such as Mathematica or Maple can be used to calculate the stresses.

3 INTEGRAL SOLUTION FOR DISTRIBUTED FORCES

When arbitrarily distributed forces acting on the surface, shown as Fig. 2, the stress and displacement fields can be obtained by superposition, through the integration of the fundamental solutions.

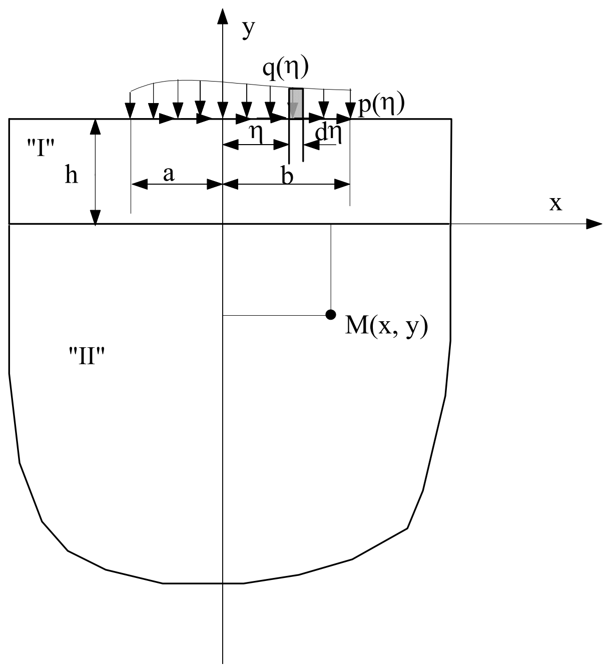


Fig. 2 Arbitrarily distributed force acting on the surface

In Fig. 2, the distribution of the shear and normal forces are $p(\eta)$ and $q(\eta)$, respectively. At the distance η away from the load point along the surface, the equivalent differential loadings are $dP_x = p(\eta)d\eta$ and $dP_y = q(\eta)d\eta$. The stresses and displacements at any point M(x, y) under dP can be calculated according to Eqs. (5) and (6), using $z-\eta$, $z_k-\eta$, and $\varsigma_k-\eta$ instead of z, z_k, and ς_k in the formulas. The results are as following:

$$\begin{aligned} d(\sigma_{yI}+i\tau_{xyI}) = \{ &\sum_{k=1}^{\infty}[A'_k(z_k-\eta)+\Phi'_k(\varsigma_k-\eta)] \\ &+\sum_{k=1}^{\infty}\left[\overline{A'_k}(z_k-\eta)+\overline{\Phi'_k}(\varsigma_k-\eta)\right] \\ &+(\bar{z}-\eta)\sum_{k=1}^{\infty}[A''_k(z_k-\eta)+\Phi''_k(\varsigma_k-\eta)] \\ &+\sum_{k=1}^{\infty}[B'_k(z_k-\eta)+\Psi'_k(\varsigma_k-\eta)]\}d\eta \end{aligned} \quad (16a)$$

$$\begin{aligned} &d(\sigma_{xI}+\sigma_{yI}) \\ &=\left\{4\,\mathrm{Re}\left(\sum_{k=1}^{\infty}[A'_k(z_k-\eta)+\Phi'_k(\varsigma_k-\eta)]\right)\right\}d\eta \end{aligned} \quad (16b)$$

$$\begin{aligned} 2\mu_I d(u_I+iv_I) = \{ &\kappa_I\sum_{k=1}^{\infty}[A_k(z_k-\eta)+\Phi_k(\varsigma_k-\eta)] \\ &-(z-\eta)\sum_{k=1}^{\infty}\left[\overline{A'_k}(z_k-\eta)+\overline{\Phi'_k}(\varsigma_k-\eta)\right] \\ &-\sum_{k=1}^{\infty}\left[\overline{B}_k(z_k-\eta)+\overline{\Psi}_k(\varsigma_k-\eta)\right]\}d\eta \end{aligned} \quad (16c)$$

$$\begin{aligned} d(\sigma_{yII}+i\tau_{xyII}) = \{ &\sum_{k=1}^{\infty}a'_k(z_k-\eta)+\sum_{k=1}^{\infty}\overline{a'_k}(z_k-\eta) \\ &+(\bar{z}-\eta)\left[\sum_{k=1}^{\infty}a''_k(z_k-\eta)\right]+\sum_{k=1}^{\infty}b'_k(z_k-\eta)\}d\eta \end{aligned} \quad (17a)$$

$$d(\sigma_{xII}+\sigma_{yII}) = \left\{4\,\mathrm{Re}\left(\sum_{k=1}^{\infty}\overline{a'_k}(z_k-\eta)\right)\right\}d\eta \quad (17b)$$

$$\begin{aligned} 2\mu_{II} d(u_{II}+iv_{II}) = \{ &\kappa_{II}\left[\sum_{k=1}^{\infty}a_k(z_k-\eta)\right] \\ &-(z-\eta)\left[\sum_{k=1}^{\infty}\overline{a'_k}(z_k-\eta)\right]-\sum_{k=1}^{\infty}\overline{b}_k(z_k-\eta)\}d\eta \end{aligned} \quad (17c)$$

