Fracture Mechanics and Failure of Multilayered Materials and Structures

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Multilayered materials and structures are of special interest to both academic researchers and industrial engineers as they have been used in an increasing number of applications, such as micro-electromechanical system (MEMS) on polymer substrate, protective coating on metal structure for anti-corrosion, ceramic coating on metal substrate for abrasion resistance, thermal barrier coatings, metal or metal oxide coating on metal-coated polymer for reflectance tuning and protection, as well as laminated composites and structures, etc. However, the surface layer and joint interface are commonly prone to premature failures because of cracking and delamination due to their different thermal and mechanical properties. In return, the premature failures will affect the performance and structural integrity of the device and eventually cause the failure of the multilayered structures to perform their functions. Therefore, it is essential to understand the mechanical behavior and corresponding failure mechanisms of the multilayered systems.

This Ph.D. dissertation focuses on the study of opening-mode fracture (OMF) behavior and interfacial delamination in different types of multilayered structures, such as the aluminum plate or wire with alumina protective coating, multilayered advanced polymeric reflectors, and asphalt pavements. In addition, another failure mechanism, i.e. the material degradation and aging, is also studied.

Firstly, a two-dimensional (2D) elastoplastic fracture model in Cartesian coordinates is developed to study the OMF in the thin alumina film fully bonded to an aluminum plate undergoing large-scale yielding. The stress field in the coating layer is described by one section between two adjacent cracks. The 2D plane strain formulations are employed to analyze the elastic field in the thin film, while a one-dimensional (1D) linear hardening plastic model is applied to account for the large plastic deformations in the substrate under substantial yielding. An elastoplastic shear lag model
is established to transfer the tensile stress in the substrate to the thin film. General formulations and explicit expressions of the elastic/elastoplastic solutions of the thin film/substrate system under different loading stages have been presented. The elastic field in the thin film is then verified with the finite element (FE) results. The fracture energy release rate (ERR) is calculated and corresponding elastoplastic fracture analysis is conducted. Experimental characterization is further conducted to validate the present model; the results show that this fracture model can capture the fracture initiation, infilling, and saturation in the thin film successfully. This model has been extended to cylindrical coordinates, where the alumina coating is fully bonded to an aluminum wire/rod. Due to the axial symmetry, the proposed 2D elastoplastic fracture model has been reproduced in polar coordinates and be used to study the OMF behavior of alumina coating fully bonded to an aluminum wire.

For the case where thermal loading is applied on coating/substrate structures, neither the plane strain nor plane stress assumption can be applied because the thermal loading would introduce multi axial normal stress, therefore, a three-dimensional (3D) elastic fracture model is then developed to study the OMF in the coating fully bonded to the elastic substrate. When the temperature change reaches a certain level, block cracking will initiate in the surface layer to release the accumulated thermal stress. For simplicity, we assume the top surface of the coating would keep flat and in a rectangular shape after deformation. Then the elastic field in both coating and substrate is analyzed and verified with the FE results. The fracture ERR is then obtained based on the solved elastic field and used to analyze the fracture initiation, infilling, and saturation. In order to verify the fracture analysis, the theoretical fracture analysis results are compared with FE simulation results based on the cohesive zone model (CZM) and experimental data from the literature. The good agreement demonstrates the accuracy of the proposed 3D fracture model. In addition, this model for coating/substrate system is extended to study multilayered structures with arbitrary number of layers. In order to verify this extended model, the predicted elastic field in an advanced polymeric solar reflector is compared with FE simulation results and parametric studies are conducted to investigate the effect of geometry on the accuracy of this model. Furthermore, the fracture behavior of the surface layer in the advanced polymeric solar reflector is studied using the calculated fracture ERR.

Additionally, the delamination behavior, as another common failure mode of the coating/substrate
structures, is then studied. The delamination fracture energy of a multilayered glass solar reflector is tested by employing the width-tapered beam method. The testing results indicate that the weakest interface of the multilayered solar reflector would be the glass-copper interface with a delamination fracture energy $4.4 \, J/m^2$. Using the tested fracture energy as an input, an FE model is built based on the CZM and the returned peeling force from simulation is then compared with the test results to verify the accuracy of the test method. The good agreement between the simulation and test results demonstrates that the width-tapered beam method is accurate enough to measure the delamination fracture energy of this multilayered solar reflector. Additionally, the effect of aging on the delamination fracture energy is investigated by measuring the delamination fracture energy after 50 hrs' accelerated aging test. The results show that the aging has minor effect of delamination fracture energy for samples with alumina ($Al_2O_3$) protective coating, while it reduces the delamination fracture energy for samples with titania ($TiO_2$) protective coating.

As another failure mechanism, the material degradation or aging behavior is studied in this dissertation. The weight percentage of oxygen (WPO) in three types of asphalt binders extracted from reclaimed asphalt pavements (RAPs) and one extracted from fresh Hot Mix Asphalt (HMA), that have been aged under continuous ultraviolet (UV) or UV/moisture/condensation exposure for different period, is measured using an energy-dispersive X-ray spectroscopy (EDX). Then the tested data are fitted based on two classic aging models, namely the fast-rate constant-rate (FRCR) and nonlinear differential dynamic (NDD) models. The good fitted results show that both FRCR and NDD models can capture the aging behavior of asphalt binders extracted from both RAPs and fresh HMA under continuous UV or UV/moisture/condensation exposure. Meanwhile, although exposed under UV for the same time, the WPO in samples after UV/moisture/condensation aging are lower than those in samples after continuous UV aging, which indicates that condensation and moisture reduce the UV-induced photo-oxidative aging rate.
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Chapter 1

Introduction

1.1 Coating/Substrate Structures

Typically a substrate-coating system is composed of a relatively brittle coating layer and a ductile substrate which interest both academic and industrial researchers for their extraordinary applications [70; 119; 214; 199; 211; 23], such as micro-electromechanical system (MEMS) on polymer substrate, protective coating on metal structure for anti-corrosion as shown as in Fig. 1.1(a) [3], the glass on hybrid solar roofing panel for protection as shown in Fig. 1.1(b) [39], protective metal oxide coating on advanced polymeric reflectors presented in Fig. 1.1(c) [1], and thermal barrier coating which is the ceramic coating on turbine housing in Fig. 1.1(d) [6]).

Owing to the advantageous properties of metal oxide such as higher hardness, perfect wear-resistance, enhanced anti-oxidation, improved thermal impact-resistance, they have wide applications in many industries such as automobile, architecture, MEMS, and surgery [42; 149; 112]. However, the metal oxide coating/substrate joint usually suffers premature failure because of cracking and delamination due to its different thermal and mechanical properties, affecting the performance and structural integrity of the device and eventually eliminating the coating’s ability to perform its function. Therefore, it is essential to understand the structural behavior and corresponding failure mechanism of the coating/substrate system.
(a) Protective coating on pipeline [3]

(b) Hybrid solar roofing panel [39]

(c) Advanced polymeric reflector with metal oxide protective coating [1]

(d) Thermal barrier coating on turbine housing [6]

Figure 1.1: Common coating/substrate systems or structures
1.2 Review of historic research

1.2.1 Two-dimensional Stress and Fracture Analysis for Coating/Substrate Structures

The cracking of a brittle film on a ductile substrate has been intensively studied both experimentally and theoretically. For sub-micron thin film coatings, uniaxial tension of a flat coating-substrate coupon is a common method to evaluate the coating fracture and interfacial strength between the coating and the substrate [9; 98; 218; 220; 34], because of the relatively simple testing configuration and well-controlled crack patterns. Channel-mode and opening-mode fractures (OMFs) have been commonly observed in thin-layer coating [134; 197; 183; 34]. Due to tensile stress, the opening-mode cracks initiate perpendicular to the tensile force and propagate in the same direction as channel mode fractures, which exhibit a three-dimensional (3D) process. To interpret such open-fracture crack patterns, 3D finite element (FE) analysis [147] was performed to study the mechanics of crack growth and decohesion in a highly compliant thin film bonded to a rigid substrate. The computed results showed that the stress intensity factor along the crack edge reaches a steady state value when the crack is about twice the film thickness and confirmed that potential decohesion of the film from the substrate arise from the existence of high interface stresses.

The stretchability of thin metal films on elastomeric substrates was originally studied by Li et al. [121]. Li and Suo [122] later found that the modes of tensile deformation can be identified depending on the stiffness of the substrate. Their next study [123] showed that interfacial sliding accommodates the necking of the film. Jia et al. [101] confirmed such tensile failures in thin film using computational modeling, where the channel cracking of the top oxide layer and the delamination along the oxide-organic interface release elastic energy and drive the tensile failure of the organic-inorganic multilayer permeation barriers. Furthermore, the real-time evolution of the crack density in thin films had been monitored inside a scanning electron microscope as a function of applied tensile strain [160]. Recently, Jia and Li [100] investigated the necking instability, which is the onset of ductile failure of substrate-supported metal layers, and showed that the necking retardation in an elastomer-supported metal layer allows more energy absorption and dissipation than an all-metal single layer. Their results also quantitatively correlated both the critical necking limit strain and the necking band orientation with the material and geometric properties of the
substrate-metal bilayer, which facilitates the optimal design of substrate-supported metal structures with enhanced deformability and energy absorbing capacity.

The finite-difference method [20; 21] simulated the deformation and fracture of composite materials with different coating thickness. The stress concentration near the interface increases as the coating thickness decreases, a result consistent with the prediction made by the theoretical solutions alternatively obtained by the strain gradient plasticity models [206; 207]. Moreover, the coating thickness effect enhances as plastic deformation develops in the substrate, amounting 25% at the pre-fracture stage. To further investigate this effect, special attention had been addressed to the mechanisms of stress concentrations near the complicated-geometry interfaces [20]. Their numerical results showed that local concentrations of tensile and compressive stresses are mainly developed throughout the interface and the serrated shape of the material-coating interface retards propagation of the main longitudinal crack, preventing the coating from peeling under external compression of the specimen. Therefore, premature failure of materials could be attributed to the presence of local tensile stresses under any type of external loading.

Even though the process itself is 3D, the two-dimensional (2D) plane strain analysis often solves the elastic fields of a steady-state channeling crack in the thin film caused by an OMF. Because a singular point exists at the crack tip located at the interface between the fractured and intact layers, many fracture studies have focused on the local elastic solution in the neighborhood of that point [26; 191; 222; 27; 118; 218; 87; 212; 198; 34; 35]. Hu [88] investigated the critical stress for the steady-state cracking of thin film coatings on ductile substrates by assuming a sliding (yielding) interface and linear elastic coating and substrate. In 1992, Beuth [26] developed a dimensionless plane strain stress intensity factor to characterize the cracking of thin films bonded to elastic substrate, where a dimensionless integral of the crack opening displacement was related to the steady-state energy release rate (ERR) for crack channeling across the film, and later extended this work to elastic-plastic substrate to account for the yielding in the ductile substrates by extracting the dimensionless integral of the crack opening displacement through FE analysis [27]. Although local solutions such as these are useful in the study of fracture propagation, they cannot be directly used to predict fracture initiation, predict fracture spacing, or study the interaction between fractures [226]. According to the studies from [16; 19; 18], to completely understand fracture spacing, an overall elastic field in the thin film that is based on the complete set of governing equations for the
elastic boundary value problems should be used.

The interpretation of fracture development often uses theoretical descriptions based on the stress transfer analysis. Yin and his colleagues proposed a 2D elastic model in [224; 225; 226; 227] successfully interpreting fracture initiation, infilling, and saturation caused by tension or temperature loads in layered materials. However, the improved 2D theoretical analysis only exhibits a high accuracy for layered materials with comparable thickness of the layers [227]. When the coating thickness is much smaller than the substrate thickness, a semi-infinite body more accurately models the substrate layer. Therefore, a one-body analysis needs to be conducted based on a frictional interface between the two surfaces while disregarding the substrate thickness [224; 225]. Moreover, this improved 2D elastic model was only developed for cases where both the sub-layers are restricted to elastic deformation. Earlier studies such as [27; 34] showed that in a thin film/substrate system, the yielding in the substrate allows a film crack to open more and further drive the channel cracking. Thus, the analytical solutions based on existing elastic models cannot accurately evaluate the real state of the film/substrate system undergoing large-scale yielding. To improve such a cracking analysis for thin bonded films where plastic yielding of the substrate is allowed, the analysis need to account for large plastic deformations developed in the ductile substrate. However, due to the complex stress/strain fields in the vicinity of the crack tips resulting from the plastic deformation developed in the film/substrate system, most existing studies turn to numerical analysis [27; 89; 34; 74]. Recently, an elastoplastic fracture model has been proposed to study the OMF in coating layered structures undergoing large-scale yielding [38].

Most of the existing studies in the literature only focused on planar structures with a thin layer of coating or film; very limited amount of studies focus on wire- or pipe-type structures. Ochiai et al. [151] found a transition of the pattern of failure in the coating/substrate system from a compressive fracture to an interfacial debonding when the coating thickness gradually increases. Shieu and Shiao [186; 184] concluded that the fracture morphology depends on the bonding strength of the interface between the coating and substrate. The traditional mechanical properties of metallic wires with different coatings without considering fracture behavior were experimentally measured [159; 210; 200]. None of the above mentioned studies considered the plastic deformation in the substrate. Therefore, the study of the fracture behavior of a coating layer on a ductile substrate wire highly demands an elastoplastic fracture model. To fill this need, He et al. [81] conducted an elastoplastic
fracture analysis in the brittle coating layered on a ductile wire.

### 1.2.2 Three-dimensional Stress and Fracture Analysis for Coating/Substrate Structures under Thermal Loading

Instead of uniaxial loading, one can instead consider the case of thermal loading applied to the coating/substrate structures. Here interconnected cracks along both longitudinal and transversal direction would form in the brittle coating driven by the residual stress caused by temperature change and divide the structural component into approximately rectangular pieces. In this case, the 2D plain strain or stress assumptions would not be applicable, therefore, a full 3D analysis is essential. Based on the literature, most studies about the residual stress and 3D fracture analysis of coating/substrate structures under thermal loading are based on experimental measurements [190; 25; 152; 177], while very seldom theoretical models can be found [63; 91; 87; 230; 10; 169]. The details about existing testing methods and theoretical models are summarized as follows.

In order to study the fracture behavior of the coating under thermal loading, the residual stress, which acts as driving force, needs to be measured or analyzed. The most commonly used approach in measuring the residual stress in the coating uses the curvature of the elastically deformed coated substrate. When the thickness of the film is small compared to that of the substrate, the following formula proposed by Stoney [190] can predict the residual stress in the coating:

\[
\sigma_{zz}^f \approx -E_s \frac{h_s^2}{6h_f R}
\]

where \(E_s\) is the Young’s Modulus of substrate, \(R\) is the radius of curvature, \(h_s\) is the thickness of substrate, and \(h_f\) is the thickness of coating. The index \(zz\) denotes the stress component in the direction of the length side of the beam. Berry [25] argued that such a substrate rather curls into an approximately cylindrical shape instead of a bowl- or cap-like deformation. In this case, the plate modulus should be used to replace \(E_s\). Later, Ohring [152] found that when measuring thin films deposited on plate-like substrate, the corresponding biaxial deformation has to be taken into account by using the biaxial modulus. In 2006, Schwarzer [177] examined different forms of Stoney’s equation by applying a correct 3D model and found that the biaxial modulus yielded an accurate result while the plate modulus would deliver a bigger stress by 20 to 30 percent. By fitting the experimental data [150] summarized an equation to predict the residual stress in coating/substrate
system based on the applied thermal loading or tensile stress, then the crack spacing of the coating was studied by employing a strength criteria.

In 1995, Evans and Hutchinson [63] presented several models for mechanisms which rise to tensile stresses in thin film deposition and gave the expression of residual stress in thin film attached to an infinite substrate. Later, Hutchinson [91] proposed a form for residual stress in thin coating when the substrate expands or shrinks freely based on the assumption that the substrate is effectively uninfluenced by the film. The substrate imposes its in-plane strains on the film and the shearing strain in the film equals that in the substrate at the area away from the edge. This model can predict the stress in the center area but needs more accurate displacement or stress distributions at the edge for cracking analysis. In 2003, Hsueh and Yanaka [87] derived a closed-form analytical solution to predict the stress distribution in a film segment when the film/substrate system is subjected to residual stresses and loading. In this model, the effects of external loading were included into the shear lag model. In addition, the cracking in coating was predicted by adopting both strength and energy threshold criteria for cracking onset based on the solved stress and displacement. However, this model only considered the stress along the same direction as external loading while ignoring the other stresses.

Following the developed theoretical solutions in [87], another study done by Hsueh and Wereszcak [86] calculated the residual stress in the coating based on multiple coating cracking. Based on the force and moment balances, Zhang et al. [230] proposed another analytical model to predict the thermal residual stress in multilayered coating systems. The total strains of the coating layer and the substrate in the model were decomposed into an in-plane strain and a bending strain. A closed-form solution of thermal stresses was obtained which possesses the merit of independence of the number of coating layers. In 2011, Ahmed et al. [10] used Micro-Raman spectroscopy to access the residual stress in a diamond coating as the function of the applied strain to the ductile substrate. In order to verify the experimental results, a new shear lag model based on Hsueh and Yanaka’s work [87] was developed considering the effect of the substrate plasticity. Recently, Roy [169] proposed another model based on the superposition method to predict the residual stress in the free expanded galvannealed coating/substrate structure and obtained the normal stress in both the coating and the substrate. The results showed that the initial thermal residual stress generated in the coating is independent of the coating thickness but depends on the temperature difference,
inherent mechanical properties of the coating, and thermal properties of the coating and the substrate. Based on the residual stress, the fracture ERRs in the coating along both the longitudinal and transverse directions were obtained and used to predict the cracking spacing. Compared with the experimental results, the predicted crack spacings are quite different from the observed results and the proposed model underestimated the crack spacing. The drawback of this proposed model is that the normal strain was assumed to be constant in the coating and it would depend on the material properties only. Therefore, this model cannot capture the strain and stress spacial distribution accurately.

1.2.3 Test Methods for Delamination Fracture Energy

From the view of fracture mechanics, the interfacial delamination fracture energy, a material property equal to the energy needed to delaminate a unit area, is used to quantify the bonding between each layer. There are many test methods that can be chosen from the literature to measure the delamination fracture energy for multilayered coating/substrate structures: the peeling test which is one of the most frequently used test methods for assessing the failure of flexible laminates, such as those employed in the packaging and electronic industries [140; 110; 142; 154; 99; 113; 96]; the micro-scratch test which is widely used to assess the adherence of thin film to substrate since it’s relatively simple to use and provides simple and rapid qualitative and semi-quantitative information [115; 127; 167; 204]; the blister test which relates the pressure at which debond initiates to the work of adhesion of the film [48; 72; 84; 141; 12]; the residual stress driven delamination or micro-strip test developed by Bagchi et al. [15]; the indent test measuring the delamination of ductile coatings on brittle substrates by using a micro-indenter to deform the coating [62; 168; 12; 57; 56]; the edge peel test during which the fracture process is largely elastic [58; 179; 15; 180; 137; 181; 182]; the method based on buckling [28; 92] or crack formation [153].

In 2016, Bosco et al. [29] developed a fracture mechanics-based approach for quantifying adhesion at every interface within the photovoltaic (PV) module laminate which may be applied at both the module and the coupon level to yield a similar and quantitative measurement. The development of a width-tapered cantilever beam test method circumvented the common requirements of monitoring crack width and specimen compliance. The first results on field exposed modules developed for over 27 years were also presented. This technique employs an elastic width-tapered cantilever
beam adhered to the layered structure of interest. When the beam is loaded at its apex, delamination will initiate at the weakest interface and advance upon continued loading. This measurement quantifies the material properties of adhesion, or the critical value of the ERR, and represents the energy required for debond extension. The beauty of this method is that the compliance of this width-tapered cantilever beam increases proportionally with the increase of crack length, therefore making the peeling force a constant.

For this width-tapered beam test method, the delamination fracture energy is given as follows:

\[
G_c = \frac{P_c \Delta_i}{2 \tan(\theta/2) a_i^2}
\]

where \(a_i\) is the crack length under a load-line displacement \(\Delta_i\), and \(\theta\) is the apex angle of the width-tapered beam. Eq. (1.2) uses the tested peeling force, \(P_c\), and the measured crack length with a load-line displacement to calculate the fracture energy. This study employs this width-tapered beam test method to measure the delamination fracture energy in the advanced polymeric solar reflectors because of the simpler test configuration and data analysis procedure. Chapter 6 includes details about the test procedures and data analysis.

1.2.4 Cohesive Zone Model in ABAQUS to Simulate Cracking and Delamination

With the development of numerical method, FE method has been widely used to simulate the development of cracking and delamination in coating/substrate structure. Initially, the crack propagation was simulated by using singularity elements or by using line spring elements with built-in fracture criteria. Recently, this task uses a more popular method based on cohesive zone model (CZM) \[8; 188; 231\]. A summary about the development of cohesive model can be found in \[8\].

In 1959, Barenblett studied the formation of equilibrium cracks during brittle fracture \[22\] and proposed the cohesive surface model, in which a hypothetical attractive force was applied to the two sides of crack. The attractive force would grow rapidly with increasing crack opening distance until a critical distance was reached, after which the attractive force rapidly falls with the increasing distance. Following the work of Barenblatt \[22\], Needleman \[148\] provided a unified framework for describing the process of void nucleation from initial debonding through complete separation by using a cohesive surface model, taking full account of finite geometry changes. The constitutive
equation for the interface used by Needleman [148] showed that the traction across the interface (surfaces of cracks) reaches a maximum, decreases, and eventually vanishes, with increasing interfacial separation, so that complete de-cohesion occurs with a certain fracture energy. The mechanical response of the interface was specified in terms of both a critical interfacial strength and the work of separation per unit area. This constitutive behavior is the most often used and computationally convenient exponential form for the traction-separation relationship. Later, Larsson [114] modeled the crack behavior for brittle materials using this model while Xia and Shih [217] simulated the crack growth in ductile materials under static loading. Tvergaard and Hutchinson [202] proposed a trapezoidal traction-separation model and evaluated the crack growth resistance in elastoplastic materials. Later in 1993, Ortiz and Suresh [155] adopted a linear cohesive law for intergranular fracture behavior where the traction increased linearly with the grain boundary opening up to a critical value and then dropping down to zero. In 1994, Xu and Needleman [221] studied the dynamic crack tip in stabilities by introducing special boundary elements, cohesive elements, between regular elements where the boundary elements obey a cohesive law. Three factors influence the cohesive law behavior: the cohesive strength; the critical separation at cohesive strength; and the fracture energy in the separation process. In 1998, Geubelle et al. [73] proposed a bilinear traction-separation law to simulate delamination of thin composite plates subjected to low-velocity impact. Park et al. [158] conducted a critical review of traction-separation relationships across fracture surfaces in 2011.

As an extension of the 2D cohesive model, Foulk et al. [68] detailed the 3D formulation for an arbitrary number of cohesive zones placed at arbitrary locations within the continuum. Foulk et al.'s formulations could help model multiple cracks and any or all can be evolving simultaneously, with the crack interaction included explicitly in the formulation. More recently, Roy and Dodds [170] described the formulation and application of a 3D interface-cohesive FE model in predicting the quasi-static ductile crack extension in thin aluminum panels for mode I loading and growth. The fracture model comprises an initially zero thickness interface element with constitutive response described by a nonlinear traction-separation relationship. In this simulation, the conventional volumetric finite elements were used to model the nonlinear (elastic-plastic) response of background (bulk) material while the interface-cohesive elements undergoing gradual de-cohesion between faces of the volumetric elements were used to create new traction-free crack faces.
1.2.4.1 Bilinear Traction-Separation Law

In cohesive elements with traction-separation behavior, the parameters characterizing the traction-separation relationship must be specified, including the initial stiffness ($K$), damage initiation threshold ($T$), and damage evolution properties ($G_c$). Fig. 1.2 shows one of the most commonly used constitutive behaviors for cohesive elements called the bilinear traction-separation law [73]. In this model, the initial response of the cohesive element is assumed to be linear until the damage initiation criterion is met. After that, the stress in the cohesive elements is released linearly until the damage evolution property is reached and the cohesive element is damaged.

![Bilinear traction-separation response of the cohesive element](image)

Figure 1.2: Bilinear traction-separation response of the cohesive element [187].

The damage evolution properties for bilinear traction-separation cohesive behavior is specified by giving the critical fracture ERR, $G_c$, equal to the area under the curve. When the fracture ERR in the cohesive element reaches $G_c$, the corresponding cohesive element is damaged.

The peak traction ($T$) in the traction-separation relation determines the damage initiation point; beyond this point damage begins to develop in the cohesive zone leading to traction reduction [173]. Diehl [50; 51; 52; 53] advocated treating the interface strengths as penalty parameters because of their difficulty in being determined for many material systems.

The penalty stiffness, $K$, of the bilinear traction-separation law is defined as

$$K = \frac{T}{\Delta^c}$$  \hspace{1cm} (1.3)
where $\Delta^c$ is the critical separation at damage initiation. Ideally, the stiffness of the cohesive element should be infinite not to affect the overall compliance of the model before the damage initiation point; however, an overly high value can lead to numerical problems [176; 187].

Currently, the cohesive element based on the bilinear traction-separation law has been integrated into the commercial FE package of ABAQUS. The FE model built using the commercial FE package, ABAQUS, based on CZM with bilinear traction-separation law will be used to simulate the cracking in the brittle coating and the delamination behavior of multilayered advanced polymeric solar reflectors in this dissertation. Chapter 4 and 5 will present more details about the determination of parameters for the CZM in the simulations of cracking and delamination, respectively.

1.2.5 Failure Mechanisms by Aging and Degradation of Asphalt Binder

As another failure mechanism, the degradation or aging in asphalt binders will be studied in this dissertation.

The reuse of reclaimed asphalt pavement (RAP) in Hot Mix Asphalt (HMA) will minimize the use of natural resources and reduce the waste of asphalt pavement maintenance and rehabilitation. This will become more important in the future because the availability of virgin aggregate and asphalt binder is decreasing in the U.S. [43; 135; 136]. Despite the advantages, the use of RAP makes it hard to predict and control the long-term performance of asphalt pavements. In 1997 a subgroup of the FHWA Super-pave Mixtures Expert Task Group developed an interim guidance for the use of RAP [33]. Later, the effects of RAP and how best to accommodate RAP in super-pave were investigated scientifically [108; 136]. These studies showed that RAP does not behave like an aggregate (black rock analogy). When the RAP content is low, the mixture’s performance is unable to be enhanced due to the lack of RAP binder in the mixture; however, when the RAP content increases, much softer virgin binders are needed to counteract the stiffening effect of the hardened RAP binder [108; 136].

As a rule of thumb, it is generally required that pavements containing recycled road materials reach similar properties or the same level of performance as any alternative pavement containing virgin materials in addition to the environmental sustainability [164]. In reality, due to asphalt aging, the life span of asphalt pavement might be shorter than expected especially for pavements produced using RAP because of the presence of aged binder in RAP [13; 144]. The short-term
oxidation and long-term aging of virgin asphalt used in the pavement are typically tested with standard test methods in design or delivery. However, the status of RAP really depends on the service life and environment, which is much more complex than that of virgin binder. It is important to understand the oxidation behavior of the RAP binder first. When RAP binder mixes with virgin binder or other additives, the effective oxidation behavior may be related to the behavior of both the RAP binder and the virgin binder.

