DELAMINATION AT FREE EDGE OF INTERFACE BETWEEN PIEZOELECTRIC THIN FILMS

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ABSTRACT

This work focuses on the delamination cracking initiated at the free edge of interface between piezoelectric thin films on a substrate, and investigates the interface strength experimentally and theoretically. At first, $Pb(Zr_{0.53},Ti_{0.47})O_3$ **(**PZT) thin film of around 2.5 μm thickness is deposited on PLT/Pt/Ti/Si substrate using magnetron sputtering technique, followed by sputtering a chromium (Cr) layer on the top surface of the PZT layer. Then, a novel experimental method of sandwiched cantilever specimen is utilized to perform the delamination tests, where the stiff steel cantilever and silicon substrate are chosen to constrain the plastic deformation of the films during the tests. The experimental results show that the delamination occurs along the thin Cr and PZT layers, and the cracking process is rather fast. These suggest that strong stress intensification prevails over the region near the free edge of the interface. Therefore, a theoretical analysis is performed on the singular behavior of the stresses near the free edge of the interface, and the stress singularity order is given for the case of Cr/PZT interface, i.e., 0.3~0.33. Finally, a criterion of interface crack initiation is proposed on the basis of fracture mechanics concept.

1 INTRODUCTION

Interfaces are intrinsic to various functional devices using piezoelectric thin films, such as ferroelectric memories and MEMS. Interfaces, however, are susceptible to delaminate in the processing and in service. Especially, the delamination crack usually initiates at the free edge of thin films due to the stress concentration originated from the mismatch of deformation. Therefore, it is of critical importance to evaluate the interface strength between the thin films.

In this study, a novel experimental method of sandwiched cantilever specimen [1] is utilized to explore the interface strength of PZT thin films deposited on silicon substrate. Furthermore, a theoretical analysis is conducted on the singular behavior of the stresses near the free edge of interface, in order to evaluate the interface strength of the PZT thin films.

2 EXPERIMENTAL METHOD

Figure 1 shows the experimental setup of the sandwiched cantilever-testing scheme. The load, P, is applied at the edge of the cantilever of stainless steel. The relatively stiff steel cantilever and silicon substrate are chosen to constrain plastic deformation of the films during the tests. A square plate of film/substrate is cut from the wafer with the PZT films and carefully glued with epoxy on the cantilever.

Table 1 lists the specimen sizes tested. A micro-material testing system, MCTE-500, is used to perform the tests. Tests are conducted in an air at a room temperature under the constant loading rate of 0.004 N/s using a remodeled micro-Vickers hardness tester. The load is applied by an electro-magnetic actuator and the displacement at the load point is monitored during the tests. After the tests, the fracture surface is observed by means of optical microscope and also examined by Auger electron spectroscopy (AES).

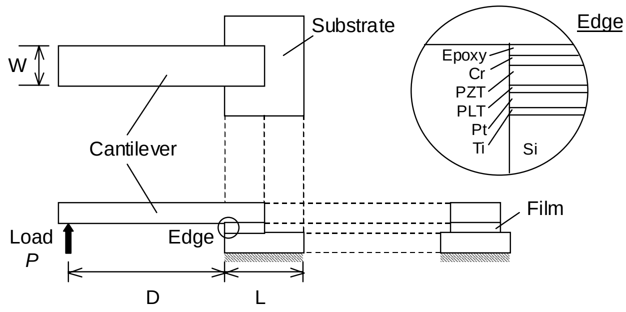

Figure 1: Schematics of PZT specimen and loading system

Table 1: Dimensions of PZT specimens

Test	L (mm)	W (mm)	D (mm)
D1	1.260	1.746	10
D2	1.484	1.725	10
D3	1.535	1.877	10

In this study, *c*-axis oriented PZT thin films are fabricated by magnetron sputtering technique [2]. The PZT layer is firstly sputtered at 700 °C with 180 W rf power, using a ceramics target of composition of $Pb(Zr_{0.53},Ti_{0.47})O_3$, on PLT/Pt/Ti/Si substrate. The as-deposited PZT films are about 2.5 μm thick. Then, a Cr layer of thickness of around 0.2 μm was deposited on the top surface of the PZT layer.

3 EXPERIMENTAL RESULTS

Table 2 lists the delamination load, P_d, the nominal fracture stress, $\sigma_d = P_d/(L \cdot W)$, and the fracture positions of the typical tests for the PZT films. The experiments reveal that: (1) delamination initiates at the left edge of all the specimens; (2) Fracture takes place abruptly after the initiation without slow stable crack growth and the fracture is brittle of nature; (3) A linear relationship between the load P and the displacement δ is shown for the specimens up to the delamination, see Fig. 2; (4) AES analyses for the fracture surfaces of the specimens confirmed that cracking goes through the interface between the thin Cr and PZT layers. These indicate that delamination could be controlled by strong stress intensification prevailed over the region near the free edge of the interface, which will be discussed next.

