A novel boundary-domain element method of initial stress, finite deformation and discrete cracks in multilayered solids

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Abstract

We introduce a novel boundary-domain element method of initial stress, finite deformation and discrete cracks in multilayered solids. Because the special Green’s function of multilayers that satisfies the interfacial continuity and surface boundary conditions is employed as the integral kernel, the numerical discretization is reduced only along the crack surfaces and over the subdomains of finite deformation. Two examples are presented. First, we simulate the interfacial cohesive delamination around a through-thickness crack in a pre-stretched thin film on a flexible substrate. The process of interfacial crack initiation and growth following the expansion of a cohesive damage front, driven by the opening through-thickness crack, is shown. Second, we simulate the buckling of a delaminated pre-compressed thin film on a flexible substrate. It is shown that the compliance of the substrate plays a significant role in the critical behavior. If the substrate is more compliant than the film, the buckling initiates as a subcritical hard bifurcation. In contrast, if the substrate is stiffer than the film, it initiates as a supercritical soft bifurcation.

Keywords: anisotropic elasticity, boundary element, post-buckling, crack, delamination, finite deformation, initial stress, multilayers, thin films.

1 Introduction

Various integral-equation (IE) formulations have been developed for Kirchoff’s thin plates [1-3], Reissner’s thick plates [4-6], and mixed thin and thick plates [7]. Because only boundary integrals are involved, they have been applied to develop numerical boundary element (BE) methods to solve related boundary
value problems. Owing to the computational efficiency and convenience in meshing, the BE methods are advantageous compared to the domain-based finite element (FE) method. However, for von Karman’s plates undergoing finite deformation, a similar IE formation involves necessarily a domain integral due to the geometrical nonlinearity in addition to the boundary integrals [8-10]. The resulting numerical method is of a boundary-domain element (BDE) type, involving discretization over the domain as well as along the boundary. Because its stiffness matrix is full, the BDE method is seemingly less favored than its FE counterpart with a sparse stiffness matrix.

Despite its aforementioned disadvantage in general, we introduce the BDE method to the special case of initial stress, finite deformation and discrete cracks in multilayered solids. We employ the special Green’s function (GF) of multilayers that satisfies the interfacial continuity and surface boundary conditions as the integral kernel. Consequently, the method requires numerical discretization only along the crack surfaces and over the subdomains of finite deformation. The significant mesh reduction makes it more efficient and hence more advantageous than the FE counterpart. It may be worthwhile mentioning that the present study was motivated by our intention to simulate the process of cracking in pre-stressed thin films on a flexible substrate. The cracking shows various intriguing patterns, such as circular, asterisk and phone-cord blisters in the case of pre-compression [11], and straight, spiral and wavy through-thickness cracks in the case of pre-stretching [12].

In Section 2, we describe the physical problem of our interest, and summarize the theory of three-dimensional (3D) finite elasticity [13]. In Section 3, the integral equation of displacement is first derived, employing the special GF of multilayers as the integral kernel as mentioned earlier. Then, the integral equation of traction is derived to accommodate cracks. Because it makes no assumption on the field in the layers, the present formulation of 3D finite elasticity applies to thick layers. In Section 4, we apply the method to simulate the interfacial delamination around a through-thickness crack in a pre-stretched thin film on a flexible substrate. The simulation shows the process of interfacial crack initiation and growth following the expansion of a cohesive damage front. Then, we simulate the buckling of a delaminated pre-compressed thin film on a flexible substrate. It is shown that the compliance of the substrate plays a significant role in the critical behavior. If the substrate is more compliant than the film, the buckling initiates as a subcritical hard bifurcation, where the blister pops up with a finite deflection. In contrast, if the film is more compliant than the substrate, it initiates as a supercritical soft bifurcation, where the blister builds up its deflection gradually with increasing driving force. The magnitude of pre-stress in the film required to trigger the buckling is much lower in the former case of compliant substrate than the other case.