Based on a survey conducted by the Federal Highway Administrations RAP Expert Task Group, up until 2014 in the United States the average RAP content in asphalt mixture was lower than 20 percent. The primary reason for this limited use was the uncertainty of the long-term performance of RAP materials [80]. Therefore, better understanding of the response of RAP binder to oxidative aging is necessary in order to increase the percentage of RAP used in asphalt mixtures.

1.2.5.1 Aging Mechanism of Asphalt Binder

Asphalt aging involves a set of complex physiochemical processes where the composition, chemical structure and morphology of asphalt may be altered after being mixed, laid on the road and exposed to the environment in the field. This includes an increase in the amount of asphaltenes and the creation of carbonyl and sulfoxide groups. These actions further influence the rheological and mechanical properties of asphalt such as an increase in the viscosity and softening point [128; 156; 162; 172]. Asphalt aging behavior may be caused by three main factors: thermal aging, moisture damage, and ultraviolet (UV) photo-oxidation aging (UV radiation aging).

The thermal-oxidation process changes the physical and chemical properties through the loss of volatiles or specimens of low molecular weight or the formation of hydrogen bonds [130; 171]. The temperature influences the asphalt binder aging process in two ways: increasing the volatilization rate of light components (saturates and aromatics) and accelerating the oxidation rate of asphalt [130; 161; 228]. Two tests are commonly used to study the thermal aging process of asphalt binders. The first one is the rolling thin film oven test (RTFO) based on ASTM D-2872, which simulates the short-term asphalt binder aging. The second one is the pressure aging vessel test (PAV) based on ASTM D-6521, which attempts to simulate the long-term aging of in-service asphalt [44; 129].

Moisture damage is usually defined as the loss of strength and durability of asphalt mixtures
caused by the presence of water [223]. At least five different stripping mechanisms have been identified in literature: detachment, displacement, spontaneous emulsification, pore pressure, and hydraulic scour [109; 195; 196]. AASHTO T283, a standard test method that evaluates the resistance of compacted asphalt mixtures to moisture-induced damage, is commonly used to test the moisture sensitivity of asphalt pavements. Additionally, the Hamburg Wheel Tracking Device test method (HWTD) and the Moisture Induced Stress Tester (MIST) are widely used to investigate the effects of moisture on the performance of asphalt pavements.

Photo-oxidation is the degradation of a material in the presence of molecular oxygen or ozone facilitated by radiant energy such as UV radiation or artificial light. The influence of solar irradiation on asphalt binders has been known since 1822 [5]. When solar irradiation reaches the surface of the asphalt pavement, it generates free radical reactions and produces an oxidized layer on the pavement surface [60]. The influence of solar radiation on asphalt binder aging has commonly been ignored as it was believed that, due to the high absorption coefficient of bitumen, it only affects the upper layers of flexible pavements [11; 205]. In the 1950s, an exposure test was developed and it was found that the effect of solar radiation depends on the nature of the bitumen [59]. Later, it was reported that the influence of UV radiation on the aging of the asphalt pavements wearing courses cannot be totally ignored as these actions occur rapidly and has been shown that 10 hours of laboratory exposure to UV radiation is equivalent to one year of oxidation in the field [60].

Therefore, any complete study on the performance of asphalt pavements must consider the effects of solar irradiation on the aging of the asphalt binder, especially in the geographical regions where high solar irradiation intensities, high temperatures, and high relative humidities occur [124]. So far there is not a standard test that quantitatively evaluates the degradation of asphalt binders caused by photo-oxidation; however many researchers have investigated it by using different UV aging methods under a variety of conditions [64; 143; 215; 219; 228]. A recent study [228] found that the influence of temperature on UV aging can be ignored when the aging temperature is lower than 50°C but that the oxidation rates of asphalt increase at 70°C. Wu et al. [215] studied the effect of the film thickness of bitumen and UV radiation intensity on UV degradation using a customized UV radiation oven and showed the significant effect of the film thickness and the direct correlation of the UV degradation rate with the intensity of the UV radiation.
1.2.5.2 Asphalt Aging Models

Various models have been developed to describe the chemical, physical, and rheological behavior of asphalt. These models are either empirical and based on laboratory results [83; 90; 116; 139; 185; 203] or semi-empirical [24; 40; 102; 120; 126; 131; 165] based on a combination of laboratory results and constitutive equations concerning material behavior [66].

Griffin et al. [77] proposed one of the first mathematical expressions for asphalt hardening, the Aging Index (AI), which represents the ratio of the viscosity of an aged asphalt binder to that of the unaged binder, both determined at the same shear rate [77]. Griffin et al. discovered that both the viscosity and the amount of absorbed oxygen initially experience a rapid increase, and then the rate of increase slowly declines, eventually reaching a constant rate. During such a constant-rate period, the carbonyl formation rate can be described through a mathematical expression [126]. Later, a similar trend was observed for the increase in the logarithmic viscosity of two asphalts aged at three constant temperatures (50, 60, and 70 °C) and an elevated pressure of 2 MPa (19.7 atm) [83]. An asphalt oxidation kinematics model in terms of carbonyl formation, which is also known as the fast-rate constant-rate (FRCR) model, has been subsequently proposed [103].

After studying eight different asphalt binders over 48 months using both temperature and oxidation treatments, Lee [116] established a hyperbolic function for estimating the evolution of the physical properties of asphalt binder. In addition to Lee’s hyperbolic model, an exponential model was proposed in 1973, this model has a stronger correlation with penetration and viscosity measurements [24]. A linear empirical model was developed based on the characteristics of 20 asphalt binders aged using the thin film oven test (TFOT) and rolling thin film oven test (RTFOT) at three different temperatures [185]. The nonlinear differential dynamic (NDD) model has been developed to describe both population growth dynamics and the rate of various chemical reactions [55]. The NDD model has been employed to model the changes in asphalt pavement properties over time [71] and it was found that the NDD model can effectively simulate the asphalt binder aging process [120].

By combining a mathematical model of asphalt oxygen diffusion and reaction kinetics with Ficks law of diffusion, Lunsford [131] developed a transport model to understand the effects of the air void structure of pavements on the aging process [165]. Mirza and Witczak [139] developed an empirical global aging system model that allows for the prediction of the change in binder viscosity.
as a function of age. By considering the activation energy from diffusion and the speed of the chemical reaction based on particle collisions, Huh and Robertson [90] proposed an exponential function to model the asphalt aging process. Chen and Huang [40] studied the effect of oxidation on asphalt and developed a chemical- mathematical model in terms of molecular association that includes the aging rate and the resulting changes in the properties of the asphalt binder.

1.3 Scope

The primary objective of this dissertation is to develop a theoretical fracture model to study the cracking behavior of the brittle coating fully bonded to the elastic or elastoplastic substrate and investigate the delamination fracture energy of the multilayered solar reflector. In addition, as another failure mechanism, the material degradation or aging behavior of asphalt is studied.

Chapter 2 [38] develops an elastoplastic fracture model to study the OMF for an alumina thin film fully bonded to an aluminum plate undergoing large-scale yielding. The stress field in the coating layer is described by one section between two adjacent cracks. A 2D plane strain formulation is employed to analyze the elastic field in the thin film while a 1D linear hardening plastic model is applied to account for the large plastic deformations in the substrate under substantial yielding. An elastoplastic shear lag model is established to transfer the tensile stress in the substrate to the thin film. General formulations and explicit expressions of the elastic/elastoplastic solutions of the thin film/substrate system under different loading stages have been developed and verified with the FE results. The fracture ERR is calculated and corresponding elastoplastic fracture analysis is presented. Experimental characterization is further conducted to validate the present model which shows that the fracture initiation, infilling, and saturation in the thin film can be successfully captured by the present model.

Chapter 3 [81] extends the developed elastoplastic fracture model in Chapter 2 from Cartesian coordinates to polar coordinates to simulate the multiple micro-cracking in the thin layer film coated onto an elastoplastic aluminum wire/rod. The thin layer of alumina coating generated by the anodic oxidation is treated as an elastic media while a bi-linear hardening plastic model characterizes the ductile substrate aluminum wire. An elastoplastic shear lag model is applied to transfer the shearing stress from the substrate layer to the thin coating layer. When the coated
structure is subjected to different applied loads, the system undergoes different stress levels and exhibits different cracking stages. Accordingly, explicit solutions corresponding to different loading stages are presented based on the equilibrium equations for axial symmetric structures. FE analysis is employed to verify the present elastic solution when the applied load is relatively small and the whole system is in the elastic state. Experimental characterization is conducted to validate the present elastoplastic solution when the substrate or interlayer undergoes large deformation. During the tests, a versatile high-fidelity optical microscope is applied to check the micro structure of the coating and continuously monitor the fracture development in the coating layer, through which valuable detailed micro-cracking information, such as critical applied load corresponding to crack initiation, crack pattern, and crack spacing, are obtained. The results show that the presented fracture model can accurately capture the stress and strain distribution in the coated structure and predict the fracture initiation, infilling, and saturation in the thin coating layer.

Chapter 4 develops a 3D model to study the fracture behavior of the metal oxide coating fully bonded to the polymer substrate under thermal loading by simplifying the advanced polymeric reflector as a two-layer structure, as the plane strain or plain stress assumptions can not be applied. The so-called plane assumption and non-shearing assumption are applied to simplify the equilibrium equations and the 3D elastic field in both coating and substrate in one section between two cracks are then solved and verified by FE results. Based on the solved elastic field, the fracture ERR is calculated and used to analyze the fracture initiation, infilling, and saturation. Finally, FE simulations based on CZM are built to validate the theoretical fracture analysis, also the theoretical predicted crack spacings are verified by experimental data from literature. The good agreement between theoretical solutions and FE simulation results and experimental data denotes that the proposed 3D fracture model can predict the elastic field accurately and capture the fracture initiation, infilling, and saturation successfully.

Chapter 5 extends the model developed in Chapter 4 to be more general to study the residual stress and displacement in multilayered structures consisting of arbitrary layers. In order to verify the extended model, the elastic field in the advanced polymeric reflector is explicitly solved and compared with FE simulation results. Parametric studies are conducted to investigate the effect of geometry, particularly the thickness of each layer, on the accuracy of the extended model. Based on the obtained elastic field, the fracture ERR in the surface layer of the advanced polymeric reflector
is calculated and used for further fracture analysis.

Chapter 6 uses the width-tapered beam method to measure the delamination fracture energy of the multilayered solar reflectors with different types of protective coatings. The tests show that the delaminated interface is the interface between the copper coating and the glass substrate for all samples, which reveals that the copper-glass interface is the weakest interface. FE simulations are run to verify the test results using the CZM by treating the tested fracture energy as an input and comparing the returned peeling force from the FE simulation with the tested peeling force. The good agreement between the FE simulation and test results indicates that the width-tapered beam method is accurate and can be applied to measure the delamination fracture energy of multilayered solar reflectors. In addition, the aging effect on the delamination fracture energy of reflectors with different protective coating is investigated.

Appendix A studies the aging behavior of asphalt by UV photo-oxidation considering the effects of moisture and condensation. Three types of asphalt binders extracted from RAPs and one extracted from fresh HMA are aged in an accelerated aging chamber under different weathering conditions for different periods of time. As an aging index, the weight percentage of oxygen (WPO) in the aged asphalt binders are measured using a energy-dispersive X-ray spectroscopy (EDX). Then the tested data are fitted using two classic aging models, namely the FRCR and NDD models. The good fitted results show that both FRCR and NDD model can simulate the aging behavior of asphalt binders under both UV and UV/moisture/condensation exposures accurately. Additionally, the effects of condensation and moisture on UV aging are evaluated by comparing the change in the WPO caused by UV radiation during the continuous UV aging with that during the UV/moisture/condensation aging tests. It was found that the increase in the WPO caused by the UV radiation during the UV/moisture/condensation aging is lower than that during the continuous UV aging, indicating that condensation and moisture effectively reduces the UV aging rate.
Chapter 2

Two-dimensional Elastoplastic Fracture Analysis in Cartesian Coordinates

This chapter develops an analytical solution for fractures in thin film layered structures undergoing large-scale yielding at the onset of fractures in the thin film which assumes the film to be fully bonded to the substrate even during the formation of the discontinuities and thus considers no delamination along the interface. Because the film is assumed to be thin and brittle, once a crack initiates, it is assumed to propagate across the thickness of the film and stop at the interface. A two-dimensional (2D) plane strain formulation is employed to analyze the elastic field in the thin film, while a one-dimensional (1D) elastoplastic model is developed to account for the large plastic deformations in the substrate under substantial yielding. An elastoplastic shear lag model is established to transfer the tensile stress in the substrate to the thin film. Explicit solutions corresponding to different loading stages are presented based on the equilibrium equations for 2D plane strain structures. Finite element (FE) simulation is employed to verify the present elastic solution when the applied load is relatively small and the whole system is in the elastic state. Experimental characterization is conducted to validate the present elastoplastic solution when the substrate or interlayer undergoes large deformation. A scanning electron microscope (SEM) is applied to check the micro-structure of the alumina coating on aluminum substrate and continuously
monitor the fracture development in the coating layer. The results show that the presented fracture model is able to accurately capture the stress and strain distribution in the coated structure and predict the fracture initiation, infilling, and saturation in the thin coating layer.

2.1 Overview

Consider two brittle coating layers (thickness $h_1$, length $2\lambda$, Young’s modulus $E_1$, Poisson’s ratio $\nu_1$) fully bonded symmetrically to a substrate layer (thickness $2h_2$, Young’s modulus $E_2$, Poisson’s ratio $\nu_2$) and subjected to a uniform tensile load in the substrate as shown in Fig. 2.1(a). When the substrate is subjected to an increasing tensile load, it is transferred to the thin film through the interface shearing stress [224; 227]. From the loading end to the center, the interface shearing stress and the tensile stress in the substrate decrease whereas the tensile stress in the thin film increases in average. When the tensile load reaches a certain level, the interface shearing stress will be high enough for yielding and then the substrate may also start to yield from the loading end towards the center. As the tensile loading in the substrate increases, a higher load is transferred to the thin film and the opening-mode fracture (OMF) will initiate in the middle range of the thin film to release the strain energy [225]. When the tensile load continues to increase, the maximum stress and strain in each fragment increases with the applied loading and the continuous stretching of the substrate breaks the film with a length of $2\lambda$ into two halves of fragmentations of the coating, with more OMFs filling in the thin film until the OMF reaches a saturation status [225]. Eventually, uniformly distributed discontinuities form across the thickness of the film. In general, these cracks grow perpendicular to the applied loading direction such that the cracks separate the coating into nearly rectangular independent fragments. The side view of the saturated OMFs in the alumina coating on aluminum substrate was examined by SEM as is shown in Fig. 2.1(b).

Usually, the thin alumina layer is relatively brittle; thus, an elastic analysis as extensively conducted in the literature can describe the OMF behavior. However, the substrate and the interface will exhibit an elastoplastic behavior characterized by the uniaxial tension test and generalized by the Von-Mises criterion for the shear yielding behavior [34]. Fig. 2.2 shows the loading curve of two aluminum samples with or without alumina coating under tensile load conducted in this experiment until the OMFs were saturated. It was observed that significant yielding occurred and large plastic
deformation developed in the aluminum substrate when the OMF reached its saturation point. Therefore, to accurately predict the fracture initiation, infilling and saturation in the thin film, a proper elastoplastic analysis has to be employed to account for this large plastic deformation.

The shear lag model scheme assumes the stress in the substrate under a uniaxial tensile loading to be transferred to the thin coating film through a very thin interlayer. Such an essential stress transfer concept in the shear lag model has found extensive applications in modeling the stress transfer between the fiber and the matrix in fiber reinforced composites [45; 105; 14; 32; 146; 145; 132]. However, in extending this shear lag model to the thin coating-layered structures, most studies were restricted to elastic cases. In some existing studies where potential large-scale yielding was
allowed, some unrealistic assumptions were often applied, such as that the substrate only yielded along the interface over a slip length [88] and that plastic deformation could only be developed in the interlayer [79; 138], which might affect the accuracy of those solutions.

As the brittle coating is very thin compared to the substrate ($h_1 \ll h_2$), the effect of the thin film layer on the global stress distribution in the substrate which exhibits an elastoplastic behavior can be neglected (which is also indicated in Fig. 2.2). Therefore, during the process of crack infilling, the tensile stress on the ends of each section is still assumed to be uniform along the depth of the substrate and equal to the averaged stress ($\sigma^0$). Because the interest of this work focuses on the OMF in the thin film, the elastic analysis will follow our previous work [224; 227], whereas the elastoplastic analysis will follow the shear lag model, in which the tensile stress in the substrate is taken into account on the average and thus a 1D analysis is conducted. Based on the above assumptions, an idealized shear lag model of the considered film/substrate system with a representative fragment can be shown in Fig. 2.3, where an interlayer with thickness of $h_0$ is modeled as a distinct layer separated from the original substrate. Here $w$ is used to denote the displacement along the $z$-direction, while $u$ is used to denote the displacement along the $x$-direction.

![Figure 2.3: Idealized shear lag model of the thin film/substrate with channel cracking](image)

The remainder of this study is organized as follows. Section 2.2 presents general formulations and explicit expressions of the elastic/elastoplastic solutions of the thin film/substrate system under different loading stages. Section 2.3 gives the elastic predictions and FE analysis verifications. Section 2.4 provides the elastoplastic solutions and further experimental validation in which the present model successfully captures the crack initiation, propagation, and saturation in the thin film. Section 2.5 arrives finally at some conclusions.
2.2 Formulation

With the increase of the tensile load, three stress phases are induced: I) when the load is small, both the thin film and the substrate are in the linear elastic range, so that elastic analysis can provide the solution, II) when the interfacial shearing stress in the interlayer or the tensile stress in the substrate is higher than the corresponding yielding strength, plastic behavior will be induced in the ductile substrate and a higher proportion of the load will be transferred to the thin film, and; III) when the strain energy density is high enough in the thin film, OMFs will be induced in the thin film and OMF initiation, infilling, and saturation will be analyzed.

2.2.1 Phase I - Linear Elastic Behavior

When the overall thin film/substrate system is under the linear elastic range, the stress field proportionally increases along with the tensile load. The elastic field in the thin film, shear interlayer, and substrate is derived as follows. In the derivations, the superscript "f", "0", and "s" are used to denote the thin film or coating, interlayer, and substrate respectively.

2.2.1.1 Elastic field in the thin film (0 < z ≤ h₁)

Following the assumption from our previous work [224; 227], we assume that all the points in the same plane parallel to the surface plane in the loading direction will remain in the same plane:

\[ w_{x,x}^f = 0 \] (2.1)

which is the so-called plane assumption that simplifies the shearing strain and stress. For the OMF analysis, a plane strain formulation will be developed using the following constitutive law as

\[ \sigma_{x}^f = \frac{E_f}{(1+\nu_f)(1-2\nu_f)} \left[ (1-\nu_f)w_{x,x}^f + \nu_f w_{x,z}^f \right] \] (2.2)

\[ \tau_{x,z}^f = \frac{E_f}{2(1+\nu_f)} w_{x,z}^f \] (2.3)

where Eq. (2.1) is used in Eq. (2.3). The above equations are substituted into the equilibrium equation in the x-direction in the absence of body force, i.e.

\[ \sigma_{x,x}^f + \tau_{x,z}^f = 0 \] (2.4)
\[
\frac{1 - \nu^f}{1 - 2\nu^f}u^f_{xx} + \frac{1}{2}u^f_{zz} = 0
\] (2.5)

Eq. (2.5) is a decoupled partial differential equation of \( u_x \). The general solution for Eq. (2.5) can be obtained by the method of separation of variables by using the following simplification

\[
u^f(x, z) = X(x)Z(z) + \frac{\varepsilon^u}{2}x
\] (2.6)

where the unknown constant \( \varepsilon^u_x \) is introduced as a uniform strain caused by the uniaxial tension. Following the same procedure in [227], plugging this general solution into the governing equation produces

\[
\frac{1 - \nu^f}{1 - 2\nu^f}X''Z + \frac{1}{2}XZ'' = 0
\] (2.7)

Two independent equations can be set equal to an independent constant \( c \) such that

\[
\frac{X''}{X} = -\frac{1 - 2\nu^f}{2(1 - \nu^f)} \frac{Z''}{Z} = c^2.
\] (2.8)

The above equation can therefore extract two ordinary differential equations and produce the general solution as

\[
u^f(x, z) = (a_1 \sin (dz) + a_2 \cos (dz)) (a_3 \sinh (cx) + a_4 \cosh (cx)) + \frac{\varepsilon^u}{2}x
\] (2.9)

where \( a_i (i = 1, \ldots, 4) \) are coefficients to be determined and

\[
\alpha = \sqrt{\frac{1}{2} - \nu^f} / (1 - \nu^f)
\] (2.10)

where \( \alpha = \sqrt{\frac{1}{2} - \nu^f} / (1 - \nu^f) \)

The symmetric condition along the \( x \) axis produces the following boundary condition:

\[
u^f|_{x=0} = 0
\] (2.11)

and the free surface of the thin film provides:

\[
\tau_{xz}|_{z=h_1} = 0
\] (2.12)

By applying the above boundary conditions to Eqs. (2.2), (2.3) and (2.9) and neglecting the normal stress along the thickness direction, the general solution of the thin film can be reduced to
\[ u^f(x, z) = A \cdot \cos(dh_1 - dz) \sinh(cx) + \varepsilon_x^u x \]  
(2.13)

\[ \sigma^f_x(x, z) = \xi_f E^f \left( \text{Accos}(dh_1 - dz) \cosh(cx) + \varepsilon_x^u \right) \]  
(2.14)

\[ \tau^f_{xz}(x, z) = G^f A \sinh(dh_1 - dz) \sinh(cx) \]  
(2.15)

where \( \xi_f = \frac{1}{1 - (\nu^f)^2}, G^f = \frac{E^f}{2(1 + \nu^f)} \), and \( A \) is an constant need to be determined later.

### 2.2.1.2 Elastic field in the shear interlayer \((-h_0 \leq z \leq 0)\)

As previously stated, the shear interlayer of a thickness \( h_0 \) mainly transfers the load between the substrate and the thin film. Also, it is assumed that the shearing stress is uniformly distributed in the thickness direction. Correspondingly, the shearing strain in the shear interlayer is also uniform across its thickness direction. The constitutive equation of the shear interlayer in the elastic stage simply reads

\[ \tau^0_{xz}(x) = G_1^0 \gamma^0_{xz}(x) \]  
(2.16)

where \( \tau^0_{xz}(x) \) and \( \gamma^0_{xz}(x) \) are the shearing stress and strain in the interlayer, respectively, and \( G_1^0 \) is the elastic shear modulus of the interlayer.

Using the shearing stress continuity condition, one can write the shearing strain in the interlayer as

\[ \gamma^0_{xz}(x) = \frac{G^f}{G_1^0} A \sin(dh_1) \sinh(cx) \]  
(2.17)

By considering the displacement continuities at the interface between the thin film and shear interlayer and between the interlayer and the substrate, the interface continuity can be expressed:

\[ u^s(x) = u^f(x, 0) - h_0 \gamma^0_{xz}(x) \]  
(2.18)

where \( u^s(x) \) is the uniaxial displacement of substrate. By substituting Eqs. (2.13) and (2.17) into Eq. (2.18), the displacement of substrate can be determined:
\[ u^s(x) = A k_1 \sinh(cx) + \varepsilon_x^s x \]  

(2.19)

where \( k_1 = -\frac{G_f}{G_1} \int_0^z \sin(dh_1) + \cos(dh_1) \).

2.2.1.3 Elastic field in the substrate\((-h_2 \leq z < -h_0)\)

Because the thickness of the thin film and interlayer are much smaller than that of the substrate, it can be assumed that the tensile load is approximately uniform in the thickness direction of the substrate layer, and thus a 1D equilibrium equation of the substrate can be written:

\[ (h_2 - h_0) \frac{d}{dx} \sigma^s(x) + \tau_{zz}^0(x) = 0 \]  

(2.20)

where \( \sigma^s(x) \) is the tensile stress in the substrate.

The constitutive equation of the substrate under a plane strain assumption in the elastic stage is

\[ \sigma^s(x) = E_1^s \varepsilon^s(x) \]  

(2.21)

where \( E_1^s \) is the stiffness of the substrate characterized by fully gripped ends, which fits the plane strain assumption very well; \( \varepsilon^s(x) \) is the tensile strain in the substrate, which relates to the displacement in the substrate \( u^s(x) \) under small displacement assumption:

\[ \varepsilon^s(x) = \frac{du^s(x)}{dx} \]  

(2.22)

Combining Eqs. (2.22), (2.21) and (2.18), Eq. (2.20) becomes:

\[ (h_2 - h_0) E_1^s u^s_{,xx} + G_f Ad \sin \left( dh_1 - dz \right) \sinh (cx) = 0 \]  

(2.23)

Substituting Eq. (2.19) into Eq. (2.23) yields:

\[ \left( -\alpha \xi_c h_0 \frac{E_1^s}{G_1} d + \frac{1}{(h_2 - h_0) d} \right) \sin (dh_1) + \alpha^2 \xi_c \frac{E_1^s}{G_f} \cos (dh_1) = 0 \]  

(2.24)

the coefficient \( d \) can be numerically obtained from Eq. (2.24), and then the tensile stress in the substrate can be determined by Eqs. (2.21) and (2.19) as
\[ \sigma^*(x) = \xi_s E_1^* (A \kappa_1 \cosh(cx) + \varepsilon^u_x) \]  \hspace{1cm} (2.25)

The boundary conditions are given as

\[ \sigma^*(x) \big|_{x=\lambda} = \sigma^0 \]  \hspace{1cm} (2.26)

\[ \int_0^{h_1} \sigma^f(x, z) \big|_{x=\lambda} dz = 0 \]  \hspace{1cm} (2.27)

Eqs. (2.26) and (2.27) can finally determine the coefficients \( A \) and \( \varepsilon^u_x \) as:

\[ \varepsilon^u_x = \frac{\sigma^0}{\xi_s E_1^* \sin(dh_1) - \kappa_1} \sin(dh_1) \] \hspace{1cm} (2.28)

\[ A = \frac{-\varepsilon^u_x h_1}{a \sin(dh_1) \cdot \cosh(c\lambda)} \] \hspace{1cm} (2.29)

### 2.2.2 Phase II - Elastoplastic Behavior

As the applied load increases, both the tensile stress in the substrate and the shearing stress in the interlayer also increase. Once each of them reaches their yielding strength, yielding will initiate either in the interlayer or substrate while the thin film is still assumed to behave linearly. Section 2.3 will show that the elastic solution (obtained in Section 2.2.1) indicates the interlayer would enter into the plastic stage prior to the substrate. Typically, the yielding initiates at the two ends in the shear interlayer and then propagates toward the inner part. For the linear hardening material, the internal stress and strain will keep developing as the applied load increases.

