On Several Problems of Macro / Micro Failure Mechanics

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Keywords: Failure Mechanics, Micromechanical Damage Model, Constitutive Relation, Brittle Material, Piezoelectric Material, Stress Shielding, Damage Localization, Manufacturing Mechanics, Bucking, Delamination, Film / Substrate Structure

ABSTRACT

In this paper, some research results obtained recently by the authors’ group on several problems of macro- and micro-failure mechanics are reviewed. These problems include the micromechanical modeling of constitutive response of microcrack-weakened brittle materials, microcrack-induced stress shielding and damage localization at a crack tip in brittle materials, damage and fracture of piezoelectric materials, buckling and growth of delamination in film/substrate structures, and structural mechanics and manufacturing mechanics in electronic packaging.

1. INTRODUCTION

Due to the increasing demand of high structural performance requirements, many advanced materials with good mechanical properties have been developed, and it becomes more and more important to gain a through understanding of materials. Under such an industrial background, the modern macro- and micro-failure theory has been attracting wider and wider attention from scientists of mechanics and materials. Following [1, 2, 3], this paper shows some research results on several problems in this field obtained recently by the authors’ group.

2. DMG MODEL AND ITS APPLICATIONS

2.1. DMG damage model

Nucleation, growth and coalescence of microcracks are typical damage mechanisms in many brittle materials such as concrete and ceramics. Due to the geometrical features of microcracks, the damage of brittle materials is often highly anisotropic. The mechanisms of growth and fracture of microcracks are so complex that brittle materials often exhibit very different macroscopic behaviors
under different loading conditions. Therefore, it is very difficult to formulate a complete three-dimensional micromechanical damage theory for brittle materials. In most of the previous damage models [4, 5], the damage state is described by internal variables in the form of scalar, vector or tensor. However, the microscopic damage is often not only very complex but also different under different loading conditions, and so how to exactly describe the damage of materials is an unsolved issue. It is also very difficult for these previous models to handle damage problems of complex loading.

Recently, Feng and Yu [6-12] developed a rather complete micromechanical model to analyze the micro-damage and constitutive relation of brittle or quasi-brittle materials subjected to triaxial tension or compression or even complex loading. This model is based on the concept of domain of microcrack growth (DMG), and so called the damage model of DMG. The DMG is defined as the possible orientation scope of all propagated microcracks after a loading path, that is, all microcracks whose normal vectors are in the orientation scope of DMG must have propagated after the loading path. Using this concept, the complex evolution of anisotropic damage in brittle materials under complex loading can be described well [6-8].

In [8, 9], the constitutive response of brittle or quasi-brittle materials was classified into four stages, namely, linear elasticity, pre-peak nonlinear hardening, rapid stress drop and post-peak strain softening. The microscopic damage mechanisms in all these stages were investigated. The influences of microscopic mechanisms including the self-similar growth of open microcracks [6-8], the frictional sliding, self-similar growth and kinking growth of closed microcracks [7] as well as damage localization [8-10, 12] were all considered in the constitutive relation. It was pointed out [8] that the regime of pre-peak nonlinear hardening corresponds to distributed damage, i.e., the stable propagation of microcracks, while the rapid stress drop and the strain softening reflect the transition from continuous distributed damage to damage localization. The constitutive relation in the four stages under triaxial tension or compression can be found in [8]. Also, the condition of axial splitting under compression was given in [9].

2.2. Residual strain of brittle materials

Both experimental observation and theoretical research indicate the necessity to incorporate residual strains caused by microcracking into modeling. Based on the DMG model, Yu and Feng [13] investigated the microscopic mechanisms of residual strains and their influences on constitutive relation in brittle or quasi-brittle materials. It was thought that there are two reasons for the occurrence of residual strains, i.e., the release of residual stresses in the materials due to microcrack growth and the microscopic plastic deformation along the front edges of propagated microcracks. Firstly, due to such reasons as thermal mismatch during formation process, there often exist residual stresses distributed in brittle materials and assumed to satisfy a certain statistical distribution rule. In order to include the residual stresses in the constitutive relation, for simplicity, consider only the statistically averaged effect of the residual stresses and assume that the residual stresses around all microcracks are of the same average values. If a microcrack radius grows from the initial value \( \sigma_r \) to \( a \) under external applied loading, the residual stresses in the interface around the microcrack will be released. After the applied loading is unloaded, the opening displacement of the microcrack will not return to zero, in other words, some residual deformation will be left. The average of the residual opening displacement of a microcrack due to the release of residual stresses was deduced and denoted by \( \bar{E}^1(a) \). Secondly, even for a very brittle material, some complex energy dissipation
mechanisms exist along the front edge of a propagating microcrack, among which the most important is often the plastic deformation in a very small zone. The microscopic plastic deformation dissipates part of external applied energy and causes microscopic damage such as nucleation and growth of microvoids in a smaller zone. Just because of the microscopic plasticity, some opening displacement will remain in the propagated microcracks after completely unloading. Under this microscopic mechanism, the average opening displacement of the microcrack after unloading was denoted by $b^{+}(a)$.