## 2 Physical problem and modeling

Consider a multilayered specimen with through-thickness and delamination cracks in the top (single or multiple) layers, as schematically shown in Fig. 1.
The cracks are caused by either compressive or tensile residual stresses in some layers. The specimen is modeled as a semi-infinite, multilayered, generally anisotropic and linearly elastic solid. The residual stresses are modeled by a planar self-balanced initial stress field—uniform in the in-plane directions but varying in the out-of-plane direction—before any cracking in the layered solid. When cracking, the initial stress field is partially relaxed to provide the necessary energy of dissipation. Finite deformation (with small strain but large rotation) is taken into account in general, which is necessary to model the post-buckling behavior of a blister. Otherwise, it is reduced to the case of infinitesimally small deformation. It means that the theory of finite deformation is applied to the entire structure at this point of theoretical development. When coming down to the point of numerical solution, the nonlinear terms of finite deformation are kept only for the part of thin films that undergo large deflection.

Our formulation of finite deformation along with initial stress follows closely the theory of incremental deformation developed by Biot [13]. The original theory applies to the finite deformation of both large strain and large rotation. Below summarized is only the special case of small strain and large rotation, which is sufficient in the modeling of buckling of thin films in the present case. The resulting formulation of buckled films is equivalent to what is behind von Karman’s plate theory [14]. However, the present formulation does not make any assumption on the stress field in the layers. Thus, it applies to 3D “thick” films. The present formulation treats the films and the substrate as an integrated structure. This is advantageous when accounting for the effect of a flexible substrate because only the crack surfaces need to be discretized numerically.

The equilibrium equation of the system as shown in Fig. 1 is given by

\[ A_{ij,j} = 0, \]  

(1)

where \( A \) is defined as

\[ A_{ij} = \tau_{ij} + \tau_{kj}w_{ik}, \]  

(2)

\[ \tau_{ij} = t_{ij} + S_{ij}, \]  

(3)

where \( t \) is the incremental stress, and \( S \) is the initial stress. In addition, \( w \), which describes the rotation of a material point, is defined as

\[ w_{ij} = \frac{1}{2}(u_{i,j} - u_{j,i}), \]  

(4)

where \( u \) is the displacement. The tensor \( A \) is related to the traction \( p \) prescribed on a boundary with outward normal \( n \) by

\[ A_{ij}n_j = p_i. \]  

(5)

The constitutive relationship between incremental stress \( t \) and nonlinear strain \( \varepsilon \) is given by
where $C$ is the elastic stiffness, and $\varepsilon$ is defined by

$$\varepsilon_{ij} = \varepsilon_{ij} + \frac{1}{2} w_{ik} w_{jk} .$$

The first term in the above equation is the linear strain tensor, defined by

$$e_{ij} = \frac{1}{2} (u_{i,j} + u_{j,i}) .$$

We model the through-thickness cracks by the linear elastic fracture mechanics while approaching the delamination cracks by the cohesive zone model. These cracks may be open, closed, or partially both. The through-thickness cracks are modeled as traction-free surfaces unless they are closed. When this happens, the condition of non-penetration of opposite crack surfaces is enforced. The resistance to relative sliding between opposite crack surfaces is modeled by the Coulomb friction law. The delamination cracks are modeled as opposite crack surfaces being bridged by a cohesive spring. When they are closed, the Coulomb friction law is applied in addition. The overall approach is suitable to a brittle film and a relatively tough interface.

### 3 Integral equation formulation

A novel IE formulation is developed for the previous problem of initial stress, finite deformation and discrete cracks in multilayered solids. It employs the GF of multilayers undergoing linear deformation as the integral kernel. It involves both boundary and domain integrals. However, as will be shown later, the domain integral can be reduced to the part of buckled films only.

The above equilibrium equation (1) can be rewritten as

$$\left(C_{ijkl} \varepsilon_{kl} \right)_{,j} + \left(\frac{1}{2} C_{ijkl} w_{km} w_{ln} + S_{ij} + \tau_{ji} w_{ik} \right)_{,j} = 0 ,$$

Figure 1: Cracking and finite deformation in multilayered structures subjected to (a) compressive and (b) tensile residual stresses.
after substituting the later equations. By considering the second term as a body force in general, the displacement field, \( \mathbf{u} \), can be derived as

\[
c_{pq}u_q = \oint_{\Gamma} \left\{ u_{pq}^*(p_i - S_j n_j) - p_{pq}^* u_i \right\} d\Gamma + \oint_{C} p_{pq}^* [u_i] d\Gamma - \int_{\Omega} u_{pq}^* N_i d\Omega ,
\]

where \( \mathbf{c} \) is a constant matrix, different for different locations of source point, \( \Gamma \) indicates the regular boundaries, \( C \) indicates one side of the crack surfaces, \( \Omega \) indicates the domain, \( [u] \) is the crack displacement jump, and the nonlinear force \( N \) due to large rotation is given by

\[
N_j = \frac{1}{2} C_{ijkl} w_{km} w_{lm} + S_{ij} w_{ik} .
\]