#### 2.2.2.1 Elastic substrate and elastoplastic interlayer

Assume that at a certain applied load (\( \sigma^0 = \sigma_1 \)) the developed yielding zone in the shear interlayer is from \( x_1 \) to \( \lambda \) (with symmetry) and the substrate is at the verge of yielding initiation. In this case, the film/substrate system needs to be divided into two continuous parts:
2.2.2.1 Elastic zone \((0 \leq x \leq x_1)\)

In this zone, both the shear interlayer and substrate are in the elastic stage making all the solutions in Section 2.2.1 applicable. Considering the slightly changed boundary conditions, all the elastic solutions for the thin film/substrate system are rewritten in the following expressions:

\[
    u^f(x, z) = A_1 \cdot \cos (d_1 h_1 - d_1 z) \sinh (c_1 x) + \varepsilon_{x_1}^u x
\]  \hspace{1cm} (2.30)

\[
    \sigma_x^f(x, z) = \xi_f E_f (A_1 c_1 \cdot \cos (d_1 h_1 - d_1 z) \cosh (c_1 x) + \varepsilon_{x_1}^u)
\]  \hspace{1cm} (2.31)

\[
    \tau_{xz}^f(x, z) = G_f (A_1 d_1 \cdot \sin (d_1 h_1 - d_1 z) \sinh (c_1 x))
\]  \hspace{1cm} (2.32)

\[
    u^s(x) = A_1 k_1 \sinh (c_1 x) + \varepsilon_{x_1}^u x
\]  \hspace{1cm} (2.33)

\[
    \sigma^s(x) = \xi_s E_s (A_1 c_1 k_1 \cosh (c_1 x) + \varepsilon_{x_1}^u)
\]  \hspace{1cm} (2.34)

where \(c_1 = c\), \(d_1 = d\) and \(c_1^2 = \alpha^2 d_1^2\) still holds.

2.2.2.1.2 Elastic-plastic zone \((x_1 \leq x \leq \lambda)\)

As the thin film is still in the elastic stage, the general expression of the displacement in the thin film in Eq. (2.9) still applies. By applying the boundary condition Eq. (2.12), the displacement of the thin film can be reduced to

\[
    u^f(x, z) = \cos (d_2 h_1 - d_2 z) \cdot (B_1 \sinh (c_2 x) + B_2 \cosh (c_2 x)) + \varepsilon_{x_2}^u x
\]  \hspace{1cm} (2.35)

where \(B_1\) and \(B_2\) are constants to be determined. The constitutive equations in Eqs. (2.2) and (2.3) simplify the normal and shearing stresses in the thin film as

\[
    \sigma_x^f(x, z) = \xi_f E_f (c_2 \cdot \cos (d_2 h_1 - d_2 z) \cdot (B_1 \cosh (c_2 x) + B_2 \sinh (c_2 x)) + \varepsilon_{x_2}^u)
\]  \hspace{1cm} (2.36)
\[
\tau^f_z(x, z) = G^f (d_2 \cdot \sin (d_2 h_1 - d_2 z) \cdot (B_1 \sinh (c_2 x) + B_2 \cosh (c_2 x)))
\] (2.37)

As the shear interlayer enters into the plastic stage, the shearing stress-strain curve for the interlayer becomes:

\[
\tau^0_{xx}(x) = G^0_{22} \gamma_{xx}(x) + \left( G^0_1 - G^0_2 \right) \gamma_Y
\] (2.38)

where \(G^0_2\) is the linear hardening rate of the shear interlayer under uniform shear, \(\gamma_Y = \frac{\tau_Y}{G^0_1}\) is the yield shearing strain, and \(\tau_Y\) is yield stress under uniform shear.

By following the similar procedures in Section 2.2.1, the displacement and normal stress of the substrate can be determined through

\[
u^s(x) = k_2 (B_1 \sinh (c_2 x) + B_2 \cosh (c_2 x)) + \varepsilon^s_{xx} x + h_0 \left( \frac{1}{G^0_2} - \frac{1}{G^0_1} \right) \tau_Y
\] (2.39)

\[
\sigma^s(x) = \xi_s E^s_{11} c_2 k_2 (B_1 \cosh (c_2 x) + B_2 \sinh (c_2 x)) + \xi_s E^s_{11} \varepsilon^s_{xx}
\] (2.40)

where \(k_2 = -\frac{G^f}{G^0_2} d_2 h_0 \cdot \sin (d_2 h_1) + \cos (d_2 h_1)\). Substituting Eqs. (2.39) and (2.40) into the equilibrium equation Eq. (2.20) and considering the shearing stress continuity between the film and interlayer yields

\[
\left( -\alpha^2 \xi_s E^s_{11} d_2 h_0 + \frac{1}{(h_2 - h_0) d_2} \right) \sin (d_2 h_1) + \alpha^2 \xi_s E^s_{11} \cos (d_2 h_1) = 0
\] (2.41)

from which the coefficient \(d_2\) can be theoretically obtained.

The boundary conditions in this case read

\[
\int_0^{h_1} \sigma^f(x) |_{x=\lambda} \ dz = 0
\] (2.42)

\[
\tau^0_{xx}(x) |_{x=x_1} = \tau_Y
\] (2.43)

\[
\sigma^s(x) |_{x=\lambda} = \sigma_1
\] (2.44)

The continuity equations read
The yielding initiation position $x_1$ can be determined by substituting Eqs. (2.48) to (2.52) into Eq. (2.47), which is simplified as

$$A_1 c_1 k_1 \cosh (c_1 x_1) + \varepsilon_{x_1}^u = c_2 k_2 (B_1 \cosh (c_2 x_1) + B_2 \sinh (c_2 x_1)) + \varepsilon_{x_2}^u$$

### 2.2.2.2 Plastic substrate and elastoplastic interlayer

As the applied load continues to increase, the yielding zone in the interlayer propagates toward the inner part, and meanwhile, the internal stress in the substrate will also keep increasing until yielding also initiates in the substrate. For the aluminum substrate, as the thin film plays minor role for carrying the externally applied load as it indicates from Fig. 2.2, the distribution of the
normal stress in the substrate will be approximately uniform along the whole span; thus we assume that the substrate will yield as a whole for simplicity once the internal stress reaches its yielding strength. Assuming that at a certain applied load \( \sigma^0 = \sigma_2 \) the developed yielding zone in the shear interlayer is \( x_2 \) to \( \lambda \) (with symmetry). In this case, the film/substrate system needs to be divided into the following two continuous parts:

### 2.2.2.2.1 Elastic zone \((0 \leq x \leq x_2)\)

In this zone, the displacement and stress in the thin film will have similar formulations as presented in the elastic zone of Section 2.2.1.1:

\[
\begin{align*}
u^f(x, z) &= A_3 \cos (d_3h_1 - d_3z) \sinh (c_3x) + \varepsilon_{x3}^u x \\
\sigma^f_x(x, z) &= \xi_f E^f (A_3 c_3 \cos (d_3h_1 - d_3z) \cosh (c_3x) + \varepsilon_{x3}^u) \\
\tau^f_x(x, z) &= G^f (A_3 d_3 \sin (d_3h_1 - d_3z) \sinh (c_3x))
\end{align*}
\]

Because the shear interlayer is in the elastic stage in this zone, Eq. (2.16) still determines the shearing stress-strain curve for the interlayer while for the substrate with assumption of linear hardening material, the uniaxial stress-strain curve of the substrate can be expressed as

\[
\sigma^s(x) = E_2^s \varepsilon^s(x) + (E_1^s - E_2^s) \varepsilon_Y
\]

where \( E_2^s \) is the linear hardening rate of the substrate under uniaxial tension, \( \varepsilon_Y = \frac{\sigma_Y}{E_1^s} \) is the yield strain, and \( \sigma_Y \) is the yield stress under uniaxial tension.

By following the similar procedures in Section 2.2.1, the displacement and normal stress of the substrate can be determined as:

\[
\begin{align*}
u^s(x) &= A_3 k_3 \sinh (c_3x) + \varepsilon_{x3}^u x \\
\sigma^s(x) &= E_2^s A_3 c_3 k_3 \cosh (c_3x) + E_2^s \varepsilon_{x3}^u + \left( 1 - \frac{E_2^s}{E_1^s} \right) \sigma_Y
\end{align*}
\]
where \( k_3 = -\frac{G_f}{G_1} d_3 h_0 \cdot \sin(d_3 h_1) + \cos(d_3 h_1) \), and \( d_3 \) can be similarly determined from the following equation,

\[
\left( -\alpha^2 \xi s \frac{E_s^g}{G_2} d_3 h_0 + \frac{1}{(h_2 - h_0) d_3} \right) \sin(d_3 h_1) + \alpha^2 \xi s \frac{E_s^g}{G_f} \cos(d_3 h_1) = 0 \quad (2.60)
\]

### 2.2.2.2 Plastic zone \((x_2 \leq x \leq \lambda)\)

In this zone, the displacement and stress in the thin film will have similar formulations as presented in the plastic zone of Section 2.2.2.1:

\[
u^f(x, z) = \cos(d_4 h_1 - d_4 z) \cdot (B_3 \sinh(c_4 x) + B_4 \cosh(c_4 x)) + \varepsilon^u_{x4} x \quad (2.61)
\]

\[
\sigma^f_x(x, z) = \xi f E_f(c_4 \cdot \cos(d_4 h_1 - d_4 z) \cdot (B_3 \cosh(c_4 x) + B_4 \sinh(c_4 x)) + \varepsilon^u_{x4}) \quad (2.62)
\]

\[
\tau^f_x(x, z) = G_f d_4 \cdot \sin(d_4 h_1 - d_4 z) \cdot (B_3 \sinh(c_4 x) + B_4 \cosh(c_4 x)) \quad (2.63)
\]

As both the shear interlayer and the substrate are in the plastic stage, the constitutive equations for them are provided by Eqs. (2.38) and (2.57), respectively. By following similar procedures as in Section 2.2.1, the displacement and normal stress of the substrate can be determined as:

\[
u_s(x) = k_4 \cdot (B_3 \sinh(c_4 x) + B_4 \cosh(c_4 x)) + h_0 \left( \frac{1}{E_2} \right) \\sigma_y \quad (2.64)
\]

\[
\sigma_s(x) = \xi s E_s^g k_4 \cdot (B_3 \cosh(c_4 x) + B_4 \sinh(c_4 x)) + \xi s E_s^g \varepsilon^u_{x4} + \left( 1 - \frac{E_s^g}{E_f^g} \right) \\sigma_y \quad (2.65)
\]

where \( k_4 = -\frac{G_f}{G_2} d_4 h_0 \cdot \sin(d_4 h_1) + \cos(d_4 h_1) \), and \( d_4 \) can be determined by

\[
\left( -\alpha^2 \xi s \frac{E_s^g}{G_2} d_4 h_0 + \frac{1}{(h_2 - h_0) d_4} \right) \sin(d_4 h_1) + \alpha^2 \xi s \frac{E_s^g}{G_f} \cos(d_4 h_1) = 0 \quad (2.66)
\]

The boundary conditions in this case read

\[
\int_0^{h_1} \sigma^f(x) \mid_{x=\lambda} \, dz = 0 \quad (2.67)
\]
The continuity equations read

\[ \tau^0_{xx}(x) \bigg|_{x=x^+_{2}} = \tau_Y \]  
\[ \sigma^*(x) \bigg|_{x=\lambda} = \sigma_2 \]  

From the boundary and continuity equations listed above, the four constants \( A_3, B_i, \) and \( \varepsilon^u_{x_2}(i = 3, 4) \) can be determined as.

\[ \varepsilon^u_{x_4} = \left( \frac{\sigma_2}{E^s} - \left( \frac{1}{E_2} - \frac{1}{E^s} \right) \right) \frac{\sigma_Y}{\sin(d_1 h_1)} \frac{\sin(d_1 h_1)}{\sin(d_1 h_1) - k_4 d_4 h_1} \]  
\[ A_3 d_4 = \frac{\gamma_Y}{G} \frac{1}{\sin(d_3 h_1) \cdot \sinh(c_3 x_2)} \]  
\[ B_3 d_4 = - \left( \frac{\gamma_Y}{G} \frac{\sinh(c_4 x_2)}{\sin(d_4 h_1)} + \varepsilon^u_{x_4} \frac{d_4 h_1}{\alpha} \right) \cosh (c_4 \lambda - c_4 x_2) \]  
\[ B_4 d_4 = \frac{\gamma_Y}{G} \frac{1}{\sin(d_4 h_1) \cdot \cosh(c_4 x_2)} - B_3 d_4 \tanh(c_4 x_2) \]  
\[ \varepsilon^u_{x_3} = \varepsilon^u_{x_4} + \left( \frac{k_4}{d_4 x_2 \sin(d_4 h_1)} - \frac{k_3}{d_3 x_2 \sin(d_3 h_1)} \right) \right) \frac{\tau_Y}{G} + \frac{h_0}{x_2} \left( \frac{1}{\alpha_2} - \frac{1}{\alpha_1} \right) \gamma_Y \]  

\( x_2 \) can be determined by substituting Eqs. (2.73) to (2.77) into Eq. (2.72), which is simplified as

\[ A_3 c_3 k_3 \cosh(c_3 x_2) + \varepsilon^u_{x_3} = c_4 k_4 \left( B_3 \cosh(c_4 x_2) + B_4 \sinh(c_4 x_2) \right) + \varepsilon^u_{x_4} \]
2.2.2.3 Plastic substrate and plastic interlayer

As the applied load continues to increase, the interlayer will eventually fully yield, getting both the interlayer and substrate into plastic stage. Following the similar procedures in Section 2.2.1 by taking the constitutive laws for interlayer and substrate to be Eqs. (2.38) and (2.57), the displacement and stress field in the film/substrate system can be determined by the following equations.

\[ u^f(x, z) = A_5 \cdot \cos (d_5 h_1 - d_5 z) \sinh (c_5 x) + \varepsilon^u_{x_5} x \]  \hspace{1cm} (2.79)

\[ \sigma^f_x(x, z) = \xi f E^f (A_5 c_5 \cdot \cos (d_5 h_1 - d_5 z) \cosh (c_5 x) + \varepsilon^u_{x_5}) \]  \hspace{1cm} (2.80)

\[ \tau^f_{xz}(x, z) = G^f (A_5 d_5 \cdot \sin (d_5 h_1 - d_5 z) \sinh (c_5 x)) \]  \hspace{1cm} (2.81)

\[ u^s(x) = A_5 k_5 \sinh (c_5 x) + \varepsilon^u_{x_5} x + h_0 \left( \frac{1}{G_2^0} - \frac{1}{G_1^0} \right) \tau_Y \]  \hspace{1cm} (2.82)

\[ \sigma^s(x) = \xi s E_2^s (A_5 c_5 k_5 \cosh (c_5 x) + \varepsilon^u_{x_5}) + \left( 1 - \frac{E_2^s}{E_1^s} \right) \sigma_Y \]  \hspace{1cm} (2.83)

where \( k_5 = -\frac{G_f}{G_2^0} d_5 h_0 \cdot \sin (d_5 h_1) + \cos (d_5 h_1) \); \( c_5 = \alpha d_5 \), \( A_5 \) and \( \varepsilon^u_{x_5} \) are determined by

\[ \varepsilon^u_{x_5} = \left( \frac{\sigma^0}{E_2^s} - \left( \frac{1}{E_2^s} - \frac{1}{E_1^s} \right) \sigma_Y \right) \frac{\sin (d_5 h_1)}{\sin (d_5 h_1) - k_5} \]  \hspace{1cm} (2.84)

\[ A_5 = \frac{h_1}{\alpha (d_5 h_1 - \sin (d_5 h_1))} \left( \frac{\sigma^0}{E_2^s} - \left( \frac{1}{E_2^s} - \frac{1}{E_1^s} \right) \sigma_Y \right) \]  \hspace{1cm} (2.85)

and \( d_5 \) can be determined by

\[ \left( -\alpha^2 \xi_e \frac{E_2^s}{G_2^0} d_5 h_0 + \frac{1}{(h_2 - h_0) d_5} \right) \sin (d_5 h_1) + \alpha^2 \xi_e \frac{E_2^s}{G^f} \cos (d_5 h_1) = 0 \]  \hspace{1cm} (2.86)
2.2.2.4 Monotonic unloading

After the applied load reaches its maximum value, it is assumed to be unloaded monotonically. During this unloading stage, the equilibrium, compatibility and continuity equations are the same as those in Section 2.2.1. It should be noted that the elastic solution of this stage is under the applied load of $\sigma^0 = \sigma_2$. Eventually, the residual displacement and stress in the film/substrate system can be determined by subtracting the solutions in Section 2.2.2.3 from those obtained in Section 2.2.1.

2.2.3 Phase III - Opening-Mode Fracture Behavior

Consider the section with two OMFs at both ends in Fig. 2.3. When the external tensile loading increases to a critical value, a new OMF may nucleate along the central line. Just before the fracture initiates, the normal stress along the central line can be obtained. After the new fracture forms, the section is cracked into two pieces and the elastic fields in each piece can be solved by replacing $\lambda$ with $\lambda/2$ in the new local coordinate system.

The stress and displacement fields obtained in the previous sections can be used to calculate the OMFs in the thin film coating. Although the coating layer fractures, the substrate layer remains intact and the fracture energy released by the new fracture can be calculated using the stress necessary to close a newly formed fracture or the normal stress in the coating layer before cracking. Based on this concept, the energy release rate (ERR) of the crack front can be obtained as the work done per unit area to close the crack opening displacement [26].

$$G = \frac{1}{2h_1} \int_0^{h_1} \sigma^f(0, z) u^f(0, z) dz$$

(2.87)

As the applied loading increases, the ERR developed in the thin film increases. Once the ERR is equal to or larger than the fracture toughness, a new fracture will nucleate. Therefore, the following criterion is used to predict the fracture spacing as the external load changes:

$$G \geq \Gamma_{cr}$$

(2.88)

where $\Gamma_{cr}$ is the fracture toughness of the thin film.
2.3 Linear Elastic Solutions and Numerical Verification

To verify the proposed model, the FE solution will validate the elastic solutions obtained in Section 2.2.1 while the experimental results conducted in Section 2.4 will be compared with the elastoplastic solutions obtained in Section 2.2.2. Table 2.1 provides the material and geometric constants of the thin film/substrate system employed in this study, where $E_1^s$ and $E_2^s$ were determined from the loading stress-strain curves for samples with significant yielding (as shown in Fig. 2.2), while the material properties of the thin film and interlayer were summarized from existing studies in the literature [31; 208; 76; 97; 2].

Table 2.1: Material and geometric properties of the alumina film/Aluminum substrate system

<table>
<thead>
<tr>
<th>Modulus (GPa)</th>
<th>Strength (MPa)</th>
<th>Geometry</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_f$</td>
<td>200.0</td>
<td>$\lambda$</td>
</tr>
<tr>
<td>$G_f$</td>
<td>80.0</td>
<td>$h_f$</td>
</tr>
<tr>
<td>$E_1^s$</td>
<td>73.5</td>
<td>$\sigma_Y$</td>
</tr>
<tr>
<td>$E_2^s$</td>
<td>1.08</td>
<td></td>
</tr>
<tr>
<td>$G_1^0$</td>
<td>56.8</td>
<td>$\tau_Y$</td>
</tr>
<tr>
<td>$G_2^0$</td>
<td>4.06</td>
<td>$h_0$</td>
</tr>
</tbody>
</table>

The FE analysis was conducted through the commercial software package Abaqus 6.12, where the plane strain element SC8R was used to model the thin film and interlayer while the truss element T2D2 was used to simulate the substrate. Refined elements were applied at the interface and free surfaces of the film/substrate system. Fig. 2.4(a) shows the FE model with mesh and Fig. 2.4(b) shows the deformed shape of the system under applied load.

Fig. 2.5(a) provides the distribution of axial displacement of the thin film across its thickness direction, which are symmetric at its two ends and reflect the real crack shape as indicated in Fig. 2.1(b). The displacement distributions of the thin film and substrate along the longitudinal direction are shown in Fig. 2.5(b). As the interlayer is much thinner than that of the thin film, the displacement of the thin film at its bottom surface and that of the substrate predicted by the present model are almost overlapped, and well agrees with the that predicted by the FE. The
shearing stress in the interlayer is provided in Fig. 2.6. Both the present solution and FE result show that the shearing stress gradually increases from the middle center toward the free end of the thin film/substrate system. High stress concentration is captured by the present model at the free end, while free stress is predicted by the FE analysis to satisfy the traction free condition. Nevertheless, at a very small distance from the free end, good agreement between the present solution and the FE simulation is observed, which demonstrates the accuracy of the present elastic solutions.
2.4 Elastoplastic Solutions and Experimental Validation

2.4.1 Elastoplastic Solutions

Fig. 2.7 presents the distributions of axial displacement of the thin film across its thickness direction at different phases: (1) Elastic stage (applied strain \( \varepsilon = 0.016\%)\); (2) Elastic substrate/elastoplastic interlayer (\( \varepsilon = 0.072\%)\), and (3) Plastic substrate/elastoplastic interlayer (\( \varepsilon = 2\%)\). Symmetric displacement distributions at both elastic and plastic stages reveal that the presented elastoplastic model is able to capture the crack shape after the channel cracks initiated in the thin film coating layer. Fig. 2.7 shows that the displacement of the thin film significantly increases from 0.012 \( \mu m \) to 1.05 \( \mu m \) as the applied strain slightly increases from 0.2 \( \sigma_Y \) to 1.35 \( \sigma_Y \), revealing the development of significant plastic deformation in the interlayer/substrate and indicating the inability of any elastic model to accurately capture such an elastoplastic fracture behavior in the thin film/substrate system.

According to the obtained displacement and stress fields provided in Section 2.2.2, the ERR can be obtained via Eq. (2.87) and will be presented in this section. The variance of the ERR with respect to the cracking spacing (\( \lambda \)) at constant film thickness \( h_1 = 16.58 \mu m \) is shown in Fig. 2.8(a). When the cracking spacing is relatively small (\( \lambda < 100 \mu m \), i.e., \( \lambda/h_1 < 6 \)), the ERR rapidly increases as the cracking spacing increases until a plateau stage is reached, indicating that,
Figure 2.7: Displacement distributions of the film/substrate system at: (a) Elastoplastic stage I; and (b) Elastoplastic stage II

Figure 2.8: Variance of ERR with respect to crack spacing and coating thickness
under the applied load ($\sigma^0 = 1.35 \sigma_Y$), the potential crack spacing of the given thin film will be in the range of (50 $\mu m$ to 100 $\mu m$). Fig. 2.8(b) shows the variance of the ERR with respect to the film thickness at the constant cracking spacing $\lambda = 80 \mu m$ under the same applied load. The ERR approximately linearly increases with the film thickness until it reaches a convex point, while beyond this point, the ERR rapidly decreases as the film thickness increases. It should be pointed out that fracture saturation reaches at this convex point ($\lambda/h_1 \simeq 5.3$) i.e., under this applied load, no more new crack will be developed when $\lambda/h_1 \simeq 5.3$.

![Image](image.png)

Figure 2.9: Variance of normalized ERR with respect to constant crack spacing or constant coating thickness

To interpret the relationship between the ERR and the cracking spacing/film thickness in a more straightforward way, the variances of the normalized ERR with respect to the crack-spacing/film-thickness ratio ($\lambda/h_1$) at constant crack spacing or film thickness are plotted in Fig. 2.9, where the two curves are overlapped to each other and the normalized ERR rapidly increases as $\lambda/h_1$ increases from 4 to 7. This indicates that cracks will more easily develop as the cracking spacing increases or film thickness decreases within this aspect ratio range under the specified applied load.

Fig. 2.10 illustrates the changing of the normalized applied tensile strain ($h_1E_f/2\Gamma)^{1/2}\varepsilon^0$ with the crack-spacing/film-thickness ratio ($\lambda/h_1$), which represents the required external tensile loading to form a new crack in the thin film with a certain $\lambda/h_1$. The fracture toughness of the thin film applied in this study is 3.5 MPa $m^{1/2}$ [97; 2]. Fig. 2.10(a) clearly shows that the externally applied strain increases as the crack spacing decreases until a saturation stage is arrived. For the specified
film thickness of $h_1 = 16.58\mu m$, the saturated crack spacing can be approximately evaluated as $\lambda_{cr} = 3.8h_1 = 63\mu m$. Fig. 2.10(b) shows the variance of the normalized tensile strain with respect to the $\lambda/h_1$ at a constant $\lambda$ and indicates that the applied strain required to initiate new cracks in the thin film at a constant crack spacing decrease as the thin film thickness decreases until a critical thickness $h_{1cr}$ is reached. For the specified crack spacing of $\lambda = 80\mu m$, the critical film thickness can be approximately evaluated as $h_{1cr} = \lambda/10 = 8\mu m$.

![Graphs](image)

Figure 2.10: Fracture spacing development with respect to the external tensile loading: (a) Constant film thickness; and (b) Constant crack spacing

### 2.4.2 Experimental Validation

To validate the plastic solution of the presented model, an experiment was designed to further explore the OMFs developed in the coating layer. A ductile aluminum plate was coated with a thin brittle material and subject to a uniform tensile load. The presented elastoplastic solution is to be used to explain the OMFs that form perpendicular to the direction of loading within the material coating. Moreover, this new formulation will also explore the phenomenon of fracture saturation and the coating’s critical thickness. In this experiment, the process of anodization grew aluminum Alloy 1100 plate with a brittle Aluminum Oxide ($Al_2O_3$) coating (also called Alumina).
2.4.2.1 Sample preparation

Four aluminum plates with dimensions of 304 mm x 304 mm and varying thicknesses of 4.8 mm, 3.0 mm, 2.2 mm, and 1.4 mm were prepared. Each plate was cut into 24 samples with a uniform width of 12.7 mm. The prepared aluminum samples were polished and cleaned with sand paper. Acetone and distilled water were then used to clean the sample surfaces. The samples were labeled with regular masking tape and then covered with acid resistant tape such that 3 inches from each end of the sample were covered as the grip for the tension test. For a given aluminum thickness, four samples were kept in the anodizing bath for the same duration, resulting in six groups of samples (each group with four replicate samples) with six different anodization duration times (t1 = 2 min, t2 = 4 min, t3 = 8 min, t4 = 15 min, t5 = 30 min, and t6 = 120 min).

![Anodization devices and prepared samples](image)

(a) Anodization devices; and (b) Prepared samples

In this study, the anodization process was developed by following procedures of [93] (see Fig. 2.11(a)), where a sulfuric electrolyte solution composed of 20% sulfuric acid and 80% distilled water by weight was placed inside the test beaker followed by the two lead cathodes. Sodium bicarbonate was kept near the solution to neutralize any spills and an anodization tank was prepared by using a 5-liter glass beaker with Teflon supports manufactured to hold the anode and the cathode in place. The aluminum anode and the lead cathode were held in place by the Teflon supports, which ensures that the lead cathodes are symmetrical spaced around the aluminum anode, thereby creating a uniform alumina layer during anodization. The power supply was adjusted to 15 volts and the current was monitored by a multimeter connected in series with the circuit. The electrolyte was kept at room temperature, which was about 24°C. From experimental observations, the
alumina growth rate from this typical anodization was found to be independent of the sample thickness. Therefore, by varying the time of anodization, the brittle material coating thickness can be approximately controlled. Based on the different aluminum thicknesses and anodizing during time, a total of 96 samples were prepared in this study. After the anodization, all the samples were labeled with colored tape, and then covered with acid-resistant tape as shown in Fig. 2.11(b).