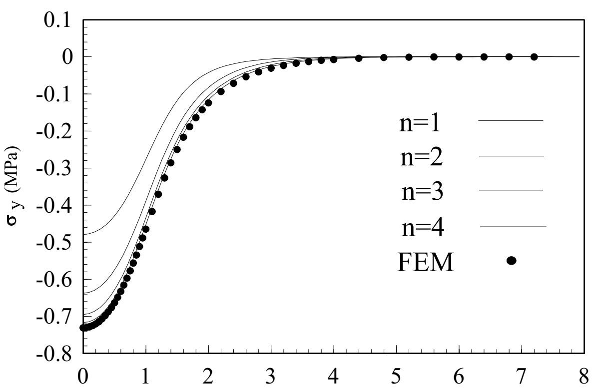
The coefficients of the stress functions in Eqs. (16) and (17) are determined by the recursive relations expressed in Eqs. (9), (10) and (11), and each term includes C or it's complex conjugate $\overline{C}$. Since $C=-\frac{P_x+iP_y}{2\pi}$ in the fundamental solutions, for the differential force dP C will be $C=-\frac{p(\eta)+iq(\eta)}{2\pi}d\eta$. Therefore, the stresses and displacements can be integrated with respect to the parameter η using Eqs. (16) and (17) for the case of distributed forces. For instance, integrating equation (16a) we can obtain the normal and shear stresses in material I, the thin layer. The integration can be carried out in complex form and then separate the solutions into real and imaginary parts, corresponding to the normal stress and the shear stress, respectively.

4 COMPARISON WITH NUMERICAL RESULTS

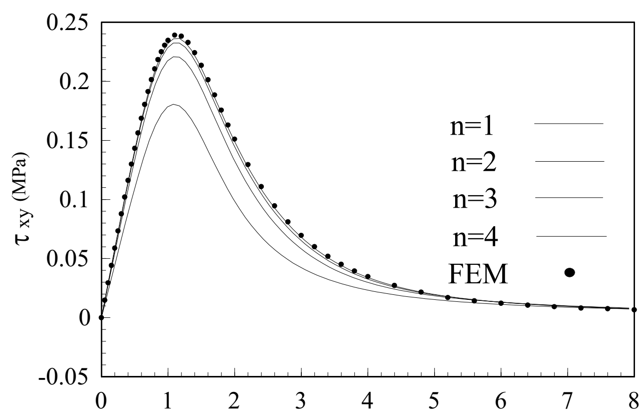
In order to validate of the analytical results presented in the previous sections, some numerical analysis based on finite element method are carried out for the case of uniform distributed normal force along the surface. In such case, $p(\eta)=0$ and $q(\eta)=\text{constant}$, the region of the distributed loading is taken from –1 to 1, and the thickness of the film is 1mm. The material constants for the coating and substrate are summarized in Table 1. The results are shown in Figs. 3(a) and 3(b).

Material	I	II
Young's Modulus E (GPa)	546	206
Poisson's Ratio ν	0.3	0.3

Table 1 Material constants



(a) Normal stress σ_y for $p(\eta)=0$, $q(\eta)=1N/mm^2$



(b) Shear stress τ_{xy} for $p(\eta)=0$, $q(\eta)=1N/mm^2$

Fig. 3 Stress distributions along the interface for the case of normal loading

In the legends of Figs. 3(a) and 3(b), n=k denotes the order of image point. With comparisons to the numerical results from finite element analysis, it can be found that the stresses increments decrease rapidly with the order of the image points increasing. And the stresses superposed with 5 image points have enough accuracy for the material combination listed in the Table 1. These results demonstrate that the convergence rate of the theoretical solutions is very fast.

5 SUMMARY

In this paper, we have formulated a framework for solving the problem of film-substrate material system subjected to distributed loads. In fact, in indentation or nanoindentation tests, the contact distributed forces are not uniformly distributed normal forces. However, many kinds of continuous distributed loads can be simulated by polynomial expression. Noting that all the stress functions are polynomial, except the stress functions corresponding to the first order image point. Therefore, Eqs. (16a) through (17c) can be integrated in closed-form.

It should be pointed out that the displacement fields are needed for validating the results in nanoindentation tests. The authors are conducting on-going research program to solve the displacement fields of this problem and to further extend the loading case to more general forms.

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