Considering both of the microscopic mechanisms, the irreversible strains induced by the growth of a single microcrack were obtained as [13]

$$\bar{\varepsilon}_p^R(a) = \pi a^{-1} [b^{+}(a) + b^{-}(a)] g_{ij} g_{ij}$$  \hspace{1cm} (1)

where $g_{ij}$ are the components of transformation matrix between the local and global coordinate systems [6, 7]. Then, based on the DMG damage model and the above results of microscopic mechanism analysis, the complete stress-strain relation of materials with residual strains was given for the four stages of linear elasticity, non-linear hardening, stress drop and strain softening [13]. This model can describe the damage and deformation behavior of brittle materials under complex loading also.

2.3. Crack tip stress shielding by microcracking

Experimental and theoretical evidences show that the profuse microcracks at the tip of a macroscopic crack may shield the crack tip from the action of remote stress and postpone the onset of unstable macroscopic crack propagation. In [14], the stress shielding effect due to microcracks at the tip of a macroscopic stationary mode-I crack was studied. The analysis method adopted combines the micromechanical approach with the effective elastic medium approach. As in most studies on this subject to date, a saturated damage stage was introduced into the micromechanics-based damage model of DMG. From this model, the constitutive relations for the three zones around the crack tip, which are the outer linear elastic zone, the inner saturated damage zone and the transition damage zone, were derived by considering the anisotropic features of microcracking damage [11]. Then, the shielding effect, which is often expressed by the ratio of the near-tip to remote stress intensity factors $K_{tip}/K_{\infty}$, was calculated by two methods, namely, the conventional $J$-integral conservation method and the modified $J$-integral method develop by Feng and Yu [14]. It was shown that the shielding ratio from the modified $J$-integral method is smaller than that from the $J$-integral conservation method, but their difference is usually not big. The result from the modified $J$-integral method accounts for the influences of such factors as the randomly distribution of microcracks in the orientation space, the anisotropic evolution of microcracking damage and the transition damage zone. Therefore, it is more reasonable than the results in the previous literature, which were often based on the approximation of path-independence of $J$-integral and the assumption of isotropic [15] or complete anisotropic [16] damage.

2.4. Damage localization at crack tip

Besides the stress shielding effect, damage localization may occur in a smaller scope around the crack tip due to the stress drop and strain softening behavior of brittle materials. Feng and Yu [17] analyzed the fracture process zone at the near tip of mode-I crack in a brittle damaged material. It
was pointed out that under external loads a narrow strip zone of damage localization, i.e., a damage localization band, will form ahead of the crack, and that it is impossible that a complete damage zone with a finite width occurs around the crack tip. The qualitative analysis of damage and the comparison of dissipated energy for different fracture mechanisms proved that the crack tip field with damage localization is more reasonable than that obtained by Bui and Ehrlicher [18]. Thus, corresponding to the four stages of the stress-strain relation of brittle materials mentioned above, the fields around the crack tip can be classified into three zones with different magnitudes of damage, namely, the elastic and undamaged zone, the distributed damage zone and the damage localization band. By using the analysis method of Dugdale-Barenblatt model, the relation between the length of damage localization band and the external loads can be obtained, as was illustrated by two examples.

3. DAMAGE AND FRACTURE OF THERMOPIEZOELECTRIC MATERIALS

Piezoelectric materials are feasible to achieve an accurate response, to monitor and provide effective control of engineering structures, and so are often used in smart structures and advanced equipment. In engineering practice, the components of smart structures are often exposed to thermal, mechanical and electric loads during service condition. Therefore, the fracture and damage behavior of microdefected smart materials requires some intensive and fundamental research.

3.1. Crack tip fields

By way of Stroh’s formula and the property on the root of multiplicity in piezoelectricity, the logarithmic singularity at a crack tip in homogeneous piezoelectric materials was investigated by Qin and Yu [19]. For a semi-infinite crack in a piezoelectric media, the study showed that both the stress and electric displacement fields at crack tips may be in the order of \( r^{-\frac{1}{2}} \), or \( r^{-\frac{1}{2}} \ln r \), or \( r^{-\frac{1}{2}} \ln^2 r \), or \( r^{-\frac{3}{2}} \ln^3 r \), as \( r \to 0 \), where \( r \) is the distance from crack tip to field point, depending on which conditions are satisfied [19].

Successively, the plane problem of a crack terminating at the interface between two piezoelectric solids was studied by using the concept of axial conjugate and the technique of singular integral equations [20, 21]. The numerical results for this problem indicated that the order of singularity in the traction-charge field at a crack tip depends strongly on the angle between the crack line and the interface.