![Image](image.png)

Figure 2.12: Thin film thickness measurement by the PEC

### 2.4.2.2 Thickness determination of the coating layer

Since the aluminum substrate used in this experiment is non-ferrous and the alumina coating is non-conducting, a pulsed eddy-current instrument (PEC) can determine the thickness of a non-conducting layer above a non-ferrous substrate [193]. In this study, a Fischer DUALSCOPE-FMP20 PEC device was used to determine these alumina layer thicknesses, which can accurately determine the coating thickness with a resolution of about 0.01 μm. During the anodization, alumina starts growing with a thickness of $d_{growth}$ from the original border of the aluminum. At the same time, there is another alumina layer that extends into the original aluminum boarder, which can be named as a penetration layer with a thickness of $d_{penetration}$. Therefore, if the original thickness of the aluminum is $H$ and after anodization the thickness is $H_0$, then $h_1 = (H_0 - H)/2$ determines the thickness of the alumina layer.

### 2.4.2.3 Uniaxial tensile testing

The Instron 5984 34k Universal Testing Machine was used to apply a uniform tensile load on each sample (see Fig. 2.13). The load was applied at a strain rate of 0.02 inch/min through a static load
cell, and the ultimate applied load for each sample was determined by the desired stress in terms of its yield stress. As the coating layer thickness varied from different groups, the applied load also varied from sample to sample, but the stress was the same for each series of samples. Since the alumina layer will fracture through its entire layer, the entirety of the stress will be carried through the intact aluminum layer. From this point of view, the ultimate stress in the substrate layer can be expressed by the applied load. After the predefined load was reached, the sample was removed from the Testing Machines with all geometric properties (i.e., thickness, color, width, apparent cracks, discontinuities) recorded.

2.4.3 Test Results and Analysis

The Hitachi S-4700 FE-SEM, a high-resolution cold field emission SEM that allows high resolution captures of thin film specimens, examined the micro-structure as well as the fracture configurations of the alumina coatings throughout the experiment. Fig. 2.14(a) shows a typical SEM image revealing the porous nature of the brittle alumina coating. This porosity allows the electrolyte solution to penetrate the electrically insulating alumina layer and reach the alumina anode during anodization [178].
2.4.3.1 Fracture spacing

The experiment was designed to ensure that periodic OMFs form when a uniform tensile load is applied. By maintaining a uniform coating thickness, OMFs were successfully induced, and were both periodically spaced and perpendicular to the direction of loading. Fig. 2.14(b) shows a typical SEM image of a fractured specimen with parallel crack spacing. It was very difficult to find any potential cracks if the applied stress in the aluminum is in its elastic stage as the crack tends to close after the applied load was removed. For this reason, considerable plastic strain was applied to each specimen, leaving the fracture separation visible.

![SEM images on fractured samples](image)

(a) Typical porous nature of the brittle alumina coating; and (b) Parallel fractures perpendicularly spaced to the applied load

Figure 2.14: SEM images on fractured samples: (a) Typical porous nature of the brittle alumina coating; and (b) Parallel fractures perpendicularly spaced to the applied load

Fig. 2.15 compares the experimental data for crack spacing as a function of film thickness with the prediction obtained by the present model. Both the test data and the theoretical solution predicted by the present model reveal that the crack spacing proportionally decreases as the thin film thickness decreases until a critical film thickness is reached, while below this thickness the crack spacing quickly increases to be infinite indicating that no new cracks will be developed. Overall, the theoretical prediction is able to well capture the varying trend of the cracking spacing with respect to the thin film thickness, which verifies the presented elastoplastic model. It’s worthy to note that all the results shown in Fig. 2.15 correspond to test samples subjected to considerable plastic strain ($\varepsilon^0 = 2\%$), which is far away from the capacities of any elastic modeling.
2.4.3.2 Critical thickness

The test showed that the crack spacing decreases as the coating thickness decreases. Therefore, a critical thickness exists below which no new crack will be initiated under the same loading. However, it will be difficult to determine the exact value of this critical thickness due to experimental restrictions such as limited samples and inaccessibility of real-time fracture observation. To approximately retrieve such a critical thickness, 7 different groups of samples with 7 different anodization time (1, 2, 4, 8, 15, 30, and 120 minutes) corresponding to 7 different aluminum coating thicknesses were prepared. Four different predetermined peak loads ($\sigma_c = 17.6$ MPa, $35.2$ MPa, $52.74$ MPa, and $70.2$ MPa) were applied to each specimen in the tensile test. After the applied load reached its desired load, the specimen was removed from the test stand and examined by SEM to check any existence of fracture. Nonexistence of any fracture indicates that the critical tensile load had not yet been reached. The test results for all the sample with the seven different coating thickness are summarized in Table 2.2. It indicates that for a load of $\sigma_c = 70.2$ MPa, the critical thickness is between $1.59 \mu m$ and $2.26 \mu m$. Moreover, for the three loads at or below $\sigma_c = 52.7$ MPa, the critical thickness is larger than $30.36 \mu m$. Although the exact critical thickness cannot be determined experimentally, this evaluation provides a good guide for comparing with the analytical results.

Fig. 2.16 shows the relationship between the fracture spacing ($\lambda$) and the thin film thickness ($h_1$) based on the present elastoplastic model under different loading levels. Fig. 2.16(a) shows
Table 2.2: Critical thin film study

<table>
<thead>
<tr>
<th>Anodization time (min)</th>
<th>Coating thickness (µm)</th>
<th>Fracture (17.6MPa)</th>
<th>Fracture (35.2MPa)</th>
<th>Fracture (52.7MPa)</th>
<th>Fracture (70.2 MPa)</th>
<th>Critical Load (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.59</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>No</td>
</tr>
<tr>
<td>2</td>
<td>1.59</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>No</td>
</tr>
<tr>
<td>4</td>
<td>2.26</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>Yes</td>
<td>66.26</td>
</tr>
<tr>
<td>8</td>
<td>6.31</td>
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<td>No</td>
<td>Yes</td>
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<td>15</td>
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<td>Yes</td>
<td>64.33</td>
</tr>
<tr>
<td>30</td>
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<td>No</td>
<td>Yes</td>
<td>62.25</td>
</tr>
<tr>
<td>120</td>
<td>30.36</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>Yes</td>
<td>57.21</td>
</tr>
</tbody>
</table>

Figure 2.16: Critical thickness at different loading levels: (a) Applied load $\sigma^0 = 70.2 Mpa$; and (b) $\sigma^0 = 52.7 Mpa$;

that, under the applied load $\sigma^0 = 70.2$ MPa, the theoretical critical thickness ($h_{1cr}$) is 2.6 µm, which is slightly larger than the higher bond one from the experimental test with a discrepancy less than 10%. When the applied load $\sigma^0 = 52.7$ MPa, the critical thickness obtained from the present model is about 38 µm as shown in Fig. 2.16(b), which is about 20 % larger than the lower bond of the value found from the test results as indicated in Table 2.2.
2.5 Conclusions

In this study, an elastoplastic fracture model has been developed to study the OMF in thin film layered structures undergoing large-scale yielding. Considering the fracture pattern with an approximately uniform fracture spacing, the stress field in the coating system is described by one section between two adjacent cracks. As the film is much thinner and more brittle than the substrate, a 2D plane strain formulation is employed to analyze the elastic field in the thin film, while a 1D linear hardening plastic model is applied to account for the large plastic deformations in the substrate under substantial yielding, and an elastoplastic shear lag model is established to transfer the tensile stress in the substrate to the thin film. An increasing tensile load induces three stress phases: linear elastic behavior, yielding of the substrate and interface, and OMF in the thin film. General formulations and explicit expressions of the elastic/elastoplastic solutions of the thin film/substrate system under different loading stages have been developed. The elastic field in the thin film has been verified with the FE results. Using the periodic condition, the fracture ERR is calculated and successfully used to predict the crack initiation, infilling, and saturation in the thin film. Under the same applied load, the crack spacing proportionally increases with the thin film thickness and a critical film thickness exists, below which no more fractures will be developed. Experimental characterization is further conducted to validate the presented elastoplastic fracture model. The present general formulation can be applied to other types of thin film-ductile substrate systems and layered material/structures.
Chapter 3

Two-dimensional Elastoplastic Fracture Analysis in Polar Coordinates

This chapter presents the two-dimensional (2D) elastoplastic fracture analysis from Cartesian coordinates extended to polar coordinates. Similar as in Chapter 2, the alumina coating generated by anodic oxidation is assumed to be elastic and fully bonded to the aluminum wire. By considering the axial symmetry, the structure is simplified as a 2D structure. As the distribution of stress in the substrate does not change much across the radial direction, the substrate is simplified as a one-dimensional (1D) bar whose plasticity is characterized by a bi-linear hardening plastic model. An elastoplastic shear lag model is employed to transfer the stress from the substrate to the coating. By solving the equilibrium equations in polar coordinates, the displacement and stress fields in the coating/substrate under different loading level are obtained and used to calculate the fracture energy release rate (ERR). Parametric studies about the change of fracture energy with respect to the geometry are done. Based on the calculated fracture ERR, the fracture initiation, infilling, and saturation are discussed. In order to verify the presented fracture model, the theoretically predicted elastic solutions are verified by the finite element (FE) results and experiments are conducted to validate the fracture analysis. The good agreements between the theoretical solutions and simulation/experimental results show that the developed 2D elastoplastic fracture model in polar...
coordinate can capture the elastic/elastoplastic field in the coating/substrate system accurately and predict the fracture initiation, infilling, and saturation successfully.

3.1 Overview

Consider a thin brittle coating layer with thickness \( b - a \), length \( 2\lambda \), Young’s modulus \( E^f \), and Poisson’s ratio \( \nu^f \) bonded to a wire substrate with radius \( a \), Young’s modulus \( E^s \), and Poisson’s ratio \( \nu^s \). Then the substrate is subjected a uniform tensile load as denoted in Fig. 3.1(left side). It was observed that no slip or debonding occurs between the substrate and the coating layer. Therefore, it is reasonable to assume that the thin film is fully bonded to the substrate [38].

Once the opening-mode fracture (OMF) initiates in the coating layer, it will propagate toward the interface between the coating layer and the substrate. Considering a section between two adjacent OMFs, as the geometry and loading are axial symmetry, a simplified 2D shear lag model is set up in the polar coordinate as shown in Fig. 3.1(right side). In this model, the thin layer of the alumina coating is treated as an elastic medium, while the ductile substrate aluminum wire is considered as an elastoplastic material. An elastoplastic shear lag model is applied to transfer the shearing stress from the substrate layer to the thin coating layer [32; 132; 37].

Fig. 3.2 shows the strain-stress curves for two aluminum rods with or without alumina coating under tensile loading. The similarity in the curves suggests that, as the brittle coating is very thin compared to the substrate \( (h_1 \ll h_2) \), the effect of the coating layer on the global stress distribution in the substrate can be neglected. Therefore, it is reasonable to assume that the tensile stress in the substrate is uniformly distributed along the radial direction; thus a 1D analysis is conducted in the substrate layer [38]. As shown in Fig. 3.2, the strains increase linearly with respect to the applied load until the yielding point is reached. After the yielding point, the strains again increase proportionally to the applied load with a much lower increasing ratio. Thus, a bi-linear model is employed to simulate the elastoplastic behavior by fitting the two sections of the stress-strain curve using two straight lines.

By following our previous work [38], as the applied tensile load continuously increases, the coating/substrate system will undergo three different stress phases.

(I) When the tensile load is small, the thin film, the interlayer, and the substrate are all in a
Figure 3.1: Schematic illustration of thin coating/substrate system with multiple parallel cracks (left); and a simplified 2D shear lag model with OMFs (right)

Figure 3.2: Tensile stress strain cure of the ductile substrate with/without coating
linear elastic range. Thus, an elastic analysis is conducted.

(II) When the interfacial shearing stress in the interlayer or the tensile stress in the substrate reaches their corresponding yielding strength, plastic behavior is induced in the ductile interlayer or the substrate.

(III) As the tensile load further increases, higher proportion of the load will be transferred to the thin film. When the strain energy developed in the thin film reaches its fracture energy, OMFs will initiate at the center of the thin film. The OMFs break the film with a length of $2\lambda$ into two halves of fragmentations. The newly formed fragments will subsequently go through the same three stress stages and more OMFs will fill in the thin film as the applied load continuously increases. However, this fracture infilling will reach a saturation point once the ratio of cracking spacing to coating thickness approaches to a critical value, upon which the stress between two adjacent cracks changes from tensile to compressive [17]. In this stage, OMF initiation, infilling, and saturation will be analyzed.

In the following, Section 3.2 will develop general formulations and provide explicit solutions of the elastic field in the coating/substrate system, which will be verified by FE analysis. Section 3.3 will conduct elastoplastic analysis of the coating/substrate system. Fracture analysis and further experimental validation will be conducted in Section 3.4, where crack initiation, infilling, and saturation in the coating will be disclosed. Some conclusive remarks will be arrived in Section 3.5.

3.2 Phase I - Elastic Analysis and Numerical Validation

3.2.1 Derivation and Formulas

When the applied load is relatively small, the coating, interlayer and substrate are all in elastic stage. This section provides the corresponding elastic solutions.

3.2.1.1 Elastic field in the thin film ($a < r \leq b$)

The equilibrium equation in the $z$-direction without body force can be written as:

$$\sigma_{z,z}^f + \tau_{r,z}^f + \frac{\tau_{r,z}}{r} = 0$$  \hspace{1cm} (3.1)
where \( \sigma_z^f \) and \( \tau_{rz}^f \) are the normal and shearing stress in the thin film, respectively. The superscript "\( f \)" denotes the coating or thin film.

By following the same principle as conducted in the planar problem \([224; 227; 38]\), we assume that all the points on the same cylindrical face parallel to the loading axis will remain on the same face, namely:

\[ u_{f, rz}^z = 0 \] (3.2)

Note that \( u_f^r \) is the radial displacement. A plane strain formulation is developed by using the following constitutive law:

\[ \sigma_z^f = \frac{E_f}{(1 + \nu^f)(1 - 2\nu^f)} \left[ (1 - \nu^f)u_{z,z}^f + \nu^f u_{r,r}^f \right] \] (3.3)

\[ \tau_{rz}^f = \frac{E_f}{2(1 + \nu^f)} u_{z,r}^f \] (3.4)

\( u_z^f \) is the displacement along the \( z \)-direction. Eq. (3.2) has been used in Eq. (3.4). By substituting Eq. (3.3) and (3.4) into Eq. (3.1), one can write

\[ \frac{2 \left( 1 - \nu^f \right)}{1 - 2\nu^f} u_{z,z}^f + \frac{1}{r} u_{z,r}^f + u_{z,rr}^f = 0 \] (3.5)

Eq. (3.5) is a decoupled partial differential equation of \( u_z^f \). By applying the method of separation of variables, the general solution of Eq. (3.5), a decoupled partial differential equation of \( u_z^f \), can be written as:

\[ u_z^f (r, z) = f(r)g(z) + \varepsilon_{z_1}^u z \] (3.6)

The unknown constant \( \varepsilon_{z_1}^u \) is introduced as a uniform strain caused by the uniaxial tension in the substrate. Substituting this general solution into Eq. (3.5) produces

\[ \frac{2 \left( 1 - \nu^f \right)}{1 - 2\nu^f} g'' f + \frac{1}{r} f' g + f'' g = 0 \] (3.7)

As \( f, f', \) and \( f'' \) are functions of \( r \), whereas \( g, g', \) and \( g'' \) are functions of \( z \), these two independent equations can be linked by an independent constant \( d_1^2 \) through

\[ - \frac{f''}{f} + \frac{1}{r} f' = \frac{2 \left( 1 - \nu^f \right) g''}{g} = d_1^2. \] (3.8)

From the above equation, the general solution of \( u_z^f \) can be written as:

\[ u_z^f (r, z) = [c_1 \sinh (e_1 z) + c_2 \cosh (e_1 z)] \left[ c_3 J_0 (d_1 r) + c_4 Y_0 (d_1 r) \right] + \varepsilon_{z_1}^u z \] (3.9)
where
\[ e_1 = \alpha d_1 \]  
\[ \alpha = \sqrt{\frac{1 - 2\nu_f}{2(1 - \nu_f)}} \]

where \( c_i (i = 1, ..., 4) \) are coefficients to be determined.

By using the symmetry of displacement along the \( z \)-direction, one additional boundary condition can be written as:
\[ u_f |_{z=0} = 0 \]  
\[ (3.12) \]

The free surface of the thin film reads
\[ \tau_{r|z} = 0 \]  
\[ (3.13) \]

By substituting Eqs. (3.12) and (3.13) into Eq. (3.9), the displacement along \( z \)-direction is reduced to
\[ u_f(r, z) = C_1 \sinh(e_1 z) [J_0(d_1 r)Y_1(d_1 b) - J_1(d_1 b)Y_0(d_1 r)] + e_{z1}^u z \]  
\[ (3.14) \]

Substituting Eq. (3.14) into the constitutive equation and neglecting the normal stress along the radial direction, the stress field in the coating layer can be written as
\[ \sigma_f(r, z) = \xi_f E_f \left[ C_1 e_1 \cosh(e_1 z) [J_0(d_1 r)Y_1(d_1 b) - J_1(d_1 b)Y_0(d_1 r)] + e_{z1}^u \right] \]  
\[ (3.15) \]
\[ \tau_{r|z} = -G_f C_1 d_1 \sinh(e_1 z) [J_1(d_1 r)Y_1(d_1 b) - J_1(d_1 b)Y_1(d_1 r)] \]  
\[ (3.16) \]

where \( \xi_f = \frac{1-\nu_f}{(1+\nu_f)(1-2\nu_f)} \) and \( G_f = \frac{E_f}{2(1+\nu_f)} \).

### 3.2.1.2 Elastic field in the shear interlayer \((R \leq r \leq a)\)

Referring to our previous study [38], the introduced shear interlayer with a thickness of \((a - R)\) mainly transfers the tensile load in the substrate to the coating layer. We also assume a uniformly distributed shearing stress and corresponding shearing strain along the radial direction.

The constitutive equation of the shear interlayer in the elastic stage reads
\[ \tau_{r|z} = G_f \gamma_{r|z} \]  
\[ (3.17) \]

where \( \tau_{r|z} \) and \( \gamma_{r|z} \) are the shearing stress and strain in the interlayer and \( G_f \) is the elastic shear modulus of the interlayer.
Considering the continuity of shearing stress between the substrate and the interlayer, we define

\[ A_1 = J_0(d_1a)Y_1(d_1b) - J_1(d_1b)Y_0(d_1a) \]  
(3.18)

and

\[ A_2 = J_1(d_1a)Y_1(d_1b) - J_1(d_1b)Y_1(d_1a) \]  
(3.19)

The shearing stress and shearing strain in the interlayer can be written as

\[ \tau_{rz}^0(z) = -GfC_1d_1A_2\sinh(e_1z) \]  
(3.20)

\[ \gamma_{rz}^0(z) = -\frac{Gf}{C_1}C_1d_1A_2\sinh(e_1z) \]  
(3.21)

Based on the assumption that there is no slip between the substrate and coating, and the shearing strain is uniform along the radial direction in the interlayer, the interface continuity can be expressed as

\[ u_s^e(z) = u_f^l(r = a, z) - (a - R)\gamma_{rz}^0(z) \]  
(3.22)

where \( u_s^e(z) \) is the displacement along the \( z \)-direction in the substrate. Substituting Eqs. (3.14) and (3.21) into Eq. (3.22), the displacement of substrate can be determined through

\[ u_s^e(z) = C_1K_1\sinh(e_1z) + \varepsilon_{z1}^u z \]  
(3.23)

where \( K_1 = A_1 + \frac{Gf}{C_1}(a - R)d_1A_2 \).

### 3.2.1.3 Elastic field in the substrate \((0 \leq r < R)\)

As mentioned before, the tensile load is approximately uniform along the radial direction in the substrate layer, and the substrate can be simplified as a 1D problem. The equilibrium equation can be expressed as

\[ \pi R^2 \frac{d}{dz} \sigma_s^e(z) + 2\pi R\tau_{rz}^0(z) = 0 \]  
(3.24)

where \( \sigma_s^e(z) \) is the normal stress in the substrate.

The constitutive equation of the substrate under a plane strain assumption in the elastic stage reads

\[ \sigma_s^e(z) = E_1^e\varepsilon_z^s(z) \]  
(3.25)
where $E_1^s$ is the stiffness of the substrate. $\varepsilon_z^s(z)$ is the tensile strain in the substrate, under small displacement assumption, it can be written as

$$
\varepsilon_z^s(z) = \frac{du_z^s(z)}{dz}
$$

(3.26)

Combining Eqs. (3.26), (3.25), and (3.20) gives the equilibrium equation as

$$
\frac{R}{2}E_1^s u_{z,zz}^s(z) - G^f C_1 d_1 A_2 sinh (e_1 z) = 0
$$

(3.27)

Substituting Eq. (3.23) into Eq. (3.27) yields

$$
\frac{E_1^s}{G^f} A_1 + \left[ \frac{E_1^s}{G_1^s} (a - R)d_1 - \frac{2}{Rd_1 \alpha^s} \right] A_2 = 0
$$

(3.28)

By solving Eq. (3.28), $d_1$ can be theoretically determined, and then the tensile stress in the substrate can be obtained by Eqs. (3.25) and (3.23) as

$$
\sigma_z^s(z) = E_1^s \left[ C_1 e_1 K_1 cosh (e_1 z) + \varepsilon_z^u \right]
$$

(3.29)

The boundary conditions are given as

$$
\sigma_z^s(z) \mid_{z=\lambda} = \sigma_1^0
$$

(3.30)

where $\sigma_1^0$ is the applied tensile load.

$$
\int_a^b 2\pi r \sigma_z^f (r, z) \mid_{z=\lambda} \, dr = 0
$$

(3.31)

As an OMF surface, the stress is supposed to be 0. However, this condition cannot be satisfied exactly due to the assumption in Eq. (3.2) and a relaxed boundary conditions is used in Eq. (3.31).

Eqs. (3.30) and (3.31) can be used finally to determine the coefficients $C_1$ and $\varepsilon_x$ as

$$
\varepsilon_z^u = \frac{\sigma_1^0}{E_1^s} \frac{A_3}{A_3 - K_1}
$$

(3.32)

$$
C_1 = -\frac{\varepsilon_z^u}{e_1 A_3 cosh(e_1 \lambda)}
$$

(3.33)

where $A_3 = \frac{2}{b^2-a^2} \int_a^b r [J_0(d_1 r) Y_1(d_1 b) - J_1(d_1 b) Y_0(d_1 r)] dr$
3.2.2 Elastic Solutions and Numerical Verification

To verify the proposed model, the elastic solutions obtained in Section 3.2.1 will be compared with FE solution. Table 3.1 provides the material and geometric constants of the coating/substrate system used in this FE analysis, where $E_1^s$, $E_2^s$ and $\sigma_Y$ are determined from Fig. 3.2, while the material properties of the thin film and interlayer are summarized from existing studies in the literature [31; 208; 76; 97; 2].

<table>
<thead>
<tr>
<th>Table 3.1: Material and geometric properties of the alumina film/Aluminum substrate system</th>
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<tr>
<td>Modulus (GPa)</td>
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<tr>
<td>$E^f$</td>
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<tr>
<td>$G^f$</td>
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<td>$E_1^s$</td>
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<td>$G_2^d$</td>
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The commercial software package ABAQUS 6.11-3 is employed to conduct the numerical simulation. In the FE model, 4-node bilinear axisymmetric quadrilateral elements CAX4 are used to model the thin film and interlayer while the 2-node linear axisymmetric membrane elements MAX1 are used to simulate the substrate. In order to better characterize the element optimization and capture the local stress field more accurately, gradient meshing has been used throughout the FE model and refined elements are applied at the interface and free surfaces of the film/substrate system as shown in Fig. 3.3(a). The element size for coating, interlayer and substrate increases from 0.04 to 2 $\mu$m from the two ends to the center point. In total, 12402 elements are generated in the coating and interlayer while 318 elements in the substrate. A constraint is applied to tie the coating layer, interlayer, and substrate together, therefore, no slipping or debonding is allowed. The deformed shape of the system under two opposite concentrated forces applied at the two ends of substrate is shown in Fig. 3.3(b).
Figure 3.3: FE model of the OMF film/substrate system

The distributions of the axial displacement across the radial direction at the two ends of coating layer as shown in Fig. 3.4(a) are symmetric and reflect the real crack shape as indicated in Fig. 3.1. Fig. 3.4(b) shows the axial displacement distributions in the interlayer and substrate. Recalling the interface continuity as Eq. (3.22), as the coating thickness is very small, therefore, the displacement of coating layer at its inner surface is almost overlapped with the displacement in the substrate, which agrees well with the result from FE simulation.

The distributions of stress in the substrate and interlayer are provided in Fig. 3.5. It shows that the normal and shearing stress from both the present model and FE results gradually increase from the middle center toward the free end. The normal stress in the substrate only varies in a very small range and can be approximately treated as uniformly distributed. For the shearing stress in the interlayer, high concentration is captured by the present model at the free end, while free
Figure 3.4: Displacement distributions of the film/substrate system: (a) Distributions of axial displacement of the coating across its radial direction at the crack ends; (b) Axial displacement distributions of the coating and substrate along $z$-direction.

Figure 3.5: Stress distributions of the film/substrate system: (a) Normal stress distribution in substrate along axial direction; (b) Shear stress distribution of the interlayer.

stress is predicted by the FE analysis which satisfies the free traction condition. Nevertheless, at a very small distance from the free end, good agreement between the present solution and the FE simulation is observed, demonstrating the accuracy of the present elastic solutions.
3.3 Phase II - Elastoplastic Behavior and Solutions

From the elastic solutions presented in Section 3.2, both the tensile stress in the substrate and the shearing stress in the interlayer increase in magnitude from the center to the end. If the shearing stress at the end of the interlayer reaches its yielding strength, while the tensile stress in substrate is still lower than its corresponding yielding stress, yielding will firstly initiate at the two ends of the interlayer and propagate toward the inner part. When the tensile load increases to a specific value, the tensile stress at the end of substrate will also reach the yielding stress. As shown in Fig. 3.5(a), the normal stress in the substrate varies within a very small range and can be approximated as uniform along the whole span. For simplicity, we assume that the substrate will yield once the loading stress reaches its yielding stress [38]. As the applied tensile load increases further, the yielding in the interlayer will propagate all the way to the center; therefore, all the interlayer and substrate get into the plastic stage.

In the following, Section 3.3.1 will provide the formulas as the substrate is in its elastic stage, while part of interlayer is in the plastic stage. Section 3.3.2 will present the analysis when the majority part of interlayer gets into plastic stage and all substrate yields. The solution for the case that both interlayer and substrate fully get into plastic stage is conducted in Section 3.3.3.

