DETERMINATION OF THE ENGINEER CONSTANTS OF PIEZOELECTRIC THIN FILM BASED ON THE PIEZOELECTRIC CONSTITUTION

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Summary Distinguishing with the previous method, the explicit expression of indentation load-depth (*P-h*) curve derived by the piezoelectric constitution is used to establish the supplemental equation, in which the electrical and mechanical properties of piezoelectric thin film are related with the maximum indentation load and maximum indentation depth. The engineer constants of piezoelectric thin film can be determined by combining nanoindentation test and finite element method (FEM).

INTRODUCTION

Recently, more and more efforts have been made to develop piezoelectric materials to apply into piezoelectric microelectromechanical systems, and they are usually in the form of film bonded to substrate. Piezoelectric thin film materials operating in many structural components and the intrinsic mechanical behaviour of piezoelectric thin film should be first known. Nanoindentation has been used to study the mechanical properties of thin film deposited on substrate [1]. Relatively few reports on the anisotropic mechanical properties are available for piezoelectric thin film in the literatures. Recently, the indentation modulus is taken as the weight average of transverse and longitudinal Young's moduli [2]. In fact, the indentation modulus is determined by the unloading part slope of indentation curve at the maximum indentation load, and interpretation of indented measurements indentation often contains a substantial error [3]. We naturally associate whether the substitution of supplemental equation based on the piezoelectric constitution can reduce the substantial error by combining nanoindentation test and FEM.

FOWARD ANALYSIS

Generally, a piezoelectric thin film is perfectly bonded to a substrate and loaded by an axisymmetric rigid indenter, and the schematic of film/substrate system is given in Fig. 1. The piezoelectric thin film is simplified as transversely isotropic [2]. For transversely isotropic piezoelectric materials, the constitutive equations can be represented as [2]

$$\sigma_{ij} = c_{ijkl} - e_{kij}E_k \quad (i, j=1, 2, 3;\ k, l=1, 2, 3) \qquad (1)$$
$$D_k = e_{ikl}\varepsilon_{kl} + \xi_{ik}E_k$$

For an idealized transversely isotropic bulk material, the loading part of *P-h* curve obeys a power function and the relationship between indentation load F and indentation depth h can be rewritten as [2]

$$F = F_{max}\left(\frac{h}{h_m}\right)^x \qquad (2)$$

where F_{max} and h_m are the maximum indentation load and the corresponding maximum penetration. According to the previous results of the transversely isotropic thin film indentation [2], the F_{max} and the x should be the functions of the material parameters and applying Buckingham Pi Theorem to the functions, they can be written as dimensionless form

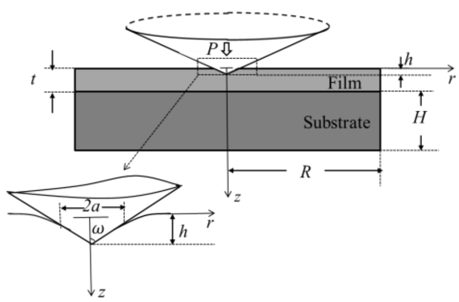

Fig. 1. The schematic of film/substrate system

$$\frac{F_{max}}{E_S h_m^{\ 2}} = \phi\left(\frac{E_T}{E_S}, \frac{E_L}{E_S}, \frac{G_L}{E_S}\right) \qquad (3)$$

$$x = \varphi\left(\frac{E_T}{E_S}, \frac{E_L}{E_S}, \frac{G_L}{E_S}\right) \qquad (4)$$

where E_T is the transverse elastic modulus, E_L the longitudinal elastic modulus, G_L the longitudinal shear modulus, E_S the elastic modulus of the substrate. Base on the piezoelectric constitution the explicit expression of *P-h* curve can directly relate the nanoindentation test with the mechanical-electrical properties, and its specific expression of the indentation load can be written as [4]

$$P_{max} = \frac{4h_m^2}{\pi \cot\omega}\frac{M_8M_5 - M_7M_6}{M_8M_1 - M_7M_2} \qquad (5)$$

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When F_{max} and h_m are extracted from the numerical loading curves to establish the dimensionless equations (3) and (4), and the E_T, E_L and G_L can be determined by solving Eqs. (3)-(5). Numerical indentation tests are simulated by using commercial numerical finite element package ABAQUS, and we adopt piezoelectric indentation (PI) mode to obtain the numerical loading curves. For Berkovich indenter, the corresponding apex angle ω of the equivalent cone was chosen as 70.3°. The numerical indentation is modelled as a two-dimensional axisymmetric problem. Film and substrate are meshed by using CAX4E and CAX4R elements [2]. For brevity, the different combinations of normalized engineer constants are fixed as E_T/E_S = (0.5, 0.8, 1.1, 1.6), E_L/E_S = (0.7, 1.0, 1.4, 1.6) and G_L/E_S = (0.2, 0.4, 0.6, 0.8). The normalized numerical loading curves under PI mode are obtained. The specific forms of Eqs. (3) and (4) can be determined by fitting the numerical results.