Further, the singular crack tip behavior for thermoelectroelastic problems was also studied [22]. By application of Fourier transformations and extended Stroh’s formula, the thermoelectroelastic problem can be reduced to a pair of dual integral equations for the temperature field with the aid of an auxiliary function. The electroelastic field is governed by another pair of dual integral equations. The inverse square root singularity is found for the temperature field while the logarithmic singularity is prevailed for the electroelastic field regardless of whether the crack lies in a homogeneous piezoelectric solid or at an interface of two dissimilar piezoelectric materials.

3.2. Overall material constants

Considering the above theoretical results, the formulation for estimating effective material constants was developed by the dilute, self-consistent, Mori-Tanaka and generalized self-consistent methods for thermopiezoelectric solids with microcracks or holes of various shapes [23-27]. These
methods are capable of determination of effective properties such as the conductivity, electroelastic moduli, thermal expansion and pyroelectric coefficients. The above material constants affected by microcracks or holes were derived by way of Stroh's formula and some recently developed explicit solutions of a crack or a hole in an infinite piezoelectric solid subjected to remote thermal, electrical and elastic loads [22, 27]. In common with the corresponding uncoupled thermal, electric and elastic behavior, the dilute and Mori-Tanaka techniques give explicit estimates of the effective thermoelectroelastic moduli. The self-consistent scheme and the generalized self-consistent scheme, however, give only implicit estimates of the effective thermoelectroelastic moduli with nonlinear algebraic matrix equations. Numerical results were given for a particular cracked material to examine the behaviors of the four micromechanics models.

4. DELAMINATION IN FILM/SUBSTRATE STRUCTURES

In the design and manufacture of advanced materials and structures such as the micro electrical-mechanical systems (MEMS), there are a lot of new mechanics problems needed to be solved, which include the mechanics analysis of manufacturing process, the meso- and micro-structural and failure mechanics analysis of the micro electrical materials, components and systems. There are many film/substrate structures in MEMS. Residual stresses are often induced in such a structure by the thermal mismatch between the film and the substrate or by the influence of complicated environment during operation. Zhang and Yu [28-31] investigated the buckling and growth problem of circular delamination in film/substrate structures.

In [28], the buckling and post-buckling of the unilateral constrained plate subjected to edge thrust and lateral pressure was analyzed by using perturbation analysis and the shooting method. The post-buckling paths of clamped and simply supported circular plates were obtained. The characteristics of buckling and post-buckling of the plates, and also the stable condition for buckling were presented. These results as well as the analysis method adopted are very useful for the investigation of the buckling and growth of delamination in film/substrate structures.

Then, the circular delamination in a film/substrate system was treated as a thin plate clamped to the substrate, as shown in Fig. 1. The first axisymmetric buckling of a circular delamination was analyzed by using the high-order perturbation analysis and the shooting method [29]. The six-order approximate results for the axisymmetric post-buckling show a good agreement with the finite element numerical results of Raju and Rao [32], as shown in Fig. 2, where $p$ and $\psi$ are the edge pressure and its critical value of buckling, $s$ is the displacement at the center of the plate. By using these results, the driving force on the interface crack and the interface toughness that is a function of the phase angle $\psi$ were deduced. It was found from the analysis that the high-order perturbation results have some characteristics evidently different to the low-order solutions. When a two-order expansion is applied, for example, it was concluded that the axisymmetric buckling and its growth are always stable [33, 34]. However, the results of higher order expansion indicate that either the stable growth or the unstable growth occurs only when their corresponding conditions are satisfied. Two characteristic blister radii, $R_s$ and $R_p$ exist under a certain residual pressure load, $p$. The delamination will buckle when the debonding dimension is larger than $R_s$, and grow along the interface when the debonding dimension is larger than $R_p$. The conditions of no growth, stable growth and unstable
growth of the delamination were all given by comparing the driving force and the resistance under different pressure.

Fig. 1. Delamination in a film/substrate system.

Fig. 2. The buckling path.

Under a higher pressure, the secondary nonaxisymmetric buckling will occur following the axisymmetric buckling, and then the toughness and the driving force of the interface crack will not be uniform along the delamination front. So the growth of circular delamination will not be in a self-similar fashion. That is to say the front of the blister will no longer be circular after some growth. The secondary nonaxisymmetric buckling of a circular delamination was studied by Zhang and Yu [30]. Some equations in closed form for the buckling and growth of the circular delamination were deduced by recourse to the moving boundary variational principle. The driving force and the mode-adjusted toughness of the interface crack are uneven along the periphery of the circular blister, because of the nonaxisymmetric deformation, as is the reason of nonaxisymmetric growth of circular delamination. The energy release rate of a mode I, II and III mixed interface crack, and the relationship between the energy release rate and the boundary configuration were obtained. Two major results about the nonaxisymmetric growth were obtained in [31]. First, the nonaxisymmetric buckling bifurcated from the axisymmetric buckling was calculated by using the perturbation expansion method. The lowest secondary critical load is much smaller than that obtained by Hutchinson, Thouless and others [33, 34]. The nonaxisymmetric buckling was considered as the mechanism of the nonaxisymmetric growth of buckling-driven circular delamination. Second, without any biased assumption regarding of the delamination front shape, the nonaxisymmetric growth with different buckling modes was simulated, and the corresponding critical loads were evaluated.