3.3.1 Elastic Substrate and Elastoplastic Interlayer

We assume that at a certain applied load ($\sigma^0 = \sigma_2^0$), the developed yielding zone in the shear interlayer is $z_1$ to $\lambda$ (with symmetry) and the substrate is still in the elastic stage. In this case, the film/substrate system needs to be divided into two continuous parts:

3.3.1.1 Elastic zone ($0 \leq z \leq z_1$)

In this zone, both the shear interlayer and substrate are in the elastic stage. Thus, all the solutions in Section 3.2.1 are applicable for this elastic zone. Considering the slightly changed boundary conditions, all the elastic solutions for the thin film/substrate system are rewritten as in the following expressions:

$$u_z^f(r, z) = C_2 \cdot sinh(\epsilon_2 z) \left[ J_0(d_2 r)Y_1(d_2 b) - J_1(d_2 b)Y_0(d_2 r) \right] + \varepsilon \frac{u_z}{r_2}$$  (3.34)
\[ \sigma^f_z(r, z) = \xi_f E^f \left[ C_2 e_2 \cdot \cosh (e_2 z) \left[ J_0 (d_2 r) Y_1 (d_2 b) - J_1 (d_2 b) Y_0 (d_2 r) \right] + \varepsilon^u_{z_2} \right] \]  

(3.35)

\[ \tau^f_{rz}(r, z) = -G^f C_2 d_2 \sinh (e_2 z) \left[ J_1 (d_2 r) Y_1 (d_2 b) - J_1 (d_2 b) Y_1 (d_2 r) \right] \]  

(3.36)

\[ u^s_z(z) = C_2 K_2 \sinh(e_2 z) + \varepsilon^u_{z_2} z \]  

(3.37)

\[ \sigma^s_z(z) = E^s \left[ C_2 e_2 K_2 \cosh(e_2 z) + \varepsilon^u_{z_2} \right] \]  

(3.38)

Similarly,

\[ K_2 = A_4 + \frac{G^f}{G_1^T} (a - R) d_2 A_5 \]  

(3.39)

\[ A_4 = J_0 (d_2 a) Y_1 (d_2 b) - J_1 (d_2 b) Y_0 (d_2 a) \]  

(3.40)

\[ A_5 = J_1 (d_2 a) Y_1 (d_2 b) - J_1 (d_2 b) Y_1 (d_2 a) \]  

(3.41)

where \( C_2 \) is a constant to be determined, \( d_2 = d_1, e_2 = e_1 \) and \( e_2^2 = \alpha^2 d_2^2 \) still holds.

### 3.3.1.2 Elastic-plastic zone \((z_1 \leq z \leq \lambda)\)

As the thin film is still in the elastic stage, the general expression of the displacement in the thin film in Eq. (3.9) is still applicable. By applying the boundary condition Eq. (3.13), the displacement of the thin film can be reduced to

\[ u^f_z(r, z) = \left[ C_3 \sinh (e_3 z) + C_4 \cosh (e_3 z) \right] \left[ J_0 (d_3 r) Y_1 (d_3 b) - J_1 (d_3 b) Y_0 (d_3 r) \right] + \varepsilon^u_{z_3} z \]  

(3.42)

where \( C_3 \) and \( C_4 \) are constants to be determined. Considering the constitutive equations in Eqs. (3.3) and (3.4), the normal and shearing stresses in the thin film can be simplified as

\[ \sigma^f_z(r, z) = \xi_f E^f \left[ e_3 \cdot \left[ C_3 \cosh (e_3 z) + C_4 \sinh (e_3 z) \right] \left[ J_0 (d_3 r) Y_1 (d_3 b) - J_1 (d_3 b) Y_0 (d_3 r) \right] + \varepsilon^u_{z_3} \right] \]  

(3.43)

\[ \tau^f_{rz}(r, z) = -G^f d_3 \left[ C_3 \sinh (e_3 z) + C_4 \cosh (e_3 z) \right] \left[ J_1 (d_3 r) Y_1 (d_3 b) - J_1 (d_3 b) Y_1 (d_3 r) \right] \]  

(3.44)

As the shear interlayer enters into the plastic stage in this zone, the shearing stress-strain curve for the interlayer becomes:

\[ \tau^0_{rz}(z) = G^0_2 \gamma_{rz}^0 (z) + \left( G^0_1 - G^0_2 \right) \gamma_y \]  

(3.45)
where $G_2^0$ is the linear hardening rate of the shear interlayer under uniform shear; $\gamma_Y = \frac{Y}{G_1}$ is the yield shearing strain and $\tau_Y$ is yield stress under uniform shear.

By following the similar procedures as in Section 3.2.1, the displacement and normal stress of the substrate can be determined by

\[
u_s^s(z) = K_3 \left[ C_3 \sinh(e_3 z) + C_4 \cosh(e_3 z) \right] + \varepsilon_3^u z + \left( a - R \right) \left( \frac{1}{G_2} - \frac{1}{G_1} \right) \tau_Y \tag{3.46}
\]

\[
\sigma_s^s(z) = E_1^s e_3 K_3 \left[ C_3 \cosh(e_3 z) + C_4 \sinh(e_3 z) \right] + E_1^s \varepsilon_3^u \tag{3.47}
\]

where

\[
K_3 = A_6 + \frac{G_f}{G_2} d_3 (a - R) A_7 \tag{3.48}
\]

\[
A_6 = J_0(d_3 a) Y_1(d_3 b) - J_1(d_3 b) Y_0(d_3 a) \tag{3.49}
\]

\[
A_7 = J_1(d_3 a) Y_1(d_3 b) - J_1(d_3 b) Y_1(d_3 a) \tag{3.50}
\]

Substituting Eqs. (3.46) and (3.47) into the equilibrium equation Eq. (3.24) and considering the shearing stress continuity between the film and interlayer yields

\[
\frac{E_1^s}{G_f} A_6 + \left[ \frac{E_1^s}{G_2^0} (a - R) d_3 - \frac{2}{R d_3 \alpha^2} \right] A_7 = 0 \tag{3.51}
\]

from which the coefficient $d_3$ can be theoretically obtained.

The boundary conditions in this case read

\[
\int_a^b 2\pi r \sigma^f_s(z) \big|_{z=\lambda} \, dr = 0 \tag{3.52}
\]

\[
\tau_{rz}^0(z) \big|_{z=\lambda} = -\tau_Y \tag{3.53}
\]

\[
\sigma_s^s(z) \big|_{z=\lambda} = \sigma_2^0 \tag{3.54}
\]

The continuity equations read

\[
\tau_{rz}^0(z) \big|_{z=z_1^-} = \tau_{rz}^0(z) \big|_{z=z_1^+} \tag{3.55}
\]

\[
u_s^s(z) \big|_{z=z_1^-} = u_s^s(z) \big|_{z=z_1^+} \tag{3.56}
\]

\[
\sigma_s^s(z) \big|_{z=z_1^-} = \sigma_s^s(z) \big|_{z=z_1^+} \tag{3.57}
\]
From the boundary and continuity equations listed above, the five constants $C_2$, $C_3$, $C_4$, and $\varepsilon^u_{z_3}(i = 2, 3)$ can be determined.

$$\varepsilon^u_{z_3} = \frac{\sigma_0^0}{E_1} \frac{A_8}{A_8 - K_3}$$  (3.58)

where $A_8 = \frac{2}{\pi^2 \alpha^2} \int_a^b r [J_0(d_3 r)Y_1(d_3 b) - J_1(d_3 b)Y_0(d_3 r)]dr$

$$C_2 = \frac{\gamma_Y}{G_f d_2 \sinh(e_2 z_1)}$$  (3.59)

$$C_3 = \frac{1}{\cosh(e_3 \lambda - e_3 z_1)} \left[ \frac{\sigma_0^0 \cosh(e_3 z_1)}{E_1 e_3 (K_2 - A_8)} - \frac{\tau_Y \sinh(e_3 \lambda)}{G_f d_3 A_7} \right]$$  (3.60)

$$C_4 = \frac{\gamma_Y}{G_f d_3 A_7 \cosh(e_3 z_1)} - C_3 \tanh(e_3 z_1)$$  (3.61)

$$\varepsilon^u_{z_2} = \varepsilon^u_{z_3} + \frac{a - R}{z_1} \left( \frac{1}{G_2} - \frac{1}{G_0} \right) \gamma_Y + \frac{\tau_Y}{G_f} \left( \frac{K_3}{d_3 A_7} - \frac{K_2}{d_2 A_5} \right)$$  (3.62)

The yielding initiation position $z_1$ can be determined by substituting Eqs. (3.58) to (3.62) into Eqs. (3.57), which is simplified as

$$C_2 e_2 K_2 \cosh(e_2 z_1) + \varepsilon^u_{z_2} = \varepsilon^u_{z_3} + C_3 \cosh(e_3 z_1) + C_4 \sinh(e_3 z_1) + \varepsilon^u_{z_3}$$  (3.63)

### 3.3.2 Plastic Substrate and Elastoplastic Interlayer

Referring to the assumption that the substrate will yield once the loading stress reaches its yielding stress, when the applied load ($\sigma^0 = \sigma_0^0$) is larger than the yielding strength of substrate, the whole substrate will get into the plastic stage and the developed yielding zone in the shear interlayer is $z_2$ to $\lambda$ (with symmetry). In this case, the film/substrate system needs to be divided into following two continuous parts:

#### 3.3.2.1 Elastic zone ($0 \leq z \leq z_2$)

In this zone, the displacement and stress in the thin film will have similar formulations as presented in the elastic zone of Section 3.2.1.1:

$$u_z^I(r, z) = C_5 \sinh(e_4 z) [J_0(d_4 r)Y_1(d_4 b) - J_1(d_4 b)Y_0(d_4 r)] + \varepsilon^u_{z_4} z$$  (3.64)
\[ \sigma_z^f(r, z) = \xi_f E_f^f \left[ C_5 e_4 \cosh(e_4 z) \left[ J_0(d_4r) Y_1(d_4b) - J_1(d_4b) Y_0(d_4r) \right] + \varepsilon_{z4}^u \right] \] (3.65)

\[ \tau_{rz}^f(r, z) = -G_f^f C_5 d_4 \sinh(e_4 z) \left[ J_1(d_4r) Y_1(d_4b) - J_1(d_4b) Y_1(d_4r) \right] \] (3.66)

As the shear interlayer is in the elastic stage in this zone, the shearing stress-strain curve for the interlayer is still determined by Eq. (3.17), while for the substrate with assumption of linear hardening material, the uniaxial stress-strain curve of the substrate can be expressed as

\[ \sigma_z^s(z) = E_2^s \varepsilon_z^s(z) + (E_1^s - E_2^s) \varepsilon_Y \] (3.67)

where \( E_2^s \) is the linear hardening rate of the substrate under uniaxial tension, \( \varepsilon_Y = \frac{\sigma_Y}{E_1^s} \) is the yield strain and \( \sigma_Y \) is the yield stress under uniaxial tension.

By following the similar procedures as in Section 3.2.1, the displacement and normal stress of the substrate can be determined by

\[ u_z^s(z) = C_5 K_4 \sinh(e_4 z) + \varepsilon_{z4}^u z \] (3.68)

\[ \sigma_z^s(z) = E_2^s C_5 e_4 K_4 \cosh(e_4 z) + E_2^s \varepsilon_{z4}^u + \left( 1 - \frac{E_2^s}{E_1^s} \right) \sigma_Y \] (3.69)

where

\[ K_4 = A_9 + \frac{G_f}{G_1^f} d_4 (a - R) A_{10} \] (3.70)

\[ A_9 = J_0(d_4a) Y_1(d_4b) - J_1(d_4b) Y_0(d_4a) \] (3.71)

\[ A_{10} = J_1(d_4a) Y_1(d_4b) - J_1(d_4b) Y_1(d_4a) \] (3.72)

d_4 can be similarly determined by the following formation:

\[ \frac{E_2^s}{G_1^f} A_9 + \left( \frac{E_2^s}{G_1^f} (a - R) d_4 - \frac{2}{R d_4 a^2} \right) A_{10} = 0 \] (3.73)

### 3.3.2.2 Plastic zone \((z_2 \leq z \leq \lambda)\)

In this zone, the displacement and stress in the thin film will have similar formulations as those presented in the plastic zone of Section 3.3.1:

\[ u_z^f(r, z) = [C_6 \sinh(e_5 z) + C_7 \cosh(e_5 z)] \left[ J_0(d_5r) Y_1(d_5b) - J_1(d_5b) Y_0(d_5r) \right] + \varepsilon_{z5}^u \] (3.74)

\[ \sigma_z^f(r, z) = \xi_f E_f^f \left[ e_5 [C_6 \cosh(e_5 z) + C_7 \sinh(e_5 z)] \left[ J_0(d_5r) Y_1(d_5b) - J_1(d_5b) Y_0(d_5r) \right] + \varepsilon_{z5}^u \right] \] (3.75)
\[ \tau^f_{rz}(r, z) = -G^f d_5 \left[ C_6 \sinh(e_5 z) + C_7 \cosh(e_5 z) \right] \left[ J_1(d_5 r) Y_1(d_5 b) - J_1(d_5 b) Y_1(d_5 r) \right] \quad (3.76) \]

As both the interlayer and the substrate are in the plastic stage, the constitutive equations for them are provided by Eqs. (3.45) and (3.67), respectively. By following the similar procedures as in Section 3.2.1, the displacement and normal stress of the substrate can be determined by

\[ u^s_z(z) = K_5 \left[ C_6 \sinh(e_5 z) + C_7 \cosh(e_5 z) \right] + \varepsilon^u_z z + (a - R) \left( \frac{1}{G_2} - \frac{1}{G_1} \right) \tau_Y \quad (3.77) \]

\[ \sigma^s_z(z) = E^s_2 K_5 \left[ C_6 \cosh(e_5 z) + C_7 \sinh(e_5 z) \right] + E^s_2 \varepsilon^u_z + \left( 1 - \frac{E^s_2}{E^s_1} \right) \sigma_Y \quad (3.78) \]

where

\[
K_5 = A_{11} + \frac{G^f}{G_2} d_5(a - R) A_{12}, \quad A_{11} = J_0(d_5 a) Y_1(d_5 b) - J_1(d_5 b) Y_0(d_5 a) \quad A_{12} = J_1(d_5 a) Y_1(d_5 b) - J_1(d_5 b) Y_1(d_5 a), \quad \text{and} \quad d_5 \text{can be determined by}
\]

\[
\frac{E^s_2}{G^f} A_{11} + \frac{E^s_2}{G_2}(a - R)d_5 - \frac{2}{Rd_5 \alpha^2} A_{12} = 0 \quad (3.79)
\]

The boundary conditions in this case read

\[
\int_a^b 2 \pi r \sigma^f_z(z) \big|_{z=\lambda} \, dr = 0 \quad (3.80)
\]

\[
\tau^0_{rz}(z) \big|_{z=z^-} = -\tau_Y \quad (3.81)
\]

\[
\sigma^s_z(z) \big|_{z=\lambda} = \sigma^0_3 \quad (3.82)
\]

The continuity equations read

\[
\tau^0_{rz}(z) \big|_{z=z^-} = \tau^0_{rz}(z) \big|_{z=z^+} \quad (3.83)
\]

\[
u^s_z(z) \big|_{z=z^-} = \nu^s_z(z) \big|_{z=z^+} \quad (3.84)
\]

\[
\sigma^s_z(z) \big|_{z=z^-} = \sigma^s_z(z) \big|_{z=z^+} \quad (3.85)
\]

From the boundary and continuity equations listed above, the four constants \( C_5, C_6, C_7 \) and \( \varepsilon^u_{z_i}(i = 4, 5) \) can be determined as.
\[
\varepsilon^u_{z5} = \frac{\sigma^0_{3} A_{13}}{E_2^0 (A_{13} - K_5)} + \left( \frac{1}{E_2^0} - \frac{1}{E_1^0}\right) \frac{\sigma_Y A_{13}}{K_5 - A_{13}} 
\]

where

\[
A_{13} = \frac{2}{b^2 - a^2} \int_a^b r [J_0(d_5r)Y_1(d_5b) - J_1(d_5b)Y_0(d_5r)] dr 
\]

\[
C_5 = \frac{\tau_Y}{G' A_{10} d_4 sinh(e_{4z2})} 
\]

\[
C_6 = -\frac{1}{cosh(e_{5\lambda} - e_{5z2})} \left[ \frac{\varepsilon^u_{z5} \cosh(e_{5z2})}{A_{13} e_5} + \frac{\tau_Y \sinh(e_{5\lambda})}{G' d_5 A_{12}} \right] 
\]

\[
C_7 = \frac{\tau_Y}{G' d_5 A_{12} \cosh(e_{5z2})} - C_6 \tanh(e_{5z2}) 
\]

\[
\varepsilon^u_{z4} = \varepsilon^u_{z5} + \frac{a - R}{z_2} \left( \frac{1}{G_0^0} - \frac{1}{G_0^1} \right) \tau_Y + \frac{\tau_Y}{G' d_5 A_{12}} \left( \frac{K_5}{d_5 A_{12}} - \frac{K_4}{d_4 A_{10}} \right) 
\]

\[
z_2 \text{ can be determined by substituting Eqs. (3.86) to (3.91) into Eqs. (3.85), which is simplified as} 
\]

\[
C_5 e_4 K_4 \cosh(e_{4z2}) + \varepsilon^u_{z4} = e_5 K_5 [C_6 \cosh(e_{5z2}) + C_7 \sinh(e_{5z2})] + \varepsilon^u_{z5} 
\]

### 3.3.3 Plastic Substrate and Plastic Interlayer

As the applied load further increases, the interlayer will eventually become fully yielded, in which case, both the interlayer and substrate will get into the plastic stage. Following similar procedures as those in Section 3.2 by replacing the constitutive equations for interlayer and substrate with Eqs. (3.45) and (3.67), the displacement and stress field in the film/substrate system can be determined by the following formulas:

\[
u^f_z(r, z) = C_8 \sinh(e_6 z) [J_0(d_6r)Y_1(d_6b) - J_1(d_6b)Y_0(d_6r)] + \varepsilon^u_{z6} z 
\]

\[
\sigma^f_z(r, z) = \xi_f E^f \left[ C_8 e_6 \cosh(e_6 z) [J_0(d_6r)Y_1(d_6b) - J_1(d_6b)Y_0(d_6r)] + \varepsilon^u_{z6} \right] 
\]

\[
\tau^f_{rz}(r, z) = -G^f C_8 d_6 \sinh(e_6 z) [J_1(d_6r)Y_1(d_6b) - J_2(d_6b)Y_1(d_6r)] 
\]

\[
u^s_z(z) = C_8 K_6 \sinh(e_6 z) + \varepsilon^u_{z6} z + (a - R) \left( \frac{1}{G_0^0} - \frac{1}{G_0^1} \right) \tau_Y 
\]

\[
\sigma^s_z(z) = E_2^0 \left[ C_8 e_6 K_0 \cosh(e_6 z) + \varepsilon^u_{z6} \right] + \left( 1 - \frac{E_2^0}{E_1^0} \right) \sigma_Y 
\]
where

\[ K_6 = A_{14} + \frac{G_f}{G_2} d_6 (a - R) A_{15} \]  
\[ A_{14} = J_0(d_6 a) Y_1(d_6 b) - J_1(d_6 b) Y_0(d_6 a) \]  
\[ A_{15} = J_1(d_6 a) Y_1(d_6 b) - J_1(d_6 b) Y_1(d_6 a) \]  

(C.8)

(C.9)

(C.10)

\[ \varepsilon_{z_6}^u = \frac{A_{16}}{A_{16} - K_6} \left[ \frac{\sigma^0}{E_s^2} - \sigma_Y \left( \frac{1}{E_s^2} - \frac{1}{E_1^s} \right) \right] \]  
\[ C_8 = -\frac{\varepsilon_{z_6}^u}{e_6 A_{16} \cosh (e_6 \lambda)} \]  

where

A_{16} = \frac{2}{b^2 - a^2} \int_a^b \int_a^b r [J_0(d_6 r)Y_1(d_6 b) - J_1(d_6 b) Y_0(d_6 r)] \, dr \]  

(C.101)

(C.102)

(C.103)

By solving the following equation, \( d_6 \) can be determined theoretically.

\[ \frac{E_s^2}{G_f} A_{14} + \left[ \frac{E_s^2}{G_2} (a - R) d_6 - \frac{2}{R d_6 a^2} \right] A_{15} = 0 \]  

(C.104)

3.3.4 Elastoplastic Solutions

The distributions of axial displacement in the thin film across its radial direction when \( \sigma^0 = 0.8 \sigma_Y \) (Elastic substrate/elastoplastic interlayer) and \( \sigma^0 = 1.2 \sigma_Y \) (Plastic substrate/elastoplastic interlayer) are shown in Fig. 3.6 and compared with the elastic solution at elastic stage (\( \sigma^0 = 0.2 \sigma_Y \)). The symmetric displacement distribution at both the elastic and the plastic stages reveal that the presented elastoplastic model is able to capture the crack evolution as the applied load increases.

Fig. 3.6(b) shows that the displacement in the thin film significantly increases from 5 \( \mu m \) to 350 \( \mu m \) as the applied strain slightly increases from 0.2 \( \sigma_Y \) to 1.2 \( \sigma_Y \), which indicates that significant plastic deformation has been developed in the interlayer/substrate. However, no elastic model in the current literature can reveal such elastoplastic behavior in the coating/substrate system and crack evolution.
3.4 Phase III - Fracture Analysis and Experimental Validation

3.4.1 Fracture Analysis

Consider the section with two OMFs at the both ends in Fig. 3.1. When the external tensile loading increases to a critical value, a steady-state channeling straight crack will initiate at the middle edge.
of the section. After cracking, the section is broken into two halves, and the displacement field in each half can also be solved by replacing $\lambda$ with $\lambda/2$ in the new local coordinate system, thus solving the crack opening displacement. To recover this OMF, the normal stress along the central line just before the fracture initiates need to be applied along the cracking surface. Therefore, the ERR can be obtained as the work done to close the crack opening displacement [26] as shown in Eq. (3.105).

$$G = \frac{1}{\pi(b^2-a^2)} \int_a^b \sigma_z^f(r,0) u_z^f(r,\frac{\lambda}{2})dr$$  \hspace{1cm} (3.105)

The ERR in the coating layer will increase as the applied load increases and once the ERR is equal to or larger than the fracture toughness, a new fracture will nucleate. Therefore, the following criterion is used to predict if new fractures will be produced or not:

$$G \geq \Gamma_{cr}$$  \hspace{1cm} (3.106)

where $\Gamma_{cr}$ is the fracture toughness of the thin film.

Based on the stress and displacement presented in Sections 3.2 and 3.3, the ERR can be obtained through Eq. (3.105). Fig. 3.7(a) shows that when the coating thickness is constant ($b-a = 20 \mu m$), the ERR increases rapidly as the cracking spacing increases from 20 to 140$\mu m$. Beyond this point the ERR does not change any more although the cracking spacing increases, indicating that, under the applied load ($\sigma^0 = 1.2 \sigma_Y$), the potential crack spacing of the given thin film will be in the range of (20 $\mu m$ to 140 $\mu m$). The variance of the ERR with respect to the coating thickness with constant cracking spacing $\lambda = 80 \mu m$ under the same applied load ($\sigma^0 = 1.2 \sigma_Y$) is shown in Fig. 3.7(b). It reveals that the ERR increases linearly as the coating thickness increases until reaching a convex point, while after this point, the ERR rapidly decreases with the increasing film thickness. Note that fracture saturation will be reached at this convex point ($\lambda/(b-a) \simeq 3.75$), therefore, no more new crack will be developed when $\lambda/(b-a) \simeq 3.75$ under this applied load.

Recalling Eq. (3.106), when the applied load reaches a critical value, a new OMF will nucleate. Fig. 3.8 illustrates the variance of the applied load required to form a new crack in the thin film with the cracking spacing/coating thickness ratio $\lambda/(b-a)$. The fracture toughness of the thin film applied in this study is 3.5 MPa $m^{1/2}$ [97; 2]. Fig. 3.8 clearly shows that the externally applied load increases as the crack spacing decreases. When $\lambda/(b-a)$ approaches 1.2, the external load
turns to infinity. Therefore, no new fractures will infill and the fracture saturation will be arrived. For this specified film thickness of $b - a = 20\mu m$, the saturated crack spacing can be approximately evaluated as $\lambda_{cr} = 1.2(b - a) = 24\mu m$.

![Figure 3.8: Fracture spacing development with respect to the external tensile loading](image)

### 3.4.2 Experimental Validation

With Section 3.2.2 verifying the elastic solution, this section will present the experiment that has been conducted to validate the plastic solution and fracture analysis. In this experiment, four aluminum alloy (A6061) rods with a brittle aluminum oxide ($Al_2O_3$) coating grown through the process of anodization were subjected to a uniform tensile load. During the tensile test, a microscope was used to monitor the crack development, through which the critical applied load that initiated the cracking in the thin film can be obtained. After reaching fracture saturation, the sample was released from the tensile machine and the cracking spacing was measured under microscope. The test results agree well with the theoretical result.

#### 3.4.2.1 Sample preparation

Four aluminum rods with a radius of 7/16 inch and a length of 1 foot were prepared. The prepared aluminum samples were polished with sand paper first and cleaned with acetone and distilled water.
The samples were covered with acid resistant tape such that 3 inches from each end of the sample were covered as the grip for tension test. These four samples were kept in the anodizing bath for four different anodization duration times \((t1 = 15\text{ min}, t2 = 30\text{ min}, t3 = 60\text{ min}, t4 = 120\text{ min})\) to obtain different coating thickness.

![Testing sample preparations](image)

Figure 3.9: Testing sample preparations: (a) Anodization devices; and (b) Prepared samples

By following the same anodization procedures as in Ref. [94] and [38], a sulfuric electrolyte solution composed of 20% sulfuric acid and 80% distilled water by weight were placed inside the test beaker followed by the cylindrical lead cathode. A Teflon support was used to fix the aluminum anode at the center of the lead cathode as shown in Fig. 3.9(a), thereby a uniform alumina layer was created on the aluminum rod surface. The power supply was adjusted to 15 volts and the electrolyte was kept at a temperature at about 22\(^\circ\) C. From the experimental observations, the alumina growth rate was found to be independent of the sample radius [38]. Therefore, by varying the anodization time, the coating thickness could be approximately controlled. Fig. 3.9(b) shows all the samples accordingly labeled according to the anodization times.

### 3.4.2.2 Uniaxial tensile testing

The Instron 5984 34k Universal Testing Machine was used to apply a uniform tensile load on each sample. The load was applied at a strain rate of 0.01 inch/min, and the ultimate applied strain for all samples was set at 2%. During the tensile test, a Keyence VHX-5000 Digital Microscope, a versatile high-fidelity optical microscope designed for high depth of field measurements, was set
up close to the sample and focused near the center of the sample (see Fig. 3.10). The VHX can recognize the focus information automatically when the field of view is moved and then create a depth composition image quickly. The purpose of this microscope is to continuously monitor the fracture development in the coating, through which valuable detailed fracture information, such as critical applied load corresponding to crack initiation, crack pattern and crack spacing, can be obtained. Once OMFs were observed in the coating, the corresponding applied load and strain were recorded. After the predefined strain was reached, the applied load was released and the sample was removed from the Testing Machines with all geometric properties (such as coating thickness, apparent cracks, and discontinuities) recorded.