Table 2: Delamination load and fracture interface

Test	Delamination load P_d, N	Nominal fracture stress, σ_d, MPa	Fracture interface
D1	1.294	0.588	Cr/PZT
D2	1.576	0.617	Cr/PZT
D3	2.136	0.741	Cr/PZT

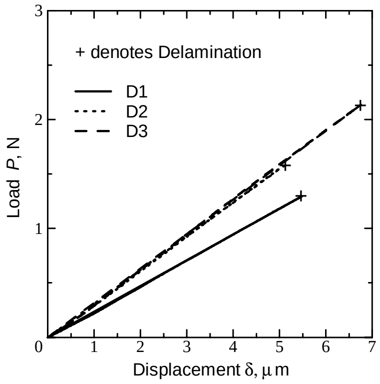

Figure 2: Load-displacement curves of PZT specimens

4 STRESS FIELDS NEAR THE INTERFACE EDGE

A two-dimensional model of linear piezoelectricity is adopted. Assume the *x-z* plane as the plane of analysis. Let (r, θ) be local polar coordinates of a point with rectangular Cartesian coordinates (x, z) in the vicinity of the interface edge Cr/PZT.

The equilibrium equations for piezoelectric materials are

$$\sigma_{ij,j} = 0, \quad D_{i,i} = 0 \tag{1}$$

where σ_{ij} and D_i are the stresses and electric displacements. To derive the eigen-equation determining the singularity order, continuity conditions at the interface Cr/PZT and electrically open boundary condition for the PZT layer are assumed.

The piezoelectric interface edge problem can be solved using the general solution developed in [3, 4], which states that displacements u_i and electric potential φ can be formulated by three quasi-harmonic potential functions ψ_i as

$$\begin{aligned} u_x &= (\psi_1 + \psi_2 + \psi_3)_{,x} \\ u_z &= (k_{11}\psi_1 + k_{12}\psi_2 + k_{13}\psi_3)_{,z} \\ \varphi &= (k_{21}\psi_1 + k_{22}\psi_2 + k_{23}\psi_3)_{,z} \end{aligned} \tag{2}$$

The potential functions applicable to the current problem take the form of

$$\psi_i = \sum_{j=0}^{\infty} (r_i)^{p+j+1} [A_{ij} \sin(p+j+1)\theta_i + B_{ij} \cos(p+j+1)\theta_i], \quad i = 1,2,3 \tag{3}$$

In eqns (2) and (3), $0 < p < 1$, A_{ij} and B_{ij} are constants, $r_i = r\cos\theta / \cos\theta_i$, $\theta_i = \arctan(s_i \tan\theta)$, k_{ij} and s_i $(i = 1,2,3)$ are the eigen-values of the PZT material.

Then, inserting the solution into the boundary and interface conditions leads to a homogeneous system of equations as

$$\mathbf{M}\,\mathbf{X} = \mathbf{0} \tag{4}$$

Here, the matrix **M** is a function of the material properties and the geometries of the interface edge. Eqn (4) has a nontrivial solution only if

$$\det \mathbf{M} = 0 \tag{5}$$

The singularity order p in the stress field near the Cr/PZT interface edge can thus be found by solving eqn (5). Then the dominant term of the stresses near the edge is given by

$$\sigma_{ij} = \frac{K_d}{r^{1-p}} f_{ij}(\theta) \tag{6}$$

Here, K_d is intensity parameter; $f_{ij}(\theta)$ are angular functions. Numerical solution of eqn (5) and finite element analysis show that the stress singularity order for the Cr/PZT interface edge is $1-p = 0.3 \sim 0.33$.

5 CRACK INITIATION CRITERION

Based on the above experimental findings and theoretical analyses, the criterion for crack initiation at the interface edge of the thin films may be considered in terms of the stress intensity parameter K_d at the delamination load, as

$$K_d \geq K_{cr} \tag{7}$$

Here, critical stress intensity parameter K_{cr} can be fracture toughness characterizing the crack initiation at the interface edge of the films/substrate material system.

6 CONCLUSIONS

Focusing on crack initiation from the free edge of the interface, the interface strength of the PZT thin films deposited on silicon substrate has been investigated experimentally and theoretically in this work. Experimental tests using the sandwiched cantilever specimen show that delamination occur along the interface Cr/PZT. Theoretical analyses give the singularity order in stresses near the interface edge Cr/PZT, i.e., 0.3~0.33. Also, the criterion for interface crack initiation is proposed.

ACKNOWLEDGMENTS

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