5. MANUFACTURING MECHANICS IN ELECTRONIC PACKAGING

5.1. Edge effect stresses in bimaterial elements

As mentioned before, the design and manufacture of MEMS need the investigation to their basic elements including the micro electrical materials, micro machines, micro sensors and actuators, and the investigation to macro- and micro structural mechanics and manufacturing mechanics. The design optimization of MEMS may be achieved with the aid of the analysis of structural and manufacturing
mechanics. Xu and Yu [35, 36] investigated the effect of geometrical configurations on the stresses in double-layer structures and the effect of edge combined configurations in multilayer structures. Their results show that the edge shape of such kinds of structures can evidently affect the magnitude of the edge stress concentration. It was suggested, therefore, that the edge shapes with smaller angles be adopted in the structural design.

The finite element analysis to stair-shaped multilayer structures shown that the specific combined configurations should be determined by considering the ratios of parameters of the adjacent materials [35, 36].

5.2. Stress analysis of manufacturing process of microelectronic components

The temperature, to which the electronic packaging is exposed, may fluctuate between 300 and 400°C during normal operation, and between 1200 and 1800 during manufacturing process. The thermal stresses developed during the manufacturing process often exert a great influence on the quality of the electronic packaging. The residual stresses of MOS components during manufacturing can be analyzed by the method developed in [35, 37]. In this method, some elements are controlled to be inactive at the specific time. Unlike most of the previous work on this subject, where only the stresses induced by the temperature history of an established structure were analyzed, the histories of both temperature and configuration variation were considered simultaneously. One example is shown in Fig. 4, where the materials SiO2, poly Si, SiO2, SiO2 and PSG are added to the single Si substrate in steps 1 to 5, respectively. This approach is proved very effective to simulate the manufacturing process of electronic packaging. Another example is the residual stress analysis of sintering of AlN multilayer ceramic substrates in electronic packaging [38].

![Fig. 3. The manufacturing process of an MOS component.](image)

5.3. Residual stresses in injection molding products

It is well known that there are very complicated relations among the temperature distribution, the metallic structure and the stress-strain state during the course of heat processing of metal due to their coupling effects [35]. Fig. 6 shows the physical mechanisms and phenomena with regard to the temperature distribution, the metallic structure and the stress-strain state. In spite of that the complexity of the relationship makes it difficult to analyze the stress distribution during heat
processing of metals, some models within the framework of continuum thermodynamics have been developed to account for their coupling effects during the welding, casting, and heat treatment of metallic materials [39].

On the basis of the Inoue's work [39], a finite element method was developed to analyze the residual stresses of polymer materials during the injection molding processes in the post-filling stage. The evolution of microstructure during the injection molding process of semi-crystalline thermoplastic polymers is very complex. In the post-filling stage, for example, crystallization and frozen in orientation often occur in the polymer materials. The influences of temperature variation, crystallization and frozen in orientation were considered in the constitutive model, and a corresponding finite element program was also developed in [35].

![Diagram](image)

**Fig. 4.** Relationship among temperature, metallic structure and stress-strain state.

6. CONCLUSIONS

The modern failure theory with the main characteristic of the combination of macro- and microscopic study has been developing rapidly. The research on damage and fracture of materials from macro- and microscopic viewpoint can show the nature of material failure clearly, model the complex behaviors of materials under various conditions, and provide the theoretical basis for using and designing materials. In spite of the great success of damage and fracture mechanics, a lot of problems, which emerge with the development of advanced materials and technologies, need to be investigated theoretically and experimentally. With regard to the fields discussed in this paper, several examples of these problems are the micromechanics-based phenomenological damage theory (or quasi-phenomenological damage theory) [5], the proper description of damage and its evolution, the mechanics analysis of manufacturing process, the meso- and micro-structural and failure mechanics analysis of the micro-electrical materials, components and systems.

**Acknowledgments:** The supports of the Doctoral Program Foundation of State Education Commission, the National Natural Science Foundation, the Post-Doctoral Science Foundation of China are gratefully acknowledged. The authors also wish to thank Dr. Q. J. Xu and Dr. X. Y. Zhang for their contribution to this paper.
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