![Figure 3.10: Uniaxial tensile configuration](image)

3.4.2.3 Test results and analysis

The micro-structures as well as the fracture configurations of the alumina coatings after tensile tests were examined by the Keyence VHX-5000 Digital Microscopic. Fig. 3.11(a) shows a typical microscope images revealing the micro structures of the brittle alumina coating. The image of a fractured specimen with parallel crack periodically spaced and perpendicular to the direction of loading is shown in Fig. 3.11(b). Note that if the applied load is within the elastic stage of the substrate, the OMF will close once the externally applied load is removed. Considering this, a relatively large plastic strain was applied to make the cracking separation visible.
Figure 3.11: SEM images on fractured samples: (a) Typical porous nature of the brittle alumina coating; and (b) Parallel fractures perpendicularly spaced to the applied load

The saturated cracking spacing observed under the digital microscopic for samples with different coating thicknesses are shown in Fig. 3.12 and the corresponding crack spacings are summarized in Table 3.2. Results from both Table 3.2 and Fig. 3.12 show that the crack spacing proportionally decreases as the thin film thickness decreases. In addition, the applied load which causes fracture initiation is listed in Table 3.2 which shows that the crack initiation load increases as the coating thickness decreases. The difference of the crack initiation loads between the case with coating thickness 9µm and 18µm is very small as the substrate has yielded; therefore, a small increase in load will cause a large increase in displacement and break the thinner coating more easily.

From the test, we found that the fracture infills the coating very quickly and once it cracks, 2 to 4 OMFs can be observed in the microscopic which is shown in Fig. 3.13. Also, because the crack opening displacement is very small at the initiation stage, high magnification (>1500 times) needs to be used for the microscope to observe the cracks clearly; thus only a very small area is monitored under the microscope (the actual length shown in Fig. 3.13 is only about 0.2mm). Therefore, once a few OMFs can be observed in the microscope, many cracks have been produced in the entire coating already and the crack initiation loads shown in Table 3.2 are slightly bigger than the exact crack initiation loads, but can still reveal the changing trends of the crack initiation load with respect to the coating thickness.
Table 3.2: Crack spacing at different coating thickness

<table>
<thead>
<tr>
<th>Coating thickness (µm)</th>
<th>Crack spacing (µm)</th>
<th>Ave. (µm)</th>
<th>Crack initiation load (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>9</td>
<td>26.9</td>
<td>26.3</td>
<td>25.5</td>
</tr>
<tr>
<td>18</td>
<td>22.0</td>
<td>22.0</td>
<td>29.6</td>
</tr>
<tr>
<td>36</td>
<td>36.6</td>
<td>30.9</td>
<td>31.4</td>
</tr>
<tr>
<td>72</td>
<td>51.7</td>
<td>52.9</td>
<td>39.9</td>
</tr>
</tbody>
</table>

Figure 3.12: Cracking spacing at different coating thickness

The comparison of cracking spacing as a function of coating thickness between the experiment results and theoretical results obtained from the presented model is shown in Fig. 3.14. Both the test data and the theoretical solution indicate that the crack spacing proportionally decreases as the thin film thickness decreases until a critical film thickness is reached. Below this thickness the
Figure 3.13: Cracks initiated in coating layer

Figure 3.14: Variance of fracture spacing with respect to thin film thickness
crack spacing quickly increases to an infinite value and no new cracks will be developed. Overall, the theoretical prediction can effectively capture the varying trend of the crack spacing with respect to the coating thickness revealed by the test results, which further demonstrates the ability of the presented model to predict the elastoplastic behavior of the coating layered structure in general, and the ability to disclose more specific details of the OMFs in the coating, such as the crack spacing and the critical coating thickness.

### 3.5 Conclusions

This study presented an elastoplastic fracture model to simulate the multiple cracking in thin layer film coated onto an elastoplastic aluminum wire. The stress field in the coating/substrate system was analyzed by one section between two adjacent cracks. The thin layer of alumina coating generated by the anodic oxidation was treated as an elastic medium, while a bi-linear hardening plastic model characterized the ductile substrate aluminum wire. In order to simulate the stress transfer between the coating layer and substrate, an elastoplastic interlayer had been employed. As the applied tensile load increased, the system would undergo three different stress stages: the elastic stage, the elastoplastic stage, and the OMFs stage. The displacement and stress distribution in the coating/substrate were firstly solved at elastic stages and verified using FE solutions. Elastoplastic solutions were further provided for the coating/substrate system as the large deformation developed with the increase of the applied load. Based on the elastoplastic solutions, the ERR at different loading stages were calculated and fracture analysis was conducted. Simulation results showed that, when the coating thickness remained constant, the load required to form a new crack increased with respect to the decrease in crack spacing and fracture saturation was reached when the cracking spacing approached 1.2 times of the coating thickness.

Experimental characterization was conducted to validate the present elastoplastic solution when the substrate or interlayer underwent large deformation. A versatile high-fidelity optical microscope was applied to check the micro structure of the coating and continuously monitor the fracture development in the coating layer, through which valuable detailed fracture information, such as the critical applied load corresponding to crack initiation, crack pattern and crack spacing, were obtained. Both experimental and theoretical results indicated that the crack spacing decreased
linearly as the thin film thickness decreased until a critical film thickness was reached, while below this critical thickness, no new cracks would be developed. Overall, the theoretical prediction can effectively capture the varying trend of the crack spacing with respect to the coating thickness revealed by the test results, which demonstrated the ability of the presented model to accurately capture the stress and strain distribution in the coated structure and predict the fracture initiation, infilling, and saturation in the thin coating layer. The present formulation is general and can be applicable to other types of coating–ductile substrate systems.
Chapter 4

Three-dimensional Elastic Fracture Analysis for Coating/Substrate Systems

Block cracks are a series of interconnected cracks that divide a structural component into approximately rectangular pieces and are often observed in multilayer-bonded infrastructures such as coating on substrates. This study develops a three-dimensional (3D) elastic fracture model to study the block cracking in multilayered advanced polymeric solar reflectors. Under thermal loading, the thin protective metal oxide coating, which is fully bonded to a silver, coating on a polymer substrate, would suffer fracture due to the material mismatch. From the proposed model, the displacement and stress fields in this multilayered advanced polymeric reflector under thermal loading are explicitly solved and validated using the finite element (FE) results. The solved displacement and stress fields are then used to obtain the energy release rate (ERR) which is further used to study the fracture initiation, infilling, and saturation. Additionally, FE simulations using the cohesive zone model (CZM) are conducted to verify the theoretical fracture analysis. The results show that the fracture model presented in this study is able to capture the displacement and stress distributions in the multilayered advanced polymeric reflector accurately and predicts the fracture initiation, infilling, and saturation successfully.
4.1 Overview

Due to its advanced mechanical and thermal properties, metal oxide thin film coating of soft structures has been widely used to improve the mechanical and thermal properties of metallic or polymeric materials [209; 189; 18; 41]. Such structures are of interest because a light and flexible substrate allows for applications across a variety of form factors and can be more cost effective than with rigid substrates [69; 107; 157; 78]. An interesting application for metal oxide coatings on a compliant (polymer) substrate is in protective coatings for silver-coated polymer film reflectors, which have found application in parabolic trough reflectors for concentrating solar power [107; 104; 192; 175] and in other applications for which a flexible reflector is desirable [36]. In these reflectors, multiple oxide layers may be used both to impart abrasion resistance [107; 104; 175] or to improve the reflectance through thin-film interference [192]. A schematic example of the construction of such a reflector as a coating/substrate system manufactured by depositing thin metal oxide and metal films on the polymer substrates is shown in Fig. 4.1. Compared with traditional mirror designs which utilize silver painted on the back of glass, this advanced front surface design attains higher reflectance and lower cost for both manufacture and installation [229]. However, under temperature changes, the brittle metal oxide coating layer on the polymer substrate may suffer premature failure because of cracking due to the significant mismatch in the thermal expansion coefficients of the materials in the stack. As a result, the cracking in the surface layer will cause the loss of its protectiveness and the reduction of its reflectance efficiency. Therefore, it is essential to understand the fracture mechanism in this advanced polymeric solar reflector.

As the thermal loading would introduce tensile stress along both the longitudinal and the transversal direction in the coating, neither the plane strain assumption nor plane stress assumption can be applied. Therefore, a full 3D fracture model is desired to study the cracking behavior of coating under thermal loading. As an initial study, the real advanced polymeric solar reflector consisting of four layers as shown in Fig. 4.1 is simplified as a two-layer structure in order to reduce the complexity of the problem as the silver and copper layer are much thinner than the metal oxide protective coating and polymer substrate. After the simplification, the problem becomes solving the elastic field and analyzing the fracture behavior of a two layers structure in which the titanium oxide coating with thickness $h_f$, Young’s modulus $E_f$, Poisson’s ratio $\nu_f$, and thermal expansion
coe

80

Figure 4.1: Schematic reflector designs [229]

coefficient $\alpha_f$ is fully bonded to the polymer substrate with thickness $h_s$, Young’s modulus $E^s$, Poisson’s ratio $\nu^s$, and thermal expansion coefficient $\alpha_s$ under a temperature change of $\Delta T$. The boundary conditions are set as follows: the displacement along the thickness direction at the bottom of the substrate is fixed while it’s free to expand along the length and width direction. Once the temperature change gets to the critical value, the opening-mode fractures (OMFs) would initiate in the coating layer and propagate toward the interface between the coating layer and the substrate. For simplification, the length and width of the model are set to be coincident and equal to $2\lambda$ as the coating would be cracked into square pieces finally if the temperature change is high enough. Considering a section between two adjacent OMFs, a simplified model is set up as shown in Fig. 4.2.

The remainder of this study is organized as follows: Section 4.2 will develop the general formulations and provide explicit solutions of the 3D elastic field in the coating/substrate system based on Yin’s work [227]. Section 4.3 will then verify the elastic field predicted by the theoretical model given in Section 4.2 through FE analysis. The fracture analysis based on the obtained elastic field will be presented in Section 4.4 while the verification of fracture analysis using FE simulation results and experimental data from literature will be given in Section 4.5. Finally, some concluding
Figure 4.2: Schematic illustration of the simplified structures

remarks will be arrived in Section 4.6.

4.2 Formulation for 3D Elastic Field Analysis

Assume the displacement is $u_x$ along $x$-direction, $u_y$ along $y$-direction, and $u_z$ along $z$-direction. For the elastic coating and substrate structure, using the small displacement assumption, the stress under a temperature change of $\Delta T$ can be written as follows:

\[
\sigma_{xx}^i = \frac{E^i}{(1 + \nu^i)(1 - 2\nu^i)}[(1 - \nu^i)u_{x,x}^i + \nu^i u_{y,y}^i + \nu^i u_{z,z}^i] - \frac{\Delta T \alpha_i E^i}{1 - 2\nu^i} \quad (4.1)
\]

\[
\sigma_{yy}^i = \frac{E^i}{(1 + \nu^i)(1 - 2\nu^i)}[(1 - \nu^i)u_{y,y}^i + \nu^i u_{x,x}^i + \nu^i u_{z,z}^i] - \frac{\Delta T \alpha_i E^i}{1 - 2\nu^i} \quad (4.2)
\]

\[
\sigma_{zz}^i = \frac{E^i}{(1 + \nu^i)(1 - 2\nu^i)}[(1 - \nu^i)u_{z,z}^i + \nu^i u_{x,x}^i + \nu^i u_{y,y}^i] - \frac{\Delta T \alpha_i E^i}{1 - 2\nu^i} \quad (4.3)
\]

\[
\tau_{xy}^i = \frac{E^i(u_{x,y}^i + u_{y,x}^i)}{2(1 + \nu^i)} \quad (4.4)
\]

\[
\tau_{xz}^i = \frac{E^i(u_{x,z}^i + u_{z,x}^i)}{2(1 + \nu^i)} \quad (4.5)
\]
\[ \tau_{yz} = \frac{E^i(u^i_{y,z} + u^i_{z,y})}{2(1 + \nu^i)} \]  

(4.6)

where the subscript and superscript \( i = (f, s) \) denote the coating (\( f \)) and substrate (\( s \)) layers, respectively. The equilibrium equations expressed in displacement read,

\[
\begin{align*}
2 \frac{(1 - \nu^i)}{1 - 2\nu^i} u^i_{x,xx} + u^i_{y,yy} + u^i_{z,zz} + \frac{1}{1 - 2\nu^i} (u^i_{y,xy} + u^i_{y,yy}) &= 0 \quad (4.7) \\
2 \frac{(1 - \nu^i)}{1 - 2\nu^i} u^i_{y,yy} + u^i_{z,zz} + u^i_{y,zz} + \frac{1}{1 - 2\nu^i} (u^i_{z,xy} + u^i_{z,yy}) &= 0 \quad (4.8) \\
2 \frac{(1 - \nu^i)}{1 - 2\nu^i} u^i_{z,zz} + u^i_{x,zz} + u^i_{x,xx} + \frac{1}{1 - 2\nu^i} (u^i_{x,xx} + u^i_{y,yz}) &= 0 \quad (4.9)
\end{align*}
\]

By following the same principle as in the 2D problem \([227; 38; 81]\), we assume that the top surface of the coating will stay flat after deformation (plane assumption) and that all lines which were parallel to y-axis or x-axis before deformation will stay parallel to the corresponding axis after deformation. More specifically, the top surface of the structure will remain square after deformation (non-shearing assumption). Mathematically, these assumptions can be expressed as

\[ u^i_{z,x} = u^i_{z,y} = 0 \quad (4.10) \]

and

\[ u^i_{x,y} = u^i_{y,x} = 0 \quad (4.11) \]

Substituting Eqs. (4.10) and (4.11) into Eq. (4.7) to (4.9), the equilibrium equations simplify to,

\[
\begin{align*}
2 \frac{(1 - \nu^i)}{1 - 2\nu^i} u^i_{x,xx} + u^i_{x,zz} &= 0 \quad (4.12) \\
2 \frac{(1 - \nu^i)}{1 - 2\nu^i} u^i_{y,yy} + u^i_{y,zz} &= 0 \quad (4.13) \\
2 \frac{(1 - \nu^i)}{1 - 2\nu^i} u^i_{z,zz} + \frac{1}{1 - 2\nu^i} (u^i_{x,xx} + u^i_{y,yz}) &= 0 \quad (4.14)
\end{align*}
\]

4.2.1 General Solution of the Displacement in \textit{x}-direction

4.2.1.1 Displacement in the coating (\( u_x^f \))

Eq. (4.12) is a decoupled partial differential equation of \( u_x \). By applying the method of separation of variables, the general solution of \( u_x \) in the coating can be written as,

\[ u_x^f = f(x)g(z) + \varepsilon u_x \quad (4.15) \]
where \( f(x) \) is a function of \( x \) while \( g(z) \) is a function of \( z \), \( \varepsilon_u \) is used to account for the uniform strain, and the superscript \( f \) stands for coating or thin film.

Substituting Eq. (4.15) into Eq. (4.12) produces:

\[
\frac{2(1 - \nu^f)}{1 - 2\nu^f} f'' + g'' = 0
\]  

(4.16)

Both \( f \) and \( f'' \) are functions of \( x \) and \( g \) and \( g'' \) are functions of \( z \), so the two terms in Eq. (4.16) can be linked by an independent constant \( C^2 \),

\[
\frac{f''}{f} = -\frac{1 - 2\nu^f}{2(1 - \nu^f)} \frac{g''}{g} = C^2
\]  

(4.17)

From Eq. (4.17), the general solution of \( u_x^f \) can be obtained as

\[
\begin{align*}
  u_x^f &= [a_1 \sinh(Cx) + a_2 \cosh(Cx)][a_3 \sin(\xi_f Cz) + a_4 \cos(\xi_f Cz)] + \varepsilon_u x \\
  \xi_f &= \sqrt{\frac{2(1 - \nu^f)}{1 - 2\nu^f}}
\end{align*}
\]  

(4.18)

where

\[
\xi_f = \sqrt{\frac{2(1 - \nu^f)}{1 - 2\nu^f}}
\]  

(4.19)

and \( a_i (i = 1, 2, 3, 4) \) are constants to be determined.

The symmetry of \( u_x^f \) at \( x = 0 \) implies

\[
u_x^f(x = 0) = 0
\]  

(4.20)

and the free shearing boundary condition at the top surface, \( \tau_{xz}(z = h) = 0 \) yields

\[
u_{x,z}^f(z = h) = 0
\]  

(4.21)

in which the assumption Eq. (4.10) has been used.

Applying Eqs. (4.20) and (4.21) to Eq. (4.18) gives

\[
a_2 = 0
\]  

(4.22)

\[
a_3 \cos(\xi_f Ch) = a_4 \sin(\xi_f Ch)
\]  

(4.23)

So the displacement along \( x \)-direction in coating is reduced to

\[
u_x^f = A \sinh(Cx) \cos(\xi_f Ch - \xi_f Cz) + \varepsilon_u x
\]  

(4.24)

where \( A, C \) and \( \varepsilon_u \) are unknowns to be determined using the boundary conditions.
4.2.1.2 Displacement in the substrate ($u_x^s$)

By repeating the same derivation as in Section 4.2.1.1, the general solution of displacement along $x$-direction in the substrate, $u_x^s$, can be written as

$$u_x^s = [b_1 \sinh(Cx) + b_2 \cosh(Cx)][b_3 \sin(\xi_s Cz) + b_4 \cos(\xi_s Cz)] + \varepsilon_u x$$

where: $\xi_s = \sqrt{\frac{2(1 - \nu^s)}{1 - 2\nu^s}}$

and $b_i (i = 1, 2, 3, 4)$ are constants to be determined.

Similarly, by applying the plane assumption (Eq. (4.11)), the free shearing stress boundary condition at the bottom, $\tau_{xz}^s (z = 0) = 0$, can be simplified as

$$u_{x,z}^s (z = 0) = 0$$

and the symmetry of $u_x^s$ at $x = 0$ is

$$u_x^s (x = 0) = 0$$

Combining Eqs. (4.27), and (4.25), the constants $b_2$ and $b_3$ reduce to

$$b_2 = 0$$

$$b_3 = 0$$

so that the general solution of $u_x^s$ becomes

$$u_x^s = B \sinh(Cx) \cos(\xi_s Cz) + \varepsilon_u x$$

Again, $B$, $C$ and $\varepsilon_u$ are unknowns to be determined using the boundary conditions.

4.2.2 General Solution of Displacement in $y$-direction

For this special case where the length and width of the structure are the same, the displacement in $y$-direction can be obtained in the same fashion. Therefore, by replacing $x$ with $y$ and $y$ with $x$ in $u_x^f$ and $u_x^s$, the displacement along $y$-direction in the coating and substrate can be obtained:

$$u_y^f = A \sinh(Cy) \cos(\xi_f Ch - \xi_f Cz) + \varepsilon_u y$$

$$u_y^s = B \sinh(Cy) \cos(\xi_s Cz) + \varepsilon_u y$$
\[ u_y = B \sinh(Cy) \cos(\xi_s Cz) + \varepsilon_u y \] (4.33)

Notice that here the block cracking exhibits a square pattern, so Eqs. (4.32) and (4.33) share
the same form as Eqs. (4.24) and (4.31), respectively.

### 4.2.3 General Solution of Displacement in z-direction

Once \( u_x \) and \( u_y \) in both coating and substrate are obtained, the general solution of \( u_z \) can be solved
based on the equilibrium equation in \( z \)-direction,

\[ u_{z,zz}^i = -\frac{1}{2 - 2\nu^i} \left( u_{x,xz}^i + u_{y,yz}^i \right) \]

(4.34)

#### 4.2.3.1 Displacement in the coating \((u_z^f)\)

Integrating the equilibrium equation along \( z \)-direction in coating twice, the general solution of
\( u_z \) can be obtained as,

\[ u_z^f = -\frac{1}{2 - 2\nu_f} \int_z u_{x,xz}^f + u_{y,yz}^f dz + f_1(x, y) \]

(4.35)

where \( f_1(x, y) \) and \( g_1(x, y) \) are functions of \( x \) and \( y \). Substituting Eq. (4.24) and (4.32) into Eq.
(4.35) yields,

\[ u_z^f = \frac{A}{(2 - 2\nu_f)\xi_f} \sin(\xi_f Cz - \xi_f Cx) [\cosh(Cx) + \cosh(Cy)] - \frac{\varepsilon_u z}{1 - \nu_f} + f_1(x, y) z + g_1(x, y) = 0 \] (4.36)

The free normal stress boundary condition at the top surface of coating is

\[ \sigma_{zz}^f(z = h) = 0 \] (4.37)

Combining Eqs. (4.3), (4.24), (4.32), (4.36), and (4.37), \( f_1(x, y) \) can be determined as

\[ f_1(x, y) = \frac{1 - 2\nu_f}{2 - 2\nu_f} [A \cosh(Cx) + A \cosh(Cy) + 2\varepsilon_u] + \frac{1 + \nu_f}{1 - \nu_f} \alpha_f \Delta T. \] (4.38)

#### 4.2.3.2 Displacement in the substrate \((u_z^s)\)

Similarly to Section 4.2.3.1, the displacement along \( z \)-direction in substrate can be written as,

\[ u_z^s = -\frac{B}{(2 - 2\nu_s)\xi_s} \sin(\xi_s Cz) [\cosh(Cx) + \cosh(Cy)] - \frac{\varepsilon_u z}{1 - \nu_s} + f_2(x, y) z + g_2(x, y) = 0 \] (4.39)
where \( f_2(x, y) \) and \( g_2(x, y) \) are functions of \( x \) and \( y \).

Applying the fixed bottom boundary condition,

\[
 u_s^z(z = 0) = 0 \tag{4.40}
\]

\( g_2(x, y) \) can be determined,

\[
 g_2(x, y) = 0 \tag{4.41}
\]

Next by considering the continuity of \( u_z \) and \( \sigma_{zz} \) at the interface,

\[
 u_f^z(z = h_s) = u_s^z(z = h_s), \tag{4.42}
\]

and

\[
 \sigma_f^{zz}(z = h_s) = \sigma_s^{zz}(z = h_s) \tag{4.43}
\]

the unknown functions \( g_1(x, y) \) and \( f_2(x, y) \) are found to be,

\[
 f_2(x, y) = \frac{E_f (1 + \nu^s)(1 - 2\nu^s)}{E_s (1 + \nu^f)(2 - 2\nu^s)} AC \left[ 1 - \cos(\xi_f Ch_f) \right] \left[ \cosh(Cx) + \cosh(Cy) \right] + \frac{1 + \nu^s}{1 - \nu^s} \alpha_s \Delta T \\
 + \frac{1 - 2\nu^s}{1 - \nu^s} \varepsilon_u + \frac{BC (1 - 2\nu^s)}{2(1 - \nu^s)} \cos(\xi_s Ch_s) \left[ \cosh(Cx) + \cosh(Cy) \right] \tag{4.44}
\]

and

\[
 g_1(x, y) = -\frac{\cosh(Cx) + \cosh(Cy)}{2} \left[ \frac{Asin(\xi_f Ch_f)}{\xi_f (1 - \nu^f)} + \frac{1 - 2\nu^f}{1 - \nu^f} ACh_s + \frac{Bsin(\xi_s Ch_s)}{(1 - \nu^s)\xi_s} \right] \\
 - \frac{1 + \nu^f}{1 - \nu^f} \alpha_f \Delta T h_s - \frac{\varepsilon_u h_s}{1 - \nu^s} + \frac{2\nu^f \varepsilon_u h_s}{1 - \nu^f} + f_2(x, y) h_s \tag{4.45}
\]

### 4.2.4 Explicit Displacement Field

The general solutions for \( u_x \), \( u_y \), and \( u_z \) have been obtained for both coating and substrate. However, there are still four unknowns \( (A, B, C, \text{ and } \varepsilon_u) \) that need to be determined. In the following section, we apply the continuity and boundary conditions to solve for all the unknowns.

#### 4.2.4.1 Continuity at the Interface

The continuity of displacement \( u_x \) and \( u_y \) at the interface, \( u_x^f(z = h_s) = u_s^x(z = h_s) \) and \( u_y^f(z = h_s) = u_y^s(z = h_s) \), yields,

\[
 A\cos(\xi_f Ch_f) = B\cos(\xi_s Ch_s) \tag{4.46}
\]
and the continuity of shearing stress at the interface, $\tau_{xz}(z = h_s) = \tau_{x}^{s}(z = h_s)$ and $\tau_{yz}(z = h_s) = \tau_{y}^{s}(z = h_s)$, yields

$$\frac{AE_f \xi_f(1 + v_f) \sin(\xi_f C_{Ch_f})}{1 + v_f} = -\frac{BE_s \xi_s(1 + v_s) \sin(\xi_s C_{Ch_s})}{1 + v_s}$$

(4.47)

By combining Eqs. (4.46) and (4.47), we find a function of only the single unknown, $C$,

$$\frac{E_f \xi_f(1 + v_f)}{E_s \xi_s(1 + v_f)} \sin(\xi_f C_{Ch_f}) \cos(\xi_s C_{Ch_s}) + \sin(\xi_s C_{Ch_s}) \cos(\xi_f C_{Ch_f}) = 0.$$  

(4.48)

By solving this nonlinear equation numerically, the unknown $C$ which is a function of material properties and thickness but independent of crack spacing can be determined.

According to [227], many solutions exist for constant $C$ because of the periodicity of the $\sin()$ and $\cos()$ functions, which suggests the need for a series-form solution. In general, the roots of $C$ in Eq. (4.48) are not periodic, which implies that the basis functions in the series-form solution are not orthonormal to each other. Therefore, the derivation of the coefficient of each basis function will be complicated and the convergence of the solution will still be open. For simplicity, this study uses the first root to demonstrate this theory. Also according to our previous works [227; 38; 81], the first root can provide sufficient accuracy. As the coating is much thinner than the substrate ($h_f << h_s$) and the thermal expansion coefficient of the substrate is larger than the coating ($\alpha_s > \alpha_f$), the shearing stress at the interface should be negative which gives the constraints $\sin(\xi_s C_{Ch_s}) > 0$, $\cos(\xi_s C_{Ch_s}) < 0$, $B > 0$, and $A < 0$.

### 4.2.4.2 Free Normal Stress at the Side Faces

After solving $C$, there are three more unknowns left, $A$, $B$, and $\varepsilon_a$, requiring three boundary conditions. Recall that in the procedure to solve $C$, only the combination of Eq. (4.46) and (4.47) was used, which means that either Eq. (4.46) or Eq. (4.47) can be further used to solve other unknowns. Therefore, two more boundary conditions are sufficient to solve all unknowns.