INVERSE ANALYSIS

Six indents were performed during the nanoindentation test. The experimental data P_{max} and h_m are obtained from the experimental indentation curve. According to the loading part of the experimental *P-h* curves, Eq. (2) can be fitted by using Origin software to determine the experimental loading curve exponent x_m. The Young's modulus of silicon substrate is assumed to be E_S=130 GPa. Substituting P_{max}, h_m, x_m and E_S into Eqs. (3)-(5), the multiple solutions will be obtained within a certain error range given in the flow chart. When the total error is least, three combinations of the elastic parameters are selected as the solutions. The three sets of selected solutions for the typical maximum indentation depths 97.7, 100.3 and 102.2 nm are given in Table 1. For each set of solution, the S3 is of the smallest total error among the solutions. In order to verify the validity of the multiple solutions, the three set of solutions are respectively inputted into ABAQUS software, and the numerical loading curves and the corresponding difference with the experimental maximum loading loads are given in Figs. 2 (a)-(c) and Table 1. Obviously, the numerical loading curves are in good agreement with the experiment loading curve. For the maximum loading load 2.73 mN and the maximum indentation depth 100.3 nm, there is the smallest difference between the numerical and experimental maximum loading loads for the S3 meanwhile the numerical loading curve is most close to the experimental curve among all of those given in Fig. 2, therefore the engineer constants are ultimately taken as E_T=101.5 GPa, E_L=154.0 GPa and G_L=42.5GPa for the solution 3 at h_m=100.3 nm, and they are reasonable comparing with the previous results of ZnO thin film [2, 5]. Consequently, the proposed method is effective to determine the engineer constants of piezoelectric thin film.

Table 1 The engineer constants for ZnO thin film

Method		E_T(GPa)	E_L(GPa)	G_L(GPa)	F_{max}-P_{max}(mN)
Experimental [5]		98.7	152.0	38.0	
Weight average [2]		104.0	152.5	38.5	
Indentation depth 97.7 nm	S1	108.5	156.0	41.5	0.034
	S2	108.5	154.0	42.0	0.028
	S3	108.0	154.0	41.5	0.020
Indentation depth 100.3 nm	S1	102.0	156.0	42.5	0.020
	S2	102.0	154.0	43.0	0.011
	S3	101.5	154.0	42.5	0.003
Indentation depth 102.2 nm	S1	89.5	154.0	46.0	0.039
	S2	89.5	152.5	46.5	0.032
	S3	89.0	152.5	46.0	0.025

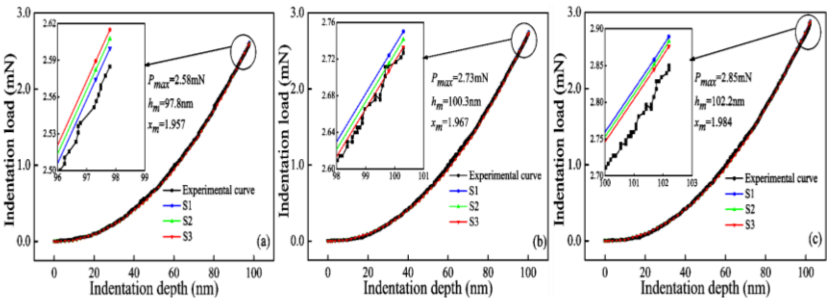

Fig. 2. The loading parts of experimental *P-h* curves and the numerical loading curves.

CONCLUSIONS

Base on the piezoelectric constitution the explicit expression of the *P-h* curve derived for conical indenter is used to establish the supplemental equation, and the method combining nanoindentation and FEM analysis is proposed to determine the engineer constants of transversely isotropic piezoelectric thin film. The numerical loading curves are obtained from the extensive FEM simulations at the moderately deep indentation for the PI mode, and the nanoindentation tests were performed on ZnO thin film to extract the maximum indentation loads, the loading curve exponents and the maximum indentation depths. The engineer constants of ZnO thin film are determined as E_T=101.5 GPa, E_L=154.0 GPa and G_L=42.5GPa, and the results are reasonable comparing with the previous results of ZnO thin film. The proposed method is effective to determine the engineer constants of piezoelectric thin film.

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