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Fracture analysis of a surface through-thickness crack in PZT thin film under a continuous laser irradiation

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ABSTRACT

In this paper, the surface crack problem in PZT thin films under a continuous laser irradiation has been investigated by the superposition principle. Using commercial (FEM) software ANSYS 9.0, the piezoelectric fields near the crack tip were solved for surface crack in the finite PZT thin film. The SIFs for crack-tip fields were obtained by using the limited stress extrapolation technique (LSET) and then the energy release rates were calculated by the relation to the intensity factors. When the irradiation time and crack location were changed, the energy release rates G, G_I, and G_e for total, mechanical terms (mode I) and electric contribution were investigated. The results show that the mechanical opening mode I is the main mode for the surface crack under a continuous laser irradiation. However, electric mode IV has inhibiting effect on crack growth. At the beginning of laser irradiation, the surface tiny crack which is close to the centre of film will propagate more easily. During the laser irradiation, the crack which is far from the centre of film will propagate more easily.

1. Introduction

Piezoelectric thin film materials, such as lead–zirconate–titanate $Pb(Zr_xTi_{1-x})O_3$ (PZT) thin films have developed rapidly in recent years due to their wide applications, including high-value capacitors, infrared detectors, sensors and actuators, optical switches, ferroelectric field-effect transistors, and non-volatile memories [1,2]. However, as is well known, because of their brittleness, piezoelectric materials including piezoelectric thin films have a tendency to develop critical cracks during the manufacturing and the service process. Because the general thin film materials operating in many structure components, especially aerospace components are ineluctably subject to severe thermal loading which may be produced by aerodynamic heating, laser irradiation, or localized intense fire [3–5]. It is natural that the film may fail due to the heating load, electric load as well as mechanical load in the case of the film at operating state. The tensile stress in thin film may cause surface cracks due to pre-existing flaws in the film [6]. A two-dimensional model of a film bonded to an elastic substrate is proposed for simulating crack propagation paths in thin elastic film under equi-biaxial residual tensile stress [7]. Vlassak detailed the elastic plane-strain problem of a crack in a coating on substrate of finite thickness [8]. Under equi-biaxial stress, the effects of crack configurations, initial crack length, substrate thickness and elastic mismatch between film and substrate on channel crack of thin film were investigated by many researchers [9–11]. The problem of crack propagation in a brittle thin film bonded to an elastic substrate was also solved by numerical analysis [12,13]. However, one of the problems that need to

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be fully understood is the behavior of the surface cracks in the piezoelectric thin films under thermal shock especially laser irradiation.

In the present work, the energy release rates for surface crack in a circular disc of PZT-6B thin film deposited on Si(100) substrate were investigated. By commercial FEM software ANSYS 9.0, the temperature, stress and electric fields in an uncracked PZT thin film were first calculated. And then crack problem was solved by using the equal and opposite of these piezoelectric fields as the crack surface loading. The SIFs at the crack tip were obtained from the stress and electric fields near the crack tip by the LSET [14,15] and then the energy release rates were calculated by the relation to the intensity factors. When the irradiation time and crack location were changed, the energy release rates G, G_I, G_e for total, mechanical terms (mode I) and electric contribution were investigated.

2. Statement of the problem

2.1. Geometrical and laser models

For the study of failure mechanism of a piezoelectric thin film system operating at laser irradiation condition, the physical map of temperature, thermal stress and electric fields should be first understood. Let us consider a geometrical model that comprises two layers in solid cylinder ($0 < r < r_0$), thin film with thickness h and substrate with thickness H, the cylindrical symmetry model consists of a piezoelectric thin film deposited on a crystal substrate, as schemed in Fig. 1. A surface crack with the initial length $2c$ is permeable through film thickness along radial direction, which LL^* and RR^* are crack front. A parameter l is used to denote the location of a surface crack in the thin film. The deformation in radial direction is much larger than that in the perpendicular direction due to the fact that the thickness of piezoelectric thin film is much smaller than the radius. Therefore, it is logical to have the following assumptions:

(1) Heat flux is absorbed in the outer surface and there is no heat source in the bodies.
(2) The heat flux across interface is continuous and the interface is completely heat contact.
(3) There is no body force, nor charge.
(4) Thermopiezoelectric fields are quasi-static and non-coupled.

The thin film is subject to continuous laser irradiation, and the function which is chosen to represent the heat absorption on the surface due to laser irradiation can be expressed as

$$Q(r) = q_0\left[f + (1-f)\left(\frac{r}{d}\right)^2\right]e^{-\left(\frac{r}{d}\right)^2} \tag{1}$$

where the parameters d and q_0 are the characteristic beam radius and the maximum incident flux for laser. When $f = 1$, it represents a Gaussian source [16].

2.2. Governing equations

In the problem considered, the heat conductivity equations for the transient temperature field $T_i(r,z,t)$ in thin film and substrate can be written as

$$\frac{\partial^2 T_i}{\partial r^2} + \frac{1}{r}\frac{\partial T_i}{\partial r} + \frac{\partial^2 T_i}{\partial z^2} = \frac{1}{\alpha_i}\frac{\partial T_i}{\partial t} \tag{2}$$

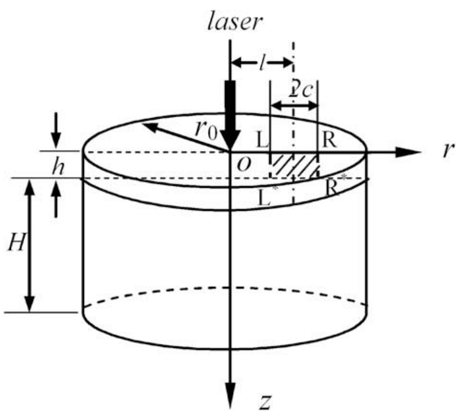

Fig. 1. Schematic of geometrical model of PZT/Si thin film system.