The normal stress at every point on the side faces for both the coating and substrate should be zero as there is no external load applied at the side faces. However, this condition cannot be satisfied exactly due to the simplifying assumptions in Eqs. (4.10) and (4.11). Instead, relaxed boundary conditions are used,

$$\int_{0}^{\lambda} \int_{h_s}^{h} \sigma_{xx}(x = \lambda) dz dy = 0$$

(4.49)
and
\[
\int_0^\lambda \int_0^{h_s} \sigma_{xx}(x = \lambda) dz dy = 0 \tag{4.50}
\]

By substituting Eqs. (4.1), (4.24), (4.31), (4.32), (4.33), (4.36), and (4.39) into Eqs. (4.49), (4.50) and combine with Eq. (4.46), all of the remaining unknowns can be determined:

\[
A = M h_f (\alpha_f \Delta T - \varepsilon_u) \tag{4.51}
\]

\[
B = \frac{A \cos(\xi_f C h_f)}{\cos(\xi_s C h_s)} \tag{4.52}
\]

\[
\varepsilon_u = \frac{\alpha_s h_s N - \alpha_f h_f M}{h_s N - h_f M} T \tag{4.53}
\]

where

\[
M = \lambda \left(1 - 2v^f\right) \frac{(1 - v^f)}{1 - v^f} \left[ (1 - v^f) \lambda \cosh(C\lambda) \sin(\xi_f C h_f)/\xi_f + v^f \sinh(C\lambda) \sin(\xi_f C h_f)/\xi_f / C \right. \\
+ \left. \left[ v^f \frac{1 - 2v^f}{2 - 2v^f} C h_f - \frac{v^f \sin(\xi_f C h_f)}{\xi_f (2 - 2v^f)} \right] \left[ \cosh(C\lambda) \lambda + \sinh(C\lambda)/C \right] \right]^{-1} \tag{4.54}
\]

\[
N = \frac{\lambda(1 - 2v^s)(1 + v^s)}{1 - v^s} \left[ (1 - v^s) \lambda \cosh(C\lambda) \sin(\xi_f C h_s) \cosh(C\lambda) \right. \\
+ \frac{v^s \cos(\xi_f C h_f) \sinh(C\lambda) \sin(\xi_s C h_s)}{\xi_s \cos(\xi_s C h_s)} - \frac{\cos(\xi_f C h_f) v^s \sin(\xi_s C h_s)}{2\xi_s (1 - v^s) \cos(\xi_s C h_s)} \left[ \lambda \cosh(C\lambda) \sinh(C\lambda) \frac{\lambda}{C} \right] \\
+ \frac{1 - 2v^s}{2 - 2v^s} C h_s v^s \cos(\xi_f C h_f) \left[ \cosh(C\lambda) \lambda + \frac{\sinh(C\lambda)}{C} \right] \\
+ \frac{C v^s h_s E^f (1 + v^s)(1 - 2v^s)}{E^s (1 + v^f)(2 - 2v^s)} \left[ 1 - \cos(\xi_f C h_f) \right] \left[ \cosh(C\lambda) \lambda + \frac{\sinh(C\lambda)}{C} \right] \right]^{-1} \tag{4.55}
\]

Now, the displacement field in both the coating and substrate have been solved explicitly. Then the stress field in the coating/substrate system can be determined by substituting the obtained displacement into the constitutive law as shown in Eqs. (4.1)-(4.6).
4.3 FE Simulation and Verification of the Theoretical Solution

To verify the proposed analytical model, a comparison will be made between the elastic field obtained in Section 4.2 and the FE simulations conducted using the commercial software ABAQUS 6.13. The material properties, which were extracted from literature [229], and geometric constants of the coating/substrate system used in this FE analysis are provided in Table 4.1 and the temperature change is set to be 40°C.

| Table 4.1: Material properties and geometric constants used in the FE model |
|------------------|------------------|------------------|-----------------|
| Modulus (GPa)    | Poisson’s Ratio  | Thermal expansion coefficient (10^{-6}/°C) | Geometry (mm)   |
| $E^f$            | $\nu^f$         | $\alpha_f$      | 9               | 2$\lambda$     | 42               |
| $E^s$            | $\nu^s$         | $\alpha_s$      | 59.4            | $h_f$           | 0.1              |
|                  |                  |                  | $h_s$           | 4.2             |

Considering the symmetry, one quarter of the structure was simulated as shown in Fig. 4.3(a). The boundary conditions were set as follows: the symmetric boundary conditions were applied at both the left side face and the front side face, while the displacement along the thickness direction at the bottom was fixed as shown in Fig. 4.3(a). Fig. 4.3(b) shows the mesh of the FE model where 3D stress 8-node linear brick elements were used to simulate both the coating and the substrate material. In order to improve the computational efficiency and accuracy, a gradient mesh was applied along the length, width, and thickness directions. From the plane of symmetry to the end faces, the mesh size increased from 0.21 mm to 1.05 mm. Four layers of elements with uniform thickness were used to mesh the coating while the thickness of elements in the substrate increased from 0.21mm to 1.05 mm from the top to the bottom. In total, 19200 elements were used for the whole model.

In order to simulate the fully bonded interface between coating and substrate, a constraint was applied to tie the coating layer and substrate together. Therefore, no slipping or debonding was allowed. The displacement fields $u_x$ and $u_z$ after deformation under a temperature change of 40°C are presented in Fig. 4.4(a) and 4.4(b) respectively. Based on the FE results, one can find that $u_x$ is almost constant throughout the width of the structure while $u_z$ varies in a very small range.
Figure 4.3: FE simulation: (a) FE model and boundary conditions; and (b) mesh of the FE model.

Figure 4.4: Displacement field in the FE model after temperature change of 40 °C: (a) \( u_x \); and (b) \( u_z \). The units of displacement fields in these figures are \( mm \).
Figure 4.5: Comparison between theoretical solutions and FE analysis results for $u^f_x$ ($\Delta T = 40^\circ C$): (a) across thickness of coating at different $y$; and (b) along width direction at different depths.

Fig. 4.5(a) shows the distribution of $u^f_x$ across the thickness of coating with different $y$-coordinates. Recalling our assumption as shown in Eq. (4.11), the theoretical prediction of $u^f_x$ is independent of $y$. Therefore, only one distribution of $u^f_x$ is obtained from the theoretical model for different $y$-coordinates. Both the theoretical solutions and the FE analysis results show that $u^f_x$ will decrease from the interface to the top surface of the coating because the thermal expansion coefficient of coating is much smaller than that of substrate and the effect of substrate on the deformation of the coating will reduce from the interface to the top surface of coating. Although the FE analysis results show that $u^f_x$ will have minor changes with the change of $y$-coordinates, the theoretical model can still capture the distribution of $u^f_x$ across the thickness of the coating at different $y$-coordinates with a maximum difference smaller than 2.5%. The distribution of $u^f_x$ along the width direction at different depths is presented in Fig. 4.5(b), both theoretical solutions and FE analysis results show that $u^f_x$ would keep constant with the change of $y$ approximately, which means our assumption in Eq. (4.11) is reasonable.

Fig. 4.6 presents the distribution of normal stress along the $x$-direction in the coating ($\sigma_{xx}^f$). Fig. 4.6(a) shows that the normal stress $\sigma_{xx}^f$ will not change with depth except at the very edge and that the theoretical solutions agree well with the FE simulation results. The maximum difference between the theoretical solutions and the FE simulation results, which is reached at the edge
Figure 4.6: Comparison between the theoretical solutions and the FE simulation results for normal stress $\sigma_{xx}^{f}$ ($\Delta T = 40^\circ C$): (a) across thickness of coating at different $y$; and (b) along width direction at different depths.

where $y = \lambda$, is smaller than 3%. The distribution of $\sigma_{xx}^{f}$ along the width direction is presented in Fig. 4.6(b), both theoretical solution and FE simulation results show that the normal stress would decrease from the center to the edge. The difference between the simulation results and the theoretical prediction is within 2%, which denotes the accuracy of our theoretical model.

### 4.4 Fracture Analysis

Consider the square section within four OMFs. When the temperature change increases to a critical value, two steady-state channeling straight cracks will initiate at the middle edge of the section. After cracking, the section is broken into four quarters, and the displacement field in each quarter can also be solved by replacing $\lambda$ with $\lambda/2$ in the new local coordinate system. Therefore, the crack opening displacement is solved. To recover this OMF, the normal stress along the central line just before the fracture initiates needs to be applied along the cracking surface. Therefore, the ERR can be obtained as the work done to close the crack opening displacement as shown in Eq. (4.56) [26].
\[ G = \frac{1}{\lambda h_f} \int_{0}^{\lambda} \int_{h_s}^{h} \sigma_{zz} (0, y, z) [u_x^f(\lambda, h_s) - u_x^f(\lambda, z)] dz dy \quad (4.56) \]

The ERR in the coating layer will increase as the temperature change increases. Once the ERR is equal to or larger than the critical fracture ERR, a new crack will nucleate. Therefore, the following criterion is used to predict whether new fractures will infill:

\[ G \geq G_{cr} \quad (4.57) \]

where \( G_{cr} \) is the critical fracture ERR of the thin film.

Using the stress and displacement presented in Section 4.2, the ERR can be obtained through Eq. (4.56). Fig. 4.7(a) shows that when the coating thickness is constant \((h_f = 100\mu m)\), the ERR increases rapidly as the crack spacing increases to \(6h_s\). Beyond this point, the ERR does not change any more even as the crack spacing increases. This indicates that under the temperature change \((\Delta T = 40^\circ C)\), the potential crack spacing of the given thin film \((h_f = 100\mu m, h_s = 4.2 mm)\) will be smaller than six times the thickness of substrate. Fig. 4.7(b) shows the variance of the ERR with respect to the coating thickness with constant crack spacing \(\lambda = 21\ mm\) under a temperature change of \(40^\circ C\) and reveals that the ERR increases linearly as the coating thickness increases until it reaches a convex point. After this point, the ERR decreases as the coating thickness increases. At this convex point \((h_f = 120\mu m)\), fracture saturation is reached, therefore, no more new crack will be developed.

Recalling Eq. (4.57), when the temperature change reaches a critical value, a new OMF will nucleate. Fig. 4.8 illustrates the variance of required temperature changes to form a new crack in the thin film. In this study, the critical fracture ERR of the thin titania film is taken to be 0.277 \(J/m^2\) [229]. Fig. 4.8(a) presents the required temperature change to crack the coating when the coating thickness is constant \((h_f = 100\mu m)\) and shows that the temperature change increases as the crack spacing decreases. When \(\lambda/h_s\) approaches 0.5, the temperature change turns to infinity which means no new fractures will infill and the fracture saturation is achieved. For this specified film thickness of \(h_f = 100\mu m\) and substrate thickness of 4.2mm, the saturated crack spacing can be approximately evaluated as \(\lambda_{cr} = 0.5h_s = 2.1 mm\). Fig. 4.8(b) shows the variance of the temperature change with respect to the coating thickness at a constant crack spacing \((\lambda = 21 mm)\) and indicates that the required temperature change to initiate a new crack in the coating will
reduce as the coating thickness decreases until a critical thickness $h_{fc}$ is reached. Under this critical coating thickness, the required temperature change to crack the coating increases to be infinite and the fracture saturation would be reached. For this study, the critical coating thickness is about 5 $\mu m$ when the crack spacing is 21 mm.

The variance of saturated crack spacing with respect to the coating thickness under the temperature change, $\Delta T = 40^\circ C$, is presented in Fig. 4.9 which shows that the crack spacing decreases as the thin film thickness decreases until a critical film thickness is reached. Below this thickness the crack spacing quickly increases to infinite and no new cracks will be developed, which means the fracture saturation is reached. For this case where the thickness of the substrate is 4.2 mm, the critical thickness is corresponding to about 70 $\mu m$ under the temperature change of 40$^\circ C$.

### 4.5 Verification of Fracture Analysis

#### 4.5.1 FE Simulation of Cracking in Coating

In order to verify the theoretical fracture analysis, the required temperature changes to crack the coating/substrate structures with different length but same coating thickness are validated by the FE simulations using ABAQUS. As we already know the path of cracks, the CZM is used to
Figure 4.8: Variance of required temperature change to create new cracks with respect to: (a) crack length \((h_f=\text{constant})\); and (b) Coating thickness \((\lambda=\text{constant})\).

Figure 4.9: Crack spacing at different coating thickness
Figure 4.10: FE model and mesh for cracking analysis

enable the cracking simulation. In order to reduce the effect of the cohesive element on the overall mechanical property, cohesive elements with zero thickness are inserted at the center of the coating. Fig. 4.10 presents the FE model and mesh. The boundary conditions used in the simulation are that the lower surface of substrate is fixed along $z$-direction ($u_s^z(z = 0) = 0$) while the center point of the bottom of substrate is fixed to get rid of any rigid body motion.

During the FE simulations, C3D8R elements are used to simulate the solid material, while 3D cohesive elements, COH3D8, are used to simulate the cracking process. In order to increase the computational efficiency and improve the accuracy of the simulation, gradient mesh is used in the substrate across the thickness direction, while uniform sized elements are used to simulate the coating. Initially, cohesive elements with specific thickness are inserted at the center of the coating in the original part then a mesh part is created and the nodes of the cohesive elements at the two sides are edited to have the same coordinates. Thus, the zero thickness cohesive elements are created. Recall that the theoretically predicted fracture ERR is an average across the thickness of the crack surface; therefore, in order to be consistent with the theoretical model, the coating is meshed by one layer of elements.

Similar to the solid elements, the constitutive behavior of the cohesive elements should be defined during the FE simulations. In this study, the bilinear traction-separation law is used for the cohesive element. For this bilinear traction-separation law, the initial response of the cohesive element is assumed to be linear until the damage initiation criterion is met. After that point, the stress in the cohesive elements would be released linearly until the damage evolution property is
reached and the cohesive element would be damaged as shown in Fig. 4.11. In this constitutive model, three parameters need to be specified: the initial strength \((T)\), the stiffness \((K)\), and the critical fracture ERR \((G_{cr})\). The initial strength defines the critical stress at which the cracking would initiate. Once the stress in the cohesive element reaches the initial strength, the stress would be released and the cracking would propagate once the fracture ERR reaches the critical value.

Figure 4.11: Bilinear traction-separation response of the cohesive element [187].

Ideally, the stiffness of the cohesive element should be infinite in order to reduce the effect of the cohesive element on the stiffness of the whole model. However, too large of a cohesive element stiffness introduces the numerical problem that the simulation cannot converge. Turon et al. [201] proposed a relationship for determining the value of the stiffness for cohesive elements based on the properties of the surrounding materials as:

\[
K = \frac{\alpha E}{t} \tag{4.58}
\]

where \(E\) is the Young’s modulus of the surrounding material, \(t\) is the initial thickness of the cohesive zone which is typically set to be 1, and \(\alpha\) is a parameter much larger than 1. As stated before, the stiffness of the cohesive elements should be large enough to avoid any effect on the overall compliance and should be small enough to get rid of the spurious oscillations in the tractions. Therefore, the parameter \(\alpha\) should provide a reasonable stiffness value and a value of 50 or larger was recommended [201]. For our case, \(\alpha\) is set to be 100, yielding a stiffness of \(2.3 \times 10^7 \frac{N}{mm^3}\). The critical fracture ERR \(G_{cr} = 0.277 J/m^2\), predicted by using the cracking saturation in [229], was
Figure 4.12: Simulated stress field in the cracking model: (a) before cracking; and (b) after cracking. used in the FE simulation. The initial strength of the cohesive elements was set to be 250 MPa.

Fig. 4.12(a) shows the stress field (Von Mises 75% average) in the coating/substrate system before the cracking initiation. Compared with the simulation results where non-cohesive elements were used, the difference is less than 1% which means the chosen stiffness of cohesive elements is reasonable. The stress field after cracking is presented in Fig. 4.12(b). It indicates that the stress is periodically distributed in each cracked piece. In the cracking simulation, the cohesive element deletion is enabled. Once the fracture ERR reaches the critical value, the cohesive element would be damaged and vanish, providing a way to monitor the cracking process. Based on the simulation, the cracks would initiate at the center and propagate to the edge of the coating. This is consistent with our theoretical prediction as the stress would decrease from the center to edge.

The simulated required temperature change to crack the coating with constant thickness is summarized in Table 4.2 and compared with the theoretical predictions in Fig. 4.13. Overall the temperature changes from the theoretical predictions agree with the simulation results well with a maximum difference of 5% at $\lambda = 0.8h_s$. In addition, the difference between the theoretical predictions and the simulation results increases as the crack spacing decreases. One potential reason is that with the decrease of crack spacing, edge effects treated approximately in our theoretical analysis would become significant. The proposed theoretical model cannot capture the stress and displacement distributions in this edge area effectively because of the application of plane and non-shearing assumptions. This problem has also been stated in [227].
Table 4.2: Simulated temperature changes for different crack spacings

<table>
<thead>
<tr>
<th>Crack Spacing</th>
<th>Theoretical Predictions</th>
<th>Simulation Results</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.8h_s</td>
<td>118</td>
<td>112</td>
</tr>
<tr>
<td>h_s</td>
<td>94</td>
<td>90</td>
</tr>
<tr>
<td>1.5h_s</td>
<td>61</td>
<td>58</td>
</tr>
<tr>
<td>2h_s</td>
<td>49</td>
<td>46</td>
</tr>
<tr>
<td>3h_s</td>
<td>40</td>
<td>38</td>
</tr>
<tr>
<td>4h_s</td>
<td>37</td>
<td>37</td>
</tr>
<tr>
<td>5h_s</td>
<td>36</td>
<td>36</td>
</tr>
</tbody>
</table>

4.5.2 Comparison with the Experimental Data

Recently, Roy and her colleague [169] proposed a simple model to predict the residual stress in the free expanded galvannealed coating/substrate structure based on Eshelby’s approach for inclusion method. In this model, the normal strain and normal stress caused by thermal loading were assumed to be uniformly distributed in the structure. The material properties used in this study are summarized in Table 4.3. Based on the obtained residual stress, the ERR in the coating along both longitudinal and transversal directions were obtained and used to predict the crack spacing. Then the crack spacing in samples with different coating thicknesses created by different thermal loadings were measured and compared with the theoretical predictions of their simplified model as shown in Table 4.4. Note that the predicted crack spacings from [169] all differ from the measured spacings by 50% or more. In addition, we point out that there appears to be large uncertainty in the experimentally produced crack spacings, as indicated by the fact that under almost identical conditions (e.g., samples 6 and 7), the measured spacings are about 14 and 25 µm, respectively. Hence, our comparisons to experiment necessarily must be made only semi-quantitatively.

In the following, we use the same material properties to calculate the ERR based on the model developed here and compare the predicted crack spacing for different samples to the experimental results [169]. Note that, the Young’s modulus of coating is smaller than that of substrate in this
analysis. This means the coefficient of the first term in Eq. (4.48) is smaller than the second term, therefore, the solution of unknown $C$ is searched near $\frac{\pi}{2h_f \xi_f}$ which make the second term of Eq. (4.48) be zero. Also based on the computational results, the value of the left part in Eq. (4.48) and the predicted crack spacing are sensitive to the value of $C$. For example, when $C$ increases by 2%, the predicted crack spacing would increase by 1.5% while the value of the left part in Eq. (4.48) would increase by 10% for this specific case whose material properties is shown in Table 4.3. Therefore, in order to predict the crack spacing accurately, $C$ should be solved with a very high accuracy. However, as Eq. (4.48) is a nonlinear equation in terms of $C$ and can only be solved numerically with some numerical errors, the presented predicted crack spacing may differ from the actual crack spacing by 1-2%.

Table 4.3: Material Properties and Geometric Constant [169]

<table>
<thead>
<tr>
<th>Modulus (GPa)</th>
<th>Poisson’s Ratio</th>
<th>Thermal expansion coefficient ($10^{-5}/^\circ C$)</th>
<th>Geometry (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E^f$</td>
<td>140</td>
<td>0.3</td>
<td>2.2</td>
</tr>
<tr>
<td>$E^s$</td>
<td>210</td>
<td>0.3</td>
<td>1.1</td>
</tr>
<tr>
<td>$\nu^f$</td>
<td></td>
<td></td>
<td>$h_s$ 1</td>
</tr>
<tr>
<td>$\nu^s$</td>
<td></td>
<td></td>
<td>$h_s$ 1</td>
</tr>
</tbody>
</table>
Fig. 4.14 presents the change of ERR with respect to the crack spacing in different samples. For these small crack spacings, the ERR would increase with the increase of the crack spacing. Based on the literature \cite{95}, the critical fracture toughness of the $\delta$ phase galvannealed coating is $2MPa \cdot m^{1/2}$, then the critical fracture ERR can be calculated based on Eq. (4.59), where $K_{ICr}^2$ is the critical fracture toughness. The horizontal line in Fig. 4.14 shows the calculated critical fracture ERR which is equal to $28.57 \frac{N}{m}$. Above this horizontal line, the ERR is higher than the critical fracture ERR, therefore, more cracks would be introduced at the center of the coating layer until the critical crack spacing, at which the ERR is smaller than or equal to the critical fracture ERR, is reached. The crack spacing at each intersection points of the horizontal line with the ERR curve for each sample shows the saturated crack spacing. These saturated crack spacing are extracted and compared with the experimental results in the literature [169], which is presented in Table 4.4. Note, first, that the predicted crack spacings all are approximately the correct value of 20 or more $\mu m$. The model derived here predicts crack spacings within 10% of the measured values for most conditions and it predicts that the crack spacing would decrease with the increase of temperature change or the decrease of coating thickness, which is coincident with the trends shown in Fig. 4.8(a) and 4.9. Also from Table 4.4, the saturated crack spacing predicted by the presented model agrees well with the experimental results, indicating that the presented model is more accurate than the model proposed by Roy [169].

$$G_{cr} = \frac{K_{ICr}^2}{E}$$  \hspace{1cm} (4.59)

<table>
<thead>
<tr>
<th>Sample number</th>
<th>1</th>
<th>3</th>
<th>2</th>
<th>7</th>
<th>6</th>
<th>4</th>
<th>5</th>
<th>8</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coating thickness ((\mu m))</td>
<td>5.9</td>
<td>6.0</td>
<td>6.6</td>
<td>6.0</td>
<td>6.0</td>
<td>6.0</td>
<td>8.0</td>
<td>9.0</td>
</tr>
<tr>
<td>Temperature change ((^\circ C))</td>
<td>-594</td>
<td>-594</td>
<td>-620</td>
<td>-591</td>
<td>-589</td>
<td>-576</td>
<td>-595</td>
<td>-512</td>
</tr>
<tr>
<td>Crack spacing ([169]) ((\mu m))</td>
<td>9.70</td>
<td>9.77</td>
<td>9.88</td>
<td>9.80</td>
<td>9.83</td>
<td>10.00</td>
<td>11.06</td>
<td>13.5</td>
</tr>
<tr>
<td>Observed crack spacing ([169]) ((\mu m))</td>
<td>20.40</td>
<td>25.68</td>
<td>33.03</td>
<td>24.89</td>
<td>14.45</td>
<td>34.22</td>
<td>19.21</td>
<td>24.78</td>
</tr>
<tr>
<td>Crack spacing (Presented model) ((\mu m))</td>
<td>21.80</td>
<td>21.99</td>
<td>22.05</td>
<td>22.11</td>
<td>22.19</td>
<td>22.75</td>
<td>25.50</td>
<td>31.02</td>
</tr>
</tbody>
</table>
Summary and Conclusions

In this study, a 3D elastic fracture model has been presented to simulate the block cracking in the advanced polymeric solar reflectors, which is modeled by a simplified bilayer structure. The displacement field in the system under a specified temperature change is obtained theoretically. The results show that the displacement along $x$-direction is nearly constant across the width which supports our assumption that $u_{x,y} = u_{y,x}$. The obtained elastic fields were verified with FE simulations. The good agreement between theoretical predictions and simulation results (maximum difference within 3%, which may caused by the singularity or edge effect) reveals the accuracy of the present fracture model and highlights the effectiveness of this approach.

Based on the elastic solutions, the ERR is calculated and shows that the ERR would increase rapidly as the crack spacing increases until a plateau stage is reached when the crack spacing approaches 6 times the substrate’s thickness. Therefore, under the temperature change of 40$^\circ$C, coating thickness 100µm, and substrate thickness 4.2 mm, the potential crack spacing is smaller than 25.2 mm. When the crack spacing is constant, the ERR approximately increases linearly with the coating thickness until it reaches the convex point, at which the fracture saturation is reached. In this case ($\Delta T = 40^\circ C, \lambda = 21mm, h_s = 4.2mm$), the critical coating thickness is 120 µm.
The fracture infilling and saturation of this specific coating/substrate system are studied based on the calculated ERR and show that, when the coating thickness remains constant, the temperature change required to form a new crack would increase as the crack spacing decreases and fracture saturation would be reached when the crack spacing approaches 0.5 times of the substrate thickness. However, when the crack spacing is constant, the required temperature change to form a new crack would decrease as the coating thickness decreases, until a critical coating thickness is reached. Under this critical thickness the required temperature change would increase to be infinite which means the fracture saturation is obtained. For the crack spacing of 21 mm, the critical coating thickness is about $5 \mu m$. Furthermore, the saturated crack spacing decreases linearly as the thin film thickness decreases until a critical film thickness is reached, while below this critical thickness ($70 \mu m$), no new cracks will be developed. This trend is consistent with our previous study [38; 81]. In order to verify the theoretical fracture analysis, FE simulations based on CZM with bilinear traction-separation constitutive behavior were conducted. The simulated temperature changes needed to initiate a new crack in the coating with different crack spacing but constant coating thickness were compared with the theoretical predictions. The good agreement between the simulation results and the theoretical solutions indicates the accuracy of the proposed fracture model. Furthermore, the predicted crack spacing in samples with various coating thicknesses under different temperature changes are compared with the experimental data from literature. The results show that the presented fracture model gives a more accurate prediction on the crack spacing than the model proposed in the literature.

Overall, the presented model is able to capture the displacement and stress distributions in the coated structure accurately and predict the fracture initiation, infilling, and saturation successfully. The present formulation is general and can be applied to other types of coating/substrate systems.
Chapter 5

Three-dimensional Elastic Fracture Analysis for Multilayered Structures

Temperature changes in multilayered structures result in residual thermal stress in multilayered structures due to the different thermal and mechanical properties of each layer. In this chapter, a three-dimensional (3D) elastic model is developed to study the residual stress in the multilayered structures, consisting of an arbitrary number of layers, under temperature change. By applying the non-shearing assumption and the assumption of free normal stress in thickness direction, the decoupled governing equations are obtained, and the general solutions of displacement and stress fields in the multilayered structures are derived by solving the elastic boundary value problem. In order to verify the proposed model, the elastic field in the advanced polymeric solar reflectors which consists of four layers are solved by applying the present model and compared with the finite element (FE) simulation. In addition, parametric studies are done to investigate the effect of the thickness ratio between each layer on the accuracy of the developed model. Based on the obtained elastic field, the fracture energy release rate (ERR) in the surface layer of the advanced polymeric reflector is obtained and used to study the fracture initiation, infilling, and saturation successfully.
5.1 Overview

Consider a multilayered structure consisting of N-layers, assume all layers are fully bonded together, therefore, there is no debonding or slipping between layers and the displacement at all interfaces would be continuous. The Young’s modulus, Poisson ratio, and the thermal expansion coefficient for each layer are denoted by $E^i$, $\nu_i$, and $\alpha_i$ respectively, where the subscript and superscript $i = 1, 2, \cdots, N$ represents the $i$th layer. The thickness of the $i$th layer is $h_i$, and the $z$-coordinate of the lower surface of the $i$th layer is $t_{i-1}$ while it is $t_i$ for the upper surface of layer $i$. The total thickness of the multilayered structure is $h$. The boundary conditions are set as follows: the displacement along the thickness direction at the bottom is fixed while it’s free to expand along the length and width direction. Once the temperature change reaches the critical value, OMFs would initiate in the brittle surface layer and propagate toward the interface. To simplify things, the length and width of the model are set to be coincident and equal to $2\lambda$ as the structure would be cracked into square pieces eventually if the temperature change is high enough. Considering a section between two adjacent OMFs a simplified model is built and shown Fig. 5.1.