The integral kernels \( u^* \) and \( p^* \) are the GFs of displacement and traction of multilayers undergoing linear deformation. An efficient scheme for evaluation of these GFs and their derivatives with respect to source point has been developed recently by Yang and Pan [15]. In deriving the above integral equation (10), the equilibrium state of the initial stress field, \( S \), and the condition of small strain relative to rotation are applied.

To solve the present problem of cracks in a single-domain formulation, the above integral equation of displacement is unworkable. Instead, the integral equation of traction is required [16, 17]. It is obtained by taking derivative of eqn (10) with respect to the coordinates of \( \mathbf{u} \) on the left-hand side and by applying the constitutive relationship; it is given by

\[
p_p^+ - \frac{1}{2} (N_p^+ + N_p^-) n_j^+ =
\]

\[
\oint_{\Gamma} \left\{ U_{pq}^* (p_i - S_j n_j) - P_{pq}^* u_i \right\} d\Gamma + \oint_{C} P_{pq}^* [u_i] d\Gamma - \int_{\Omega} U_{pq}^* N_j d\Omega ,
\]

where the superscript + and – respectively indicate the two opposite sides of a crack, and \( U^* \) and \( P^* \) are corresponding functions derived from \( u^* \) and \( p^* \).

In addition, the integral equation of rotation is required in solving the present problem of finite deformation. It is obtained by taking derivative of eqn (10) and by applying the definition of rotation tensor, eqn (4),

\[
w_{pq} = \oint_{\Gamma} \left\{ w_{pq}^* (p_i - S_j n_j) - \tau_{pq}^* u_i \right\} d\Gamma + \oint_{C} \tau_{pq}^* [u_i] d\Gamma - \int_{\Omega} w_{pq}^* N_j d\Omega ,
\]

where \( w^* \) and \( \tau^* \) are corresponding functions derived from \( u^* \) and \( p^* \). Necessarily considered in eqn (13) is the case when the source point is interior.

In the present case of initial stress-driven cracking, no external loading is applied. It means that the first term on the right-hand side of the above integral equations (10), (11) and (12) vanishes. Furthermore, it is expected that the nonlinear force due to large rotation, \( N \), is negligible in domains other than the buckled films undergoing large deflection. Thus, the term of domain integral can be reduced to the buckled films. In solving the problem, only the last two integral equations of traction and rotation are needed.
The standard numerical procedure is applied to the final boundary-domain integral equations of traction and rotation. The involved crack surface $C$ and domain $B$ are discretized into surface and volume elements, correspondingly. In each element, a number of nodes are planted, and a quantity is interpolated by the nodal values. Substituting the approximating fields into the integral equations and assigning the traction and rotation on the left-hand side of the equations to be the $m$th nodal values, a set of algebraic equations is obtained,

$$P_p^{+(m)} - \frac{1}{2} (N^{+(m)}_{pq} + N^{-(m)}_{pq}) n_i^{+(m)} = \int_H (\nu^{mn}_{pi}) - G^{mn}_{pi,j} N_{ij}^{(n)} \ ,$$  

$$w_{pq}^{(m)} = \int_T (\nu^{mn}_{qi}) - W_{pi,j}^{mn} N_{ij}^{(n)} \ ,$$

where the matrices $H$, $G$, $T$ and $W$ are integrals of the corresponding GFs within the $n$th element. Appropriate (boundary) conditions need to be imposed to ensure a unique solution to the set of equations. These conditions are given by an appropriate model of the crack surfaces. Since the general case of cracks that may be traction-free, in frictional contact, or bridged by a cohesive spring is considered, the problem is nonlinear even if the finite deflection, i.e., geometrical nonlinearity, is absent. Therefore, an iterative scheme is necessary to solve the set of equations. In the present study, the iterative solver of successive over-relaxation is adopted. Its efficiency has been demonstrated by the successful applications to similar cases of 2D and 3D cracks and 3D bolted joint [16, 18, 19]. One may refer to the cited papers for detail of the iterative scheme.

4 Numerical examples

In the section, we present two simulations within the preceding formulation: cohesive delamination around a through-thickness crack, and post-buckling of a delaminated film, on a flexible substrate. In both cases, the fracture is driven by the residual stress in the film, tensile or compressive, correspondingly.

In the first case, we consider a Si thin film coherently bonded to a Ge substrate. A tensile misfit strain of 4% is built in the Si film according to their difference in lattice constant. A through-thickness crack is introduced to the film. Due to the tensile residual stress, the crack is opened, driving delamination along the interface. In the simulation, we loaded the film up to the full amount of misfit strain in four incremental steps, each of 1%. Figure 2 shows the progression of damage front and the initiation of crack. Note that when the delamination damage and crack progress, the through-thickness crack would suffer increasing intensity of singular stress at the tips. It would propagate as well. A simulation of the simultaneous growth of through-thickness and delamination cracks and a parametric study of the behavior are in progress.

In the second case, we consider an isotropic system of film bonded to a substrate. Their Poisson’s ratios are the same, but Young’s moduli are different. A circular delamination crack is introduced at the interface. The film is subjected to a compressive residual strain. We carried out simulation of the system under
residual strain of various magnitudes but without crack growth. Two cases are considered, with modulus ratio of film to substrate equal to 1/3 and 1/0.5, respectively. The results of maximal deflection are shown as a function of residual strain magnitude in Figs. 3 (a) and (b). Note that a very small pressure was applied on the crack surfaces to trigger the buckling. In both cases, a sudden increase of deflection over a critical residual strain is observed, indicating the buckling initiation. However, in the case that the film is more compliant, the buckling happens as a supercritical soft bifurcation, indicated by a kink of slope in the maximum deflection-loading variation. In the other case that the film is stiffer, it happens as a subcritical hard bifurcation, indicated by a jump of deflection at the critical point. In addition, it is observed that a much larger magnitude of residual strain is needed to trigger the buckling if the substrate is stiffer. This is understood as a result of the stiffer constraint on rotation at the crack front. The lateral relaxation of the film on a compliant substrate plays a secondary role in the critical process.

Figure 2: Contours of traction magnitude along interface around a through-thickness crack in a system of pre-stretched film at increasing magnitude of residual strain (a) 0.02; (b) 0.03; (c) 0.04. (The normal traction component is not counted if it is in compression, which occurs right outside the damage zone.) The figure shows the progression of delamination damage zone (a, b) and further development into a crack (c) as the residual strain increases. A cohesive force law of truncated plateau is used—the traction magnitude in the damage zone is thus uniform.

5 Conclusion

We have developed a novel IE formation of initial stress, finite deformation and discrete cracks in multilayered solids within the theory of anisotropic finite
elasticity. The integral equations of displacement, traction and rotation are presented. It has been further developed into a numerical BDE method to solve related boundary value problems. Because the special GF of multilayers that satisfies the interfacial continuity and boundary conditions is employed as the integral kernel, the BDE method requires numerical discretization only along one side of the cracks and over the subdomains of finite deformation. This results in a significant reduction in meshing and hence improved efficiency/accuracy in the numerical solution compared to the conventional IE formulations and the FE counterpart.

Figure 3: Variation of maximum deflection of a delaminated film on a flexible substrate with modulus ratio of film to substrate equal to (a) 1/3; (b) 1/0.5.

Two numerical examples are presented. In the first example, we simulated the initiation and growth of a delamination crack following a cohesive damage front around a through-thickness crack opened by tensile residual stress in a thin-film-on-substrate structure. In the second example, we simulated the buckling of a delaminated thin film under compressive residual stress on a flexible substrate. In this work, the focus is on the effect of compliance of the substrate on the critical behavior of buckling. It is shown that if the film is more compliant than the substrate, the buckling initiates in a stable fashion, a second-order phase transition, or say, a supercritical soft bifurcation. In contrast, if the substrate is
more compliant, it initiates in an unstable fashion, a first-order phase transition, or say, a subcritical hard bifurcation. These examples have demonstrated the validity and efficiency of the method.

References