![Figure 5.1: Schematic illustration of the multilayered structure](image)

The remainder of this chapter is organized as follows: Section 5.2 will develop the general
formulations and provide explicit solutions of the 3D elastic field in the multilayered structure. Section 5.3 will study the distribution of residual stress and displacement in an advanced polymeric solar reflector based on the developed formulations in Section 5.2. Parametric studies are included in Section 5.3 to investigate the applicability of the proposed model to structures with different thicknesses by comparing the theoretical predictions with FE analysis results. The calculation of fracture ERR based on the obtained elastic field and some discussions about the fracture analysis will be presented in Section 5.4. Finally, some conclusive remarks will be arrived in Section 5.5.

5.2 Formulations for 3D Elastic Field Analysis

Applying the small displacement assumption, the residual stress, caused by a temperature change of $\Delta T$, in the multilayered structures can be written as:

$$
\sigma_{xx}^i = \frac{E^i}{(1 + \nu_i)(1 - 2\nu_i)} [(1 - \nu_i)u_{x,x}^i + \nu_i u_{y,y}^i + \nu_i u_{z,z}^i] - \frac{\Delta T \alpha_i E^i}{1 - 2\nu_i} \tag{5.1}
$$

$$
\sigma_{yy}^i = \frac{E^i}{(1 + \nu_i)(1 - 2\nu_i)} [(1 - \nu_i)u_{y,y}^i + \nu_i u_{x,x}^i + \nu_i u_{z,z}^i] - \frac{\Delta T \alpha_i E^i}{1 - 2\nu_i} \tag{5.2}
$$

$$
\sigma_{zz}^i = \frac{E^i}{(1 + \nu_i)(1 - 2\nu_i)} [(1 - \nu_i)u_{z,z}^i + \nu_i u_{x,x}^i + \nu_i u_{y,y}^i] - \frac{\Delta T \alpha_i E^i}{1 - 2\nu_i} \tag{5.3}
$$

$$
\tau_{xy}^i = \frac{E^i(u_{x,y}^i + u_{y,x}^i)}{2(1 + \nu_i)} \tag{5.4}
$$

$$
\tau_{xz}^i = \frac{E^i(u_{x,z}^i + u_{z,x}^i)}{2(1 + \nu_i)} \tag{5.5}
$$

$$
\tau_{yz}^i = \frac{E^i(u_{y,z}^i + u_{z,y}^i)}{2(1 + \nu_i)} \tag{5.6}
$$

where $u_{x}^i$, $u_{y}^i$, and $u_{z}^i$ are the displacements along $x$-direction, $y$-direction, and $z$-direction in the $i$th layer respectively.

Substituting the stress into the equilibrium equations yields:

$$
\frac{2(1 - \nu_i)}{1 - 2\nu_i} u_{x,xx}^i + u_{x,yy}^i + u_{x,zz}^i + \frac{1}{1 - 2\nu_i} (u_{y,xy}^i + u_{z,zz}^i) = 0 \tag{5.7}
$$

$$
\frac{2(1 - \nu_i)}{1 - 2\nu_i} u_{y,yy}^i + u_{y,xx}^i + u_{y,zz}^i + \frac{1}{1 - 2\nu_i} (u_{x,xy}^i + u_{z,yz}^i) = 0 \tag{5.8}
$$
Although the multilayered structure is fixed along the thickness direction at the bottom, the material mismatch has only minor effect on the displacement and normal stress along the thickness direction, therefore, it is reasonable to assume the normal stress along the $z$-direction is zero ($\sigma^i_{zz} = 0$, assumption of free normal stress along thickness direction) [150]:

$$\sigma^i_{zz} = 0$$  \hspace{1cm} (5.9)

Combine Eqs. (5.3) and (5.9), the normal strain in $z$-direction ($u^i_{z,z}$) can be written as a function of the strain along $x$ and $y$-directions:

$$u^i_{z,z} = \frac{1 + v_i}{1 - v_i} \Delta T \alpha_i - \frac{v_i}{1 - v_i} (u^i_{x,x} + u^i_{y,y})$$  \hspace{1cm} (5.10)

In addition, we assume that all lines which were parallel to $x$ or $y$-axis before deformation will stay parallel to the corresponding axis after deformation, indicating that every cross-section perpendicular to $z$-axis will keep be square after deformation (non-shearing assumption). Mathematically, this assumption results in:

$$u^i_{x,y} = u^i_{y,x} = 0$$  \hspace{1cm} (5.11)

Substitute Eqs. (5.10) and (5.11) into Eq. (5.7) and (5.8), the equilibrium equations are simplified as:

$$\frac{2 - \nu^i}{1 - \nu_i} u^i_{x,xx} + u^i_{x,zz} = 0$$  \hspace{1cm} (5.12)

$$\frac{2 - \nu^i}{1 - \nu_i} u^i_{y,yy} + u^i_{y,zz} = 0$$  \hspace{1cm} (5.13)

### 5.2.1 General Solution of the Displacement in $x$-direction

Eq. (5.12) is a decoupled partial differential equation of $u^i_x$. By applying the method of separation of variables, the general solution of $u^i_x$ can be written as:

$$u^i_x = f(x)g(z) + \varepsilon_u x$$  \hspace{1cm} (5.14)
where \( f(x) \) is a function of \( x \) while \( g(z) \) is a function of \( z \), \( \varepsilon_u \) is used to account for the uniform strain.

Substitute Eq. (5.14) into Eq. (5.12) produces:

\[
\frac{2 - \nu_i f''}{1 - \nu_i f} + \frac{g''}{g} = 0
\]  

(5.15)

As \( f \) and \( f'' \) are functions of \( x \) while \( g \) and \( g'' \) are functions of \( z \), these two terms in Eq. (5.15) can be linked by an independent constant \( C^2 \):

\[
\frac{f''}{f} = \frac{1 - \nu_i g''}{2 - \nu_i g} = C^2
\]  

(5.16)

From Eq. (5.16), the general solution of \( u_x^i \) can be obtained:

\[
u_x^i = [a_1^i \sinh(Cx) + a_2^i \cosh(Cx)][a_3^i \sin(\xi_i Cz) + a_4^i \cos(\xi_i Cz)] + \varepsilon_u x
\]  

(5.17)

where:

\[
\xi_i = \sqrt{\frac{2 - \nu_i}{1 - \nu_i}}
\]  

(5.18)

and \( a_1^i, a_2^i, a_3^i, \) and \( a_4^i \) are constants to be determined.

The symmetry of \( u_x^i \) at \( x = 0 \) reads:

\[
u_x^i(x = 0) = 0
\]  

(5.19)

Applying Eq. (5.19) into Eq. (5.17) yields \( a_2^i = 0 \) and the general solution of \( u_x^i \) reduces to be:

\[
u_x^i = \sinh(Cx)[A_i \sin(\xi_i Cz) + B_i \cos(\xi_i Cz)] + \varepsilon_u x
\]  

(5.20)

where \( A_i \) and \( B_i \) are unknowns to be determined in each layer.

As stated before, the material mismatch has minor effect on the displacement along the \( z \)-direction and \( u_z^i \) is mainly controlled by the thermal expansion and Poisson ratio’s effect, therefore, \( u_{x,z}^i << u_{z,x}^i \) and we can ignore the contribution of \( u_{z,x}^i \) to the shearing stress of \( \tau_{xz}^i \). Based on this fact, the shearing stress \( \tau_{xz}^i \) can be reduced to be:

\[
\tau_{xz}^i = \frac{E_i \xi_i C}{2(1 + \nu_i)} \sinh(Cx)[A_i \cos(\xi_i Cz) - B_i \sin(\xi_i Cz)]
\]  

(5.21)
5.2.1.1 Displacement in layer 1

For layer 1, the general solution of $u_1^x$ and $\tau_{xz}^1$ can be written as:

$$u_1^x = \sinh(Cx)[A_1\sin(\xi_1Cz) + B_1\cos(\xi_1Cz)] + \varepsilon_u x \quad (5.22)$$

and

$$\tau_{xz}^1 = \frac{E^1\xi_1C}{2(1 + \nu_1)}\sinh(Cx)[A_1\cos(\xi_1Cz) - B_1\sin(\xi_1Cz)] \quad (5.23)$$

The zero shearing stress boundary condition at the bottom, $\tau_{xz}^1(z = 0) = 0$, gives $A_1 = 0$. Then Eqs. (5.22) and (5.23) reduce to be:

$$u_1^x = B_1\sinh(Cx)\cos(\xi_1Cz) + \varepsilon_u x \quad (5.24)$$

and

$$\tau_{xz}^1 = \frac{-B_1E^1\xi_1C}{2(1 + \nu_1)}\sinh(Cx)\sin(\xi_1Cz) \quad (5.25)$$

where $B_1$, $C$ and $\varepsilon_u$ are unknowns to be determined using the boundary conditions.

In order to get a uniform expression for the displacement in every layer, make:

$$H_{11} = 0 \quad (5.26)$$

$$H_{12} = 1 \quad (5.27)$$

then we have:

$$u_1^x = B_1\sinh(Cx)[H_{11}\sin(\xi_1Cz) + H_{12}\cos(\xi_1Cz)] + \varepsilon_u x \quad (5.28)$$

$$\tau_{xz}^1 = \frac{B_1E^1\xi_1C}{2(1 + \nu_1)}\sinh(Cx)[H_{11}\cos(\xi_1Cz) - H_{12}\sin(\xi_1Cz)] \quad (5.29)$$
5.2.1.2 Displacement in layer 2

Eqs. (5.20) and (5.21) give the general solution of $u_x^2$ and $\tau_{xz}^2$:

$$u_x^2 = sinh(Cx)[A_2\sin(\xi_2 Cz) + B_2\cos(\xi_2 Cz)] + \varepsilon u x$$  \hspace{1cm} (5.30)

and

$$\tau_{xz}^2 = \frac{E^2\xi_2 C}{2(1 + \nu_2)} sinh(Cx)[A_2\cos(\xi_2 Cz) - B_2\sin(\xi_2 Cz)]$$  \hspace{1cm} (5.31)

Consider the continuity of the displacement and shearing stress at the interface of layer 1 and 2, $u_x^1(z = t_1) = u_x^2(z = t_1)$ and $\tau_{xz}^1(z = t_1) = \tau_{xz}^2(z = t_1)$, the following relationships can be obtained:

$$A_2\sin(\xi_2 C t_1) + B_2\cos(\xi_2 C t_1) = B_1[H_{11}\sin(\xi_1 C t_1) + H_{12}\cos(\xi_1 C t_1)]$$  \hspace{1cm} (5.32)

$$A_2\cos(\xi_2 C t_1) - B_2\sin(\xi_2 C t_1) = \frac{B_1}{E^2\xi_2(1 + \nu_1)} \left[H_{11}\cos(\xi_1 C t_1) - H_{12}\sin(\xi_1 C t_1)\right]$$  \hspace{1cm} (5.33)

Based on Eqs. (5.32) and (5.33), the unknowns in layer 2, $A_2$ and $B_2$, are solved as:

$$A_2 = H_{21}B_1$$  \hspace{1cm} (5.34)

$$B_2 = H_{22}B_1$$  \hspace{1cm} (5.35)

where:

$$H_{21} = \left[H_{11}\sin(\xi_1 C t_1) + H_{12}\cos(\xi_1 C t_1)\right]\sin(\xi_2 C t_1) + \frac{E^1\xi_1(1 + \nu_2)}{E^2\xi_2(1 + \nu_1)} [H_{11}\cos(\xi_1 C t_1) - H_{12}\sin(\xi_1 C t_1)]\cos(\xi_2 C t_1)$$  \hspace{1cm} (5.36)

$$H_{22} = \left[H_{11}\sin(\xi_1 C t_1) + H_{12}\cos(\xi_1 C t_1)\right]\cos(\xi_2 C t_1) - \frac{E^1\xi_1(1 + \nu_2)}{E^2\xi_2(1 + \nu_1)} [H_{11}\cos(\xi_1 C t_1) - H_{12}\sin(\xi_1 C t_1)]\sin(\xi_2 C t_1)$$  \hspace{1cm} (5.37)
5.2.1.3 Displacement in layer $i$ ($2 < i < N$)

Repeat the same procedures as in Section 5.2.1.2, for layer 3, 4, $\cdots$, $N-1$, the displacement and shearing stress for layer $i$ can be summarized as:

$$u_i^x = B_1 \sinh(Cx)[H_{i1}\sin(\xi_iCz) + H_{i2}\cos(\xi_iCz)] + \varepsilon_u x$$ (5.38)

$$\tau_{xz}^i = \frac{B_1 E^i \xi_i C}{2(1 + \nu_i)} \sinh(Cx)[H_{i1}\cos(\xi_iCz) - H_{i2}\sin(\xi_iCz)]$$ (5.39)

where:

$$H_{i1} = [H_{(i-1)1}\sin(\xi_{i-1}Ct_{i-1}) + H_{(i-1)2}\cos(\xi_{i-1}Ct_{i-1})]\sin(\xi_iCt_{i-1})$$

$$+ \frac{E^{i-1}\xi_{i-1}(1 + \nu_i)}{E^i \xi_i (1 + \nu_i)} [H_{(i-1)1}\cos(\xi_{i-1}Ct_{i-1}) - H_{(i-1)2}\sin(\xi_{i-1}Ct_{i-1})]\cos(\xi_iCt_{i-1})$$ (5.40)

$$H_{i2} = [H_{(i-1)1}\sin(\xi_{i-1}Ct_{i-1}) + H_{(i-1)2}\cos(\xi_{i-1}Ct_{i-1})]\cos(\xi_iCt_{i-1})$$

$$- \frac{E^{i-1}\xi_{i-1}(1 + \nu_i)}{E^i \xi_i (1 + \nu_i)} [H_{(i-1)1}\cos(\xi_{i-1}Ct_{i-1}) - H_{(i-1)2}\sin(\xi_{i-1}Ct_{i-1})]\sin(\xi_iCt_{i-1})$$ (5.41)

5.2.1.4 Displacement in layer N

For the surface layer, the general solution of $u_x^N$ and $\tau_{xz}^N$ can be written as:

$$u_x^N = \sinh(Cx)[A_N\sin(\xi_NCz) + B_N\cos(\xi_NCz)] + \varepsilon_u x$$ (5.42)

and

$$\tau_{xz}^N = \frac{E^N \xi_NC}{2(1 + \nu_N)} \sinh(Cx)[A_N\cos(\xi_NCz) - B_N\sin(\xi_NCz)]$$ (5.43)

Applying the free shearing stress boundary condition at the top surface, $\tau_{xz}^N(z = h) = 0$, $A_N$ and $B_N$ are related by the following equation,

$$A_N\cos(\xi_NCh) = B_N\sin(\xi_NCh)$$ (5.44)

Therefore, Eqs. (5.42) and (5.43) are further simplified as:

$$u_x^N = D_N\sinh(Cx)\cos(\xi_NCh - \xi_NCz) + \varepsilon_u x$$ (5.45)
\[
\tau_{yx}^N = \frac{D_N E_N^N \xi_N C}{2(1 + \nu_N)} \sinh(Cx)\sin(\xi_N Ch - \xi_N Cz) 
\]
(5.46)

where \(D_N\) is a constant to be determined.

### 5.2.2 General Solution of the Displacement in \(y\)-direction

For this special case where the length and width of the structure are coincident, the displacement in \(y\)-direction can be obtained in the same fashion. Therefore, by replacing \(x\) with \(y\) and \(y\) with \(x\) in \(u_x^i\), the displacement and shearing stress along \(y\)-direction can be obtained.

For layer 1 to layer \(N - 1\):

\[
\begin{align*}
    u_y^i & = B_i \sinh(Cy) [H_{i1} \sin(\xi_i Cz) + H_{i2} \cos(\xi_i Cz)] + \varepsilon_{u y} \\
    \tau_{yx}^i & = \frac{B_i E_i \xi_i C}{2(1 + \nu_i)} \sinh(Cy) [H_{i1} \cos(\xi_i Cz) - H_{i2} \sin(\xi_i Cz)]
\end{align*}
\]
(5.47) (5.48)

For layer \(N\):

\[
\begin{align*}
    u_y^N & = D_N \sinh(Cy) \cos(\xi_N Ch - \xi_N Cz) + \varepsilon_{u x} \\
    \tau_{yz}^N & = \frac{D_N E_N \xi_N C}{2(1 + \nu_N)} \sinh(Cy) \sin(\xi_N Ch - \xi_N Cz)
\end{align*}
\]
(5.49) (5.50)

In which Eqs. (5.26), (5.27), (5.36), (5.37), (5.40), and (5.40) still hold.

### 5.2.3 General Solution of the Displacement in \(z\)-direction

Once \(u_x\) and \(u_y\) are solved for each layer, the general solution of \(u_z^i\) can be determined by integrating Eq. (5.10) along the \(z\)-direction for each layer. Note that, the integration of Eq. (5.10) along \(z\)-direction would introduce an unknown function \(F_i(x, y)\) for each layer, by applying the fixed boundary condition at the bottom \((u_z^1(z = 0) = 0)\) and the continuity of \(u_z\) at each interface, \(N\) equations would be obtained which can used to solve the \(N\) unknown functions \(F_i(x, y), i = 1, 2, \ldots, N\). As this
study focuses on the opening-mode fracture (OMF) analysis, therefore, the displacement and normal stress along $z$-direction is less interesting compared with the displacement and normal stresses along $x$ and $y$-directions, which are essential for the OMF analysis. Based on Eqs. (5.1) and (5.2), the normal stress $\sigma^i_{xx}$ and $\sigma^i_{yy}$ are functions of $u^i_{z,z}$, which can be obtained through Eq. (5.10) after solving $u^i_x$ and $u^i_y$. Therefore, the detail about the derivation of displacement along $z$-direction, $u^i_z$, will not be presented here.

5.2.4 General Solution of the Normal Stress

By applying the solved displacement for each layer into Eq. (5.10), the strain along the $z$-direction, $u_{z,z}$ can be obtained. Substitute the solved $u_{z,z}$, $u_x$, and $u_y$ into Eqs. (5.1) and (5.2), the general solution of the in plane normal stress for layers $i$, $i \in [1, N - 1]$, can be determined as:

$$
\sigma^i_{xx} = \frac{E^i}{1 - \nu_i^2} \left[ B_1 C \left[ H_i \sin(\xi_i Cz) + H_{i2} \cos(\xi_i Cz) \right] \cosh(Cx) + \nu_i \cosh(Cy) \right] + (1 + \nu_i)(\varepsilon_u - \Delta T \alpha_i) \tag{5.51}
$$

$$
\sigma^i_{yy} = \frac{E^i}{1 - \nu_i^2} \left[ B_1 C \left[ H_i \sin(\xi_i Cz) + H_{i2} \cos(\xi_i Cz) \right] \cosh(Cy) + \nu_i \cosh(Cx) \right] + (1 + \nu_i)(\varepsilon_u - \Delta T \alpha_i) \tag{5.52}
$$

While the normal stress in the surface layer reads:

$$
\sigma^N_{xx} = \frac{E^N}{1 - \nu_N^2} \left[ B_N C \cos(\xi_N Ch - \xi_N Cz) \cosh(Cx) + \nu_N \cosh(Cy) \right] + (1 + \nu_N)(\varepsilon_u - \Delta T \alpha_N) \tag{5.53}
$$

$$
\sigma^N_{yy} = \frac{E^N}{1 - \nu_N^2} \left[ B_N C \cos(\xi_N Ch - \xi_N Cz) \cosh(Cy) + \nu_N \cosh(Cx) \right] + (1 + \nu_N)(\varepsilon_u - \Delta T \alpha_N) \tag{5.54}
$$

5.2.5 Explicit Displacement Field

Until now, the general solution of the displacement field in the multilayered structures has been solved. However, there are still four unknowns ($B_1$, $D_N$, $C$, and $\varepsilon_u$) need to be determined. In the following section, the continuity and boundary conditions would be applied to determine these unknowns.
5.2.5.1 Continuity at the interface

Consider the continuity of displacement and shearing stress at the interface between layer \(N - 1\) and layer \(N\), \(u_{x}^{N-1}(z = t_{N-1}) = u_{x}^{N}(z = t_{N-1})\) and \(\tau_{xz}^{N-1}(z = t_{N-1}) = \tau_{xz}^{N}(z = t_{N-1})\), we have:

\[D_{N}\cos(\xi_{N}Ch_{N}) = B_{1}[H_{(N-1)1}\sin(\xi_{N-1}Ct_{N-1}) + H_{(N-1)2}\cos(\xi_{N-1}Ct_{N-1})]\] (5.55)

\[D_{N}\sin(\xi_{N}Ch_{N}) = \frac{B_{1}E_{N}^{-1}\xi_{N-1}(1 + \nu_{N})}{E_{N}\xi_{N}(1 + \nu_{N})}[H_{(N-1)1}\cos(\xi_{N-1}Ct_{N-1}) - H_{(N-1)2}\sin(\xi_{N-1}Ct_{N-1})]\] (5.56)

Combine Eqs. (5.55) and (5.56) a nonlinear equation in terms of \(C\) is obtained,

\[\frac{[H_{(N-1)1}\sin(\xi_{N-1}Ct_{N-1}) + H_{(N-1)2}\cos(\xi_{N-1}Ct_{N-1})]}{\sin(\xi_{N}Ch_{N})} = \frac{E_{N}^{-1}\xi_{N-1}(1 + \nu_{N})}{E_{N}\xi_{N}(1 + \nu_{N-1})}[H_{(N-1)1}\cos(\xi_{N-1}Ct_{N-1}) - H_{(N-1)2}\sin(\xi_{N-1}Ct_{N-1})]\cos(\xi_{N}Ch_{N})\] (5.57)

As \(H_{(N-1)1}, H_{(N-1)2}, H_{N1},\) and \(H_{N1}\) are functions of material properties and geometric constants, therefore, the only unknown in Eq. (5.57) is \(C\). By solving this nonlinear equation numerically, the unknown \(C\) which is a function of material properties and thickness but independent of the length and width can be determined. According to [227], many solutions exist for constant \(C\) because of the periodicity of the \(\sin()\) and \(\cos()\) functions, which suggests the need for a series-form solution. In general, the roots of \(C\) in Eq. (5.57) are not periodic, which implies that the basis functions in the series-form solution are not orthonormal to each other. Therefore, the derivation of the coefficient of each basis function will be complicated and the convergence of the solution will still be open. As in Chapter 4, for simplicity, this study uses the first root to demonstrate this theory.

5.2.5.2 Free normal stress at the side faces

After solving \(C\), there are three unknowns left, \(B_{1}\), \(D_{N}\), and \(\varepsilon_{u}\), which require three more boundary conditions to be determined. As the combination of Eq. (5.55) and (5.56) is used to solve \(C\), therefore, either Eq. (5.55) or Eq. (5.56) can be further used to determine other unknowns. Based on this fact, two more boundary conditions are sufficient in order to get the explicit elastic solution.
As there are no external loading applied at the side faces, the normal stress at every point on the side faces for each layer should be zero. However, this condition can not be satisfied exactly due to the assumptions in Eqs. (5.9) and (5.11). Instead, relaxed boundary conditions will be used by setting the integral or the average of the normal stress on side faces be zero. As stated before, the surface layer which typically acts as a protective layer made by brittle metal oxide is easier to be cracked, therefore, in order to predict the fracture ERR or the maximum stress in the surface layer more accurately, the zero averaged normal stress at the side face of surface layer is used as one boundary condition while the integral of the normal stress across the side faces for all other layers is set to be zero to provide the other boundary condition as follows:

\[
\int_0^\lambda \int_{t_{N-1}}^h \sigma_{xx}^N(x = \lambda)dzdy = 0 \tag{5.58}
\]

\[
\int_0^\lambda \sum_{i=1}^{N-1} \left[ \int_{t_{i-1}}^{t_i} \sigma_{xx}^i(x = \lambda)dz \right] dy = 0 \tag{5.59}
\]

Substitute Eqs. (5.51) and (5.53) into Eqs. (5.58) and (5.59) yields:

\[
B_1 \sum_{i=1}^{N-1} K_{i1} + \varepsilon_u \sum_{i=1}^{N-1} K_{i2} - \Delta T \sum_{i=1}^{N-1} (\alpha_i K_{i2}) = 0 \tag{5.60}
\]

\[
B_N K_{N1} + \varepsilon_u K_{N2} - \Delta T \alpha_N K_{N2} = 0 \tag{5.61}
\]

where:

\[
K_{i1} = \begin{cases} 
\frac{E_i}{\xi_i(1-\nu_i)} Q_i \left[ \lambda \cosh(C\lambda) + \frac{\nu_i}{\xi_i} \sinh(C\lambda) \right], & i \in [1, N-1] \\
\frac{E_N}{\xi_N(1-\nu_N)} \sin(\xi_N Ch_N) \left[ \lambda \cosh(C\lambda) + \frac{\nu_N}{\xi_N} \sinh(C\lambda) \right], & i = N
\end{cases} \tag{5.62}
\]

\[
Q_i = H_{i2} \sin(\xi_i Ct_i) - H_{i2} \sin(\xi_i Ct_{i-1}) - H_{i1} \cos(\xi_i Ct_i) + H_{i1} \cos(\xi_i Ct_{i-1}) \tag{5.63}
\]

and

\[
K_{i2} = \frac{E_i}{1-\nu_i} \lambda h_i, \quad i \in [1, N] \tag{5.64}
\]

Combine Eqs. (5.60), (5.61), and (5.55), all unknowns can be determined as:
\[ B_1 = \Delta T \frac{K_{N2} \sum_{i=1}^{N-1} (\alpha_i K_{i2}) - \alpha_N K_{N2} \sum_{i=1}^{N-1} K_{i2}}{K_{N2} \sum_{i=1}^{N-1} K_{i1} - K_{N1} K \sum_{i=1}^{N-1} K_{i2}} \]  

(5.65)

\[ D_N = K B_1 \]  

(5.66)

\[ \varepsilon_u = \frac{\Delta T K_{N2} \alpha_N - B_1 K_{N1} K}{K_{N2}} \]  

(5.67)

where

\[ K = \frac{H_{(N-1)} \sin(\xi_{N-1} C t_{N-1}) + H_{(N-1)} \cos(\xi_{N-1} C t_{N-1})}{\cos(\xi_N C h_N)} \]  

(5.68)

5.3 Numerical Verification of the General Solutions

In this section, the displacement and residual stress fields in the advanced polymeric solar reflectors, driven by a temperature change, would be solved using the solution developed in Section 5.2. In order to verify the proposed model and investigate its applicability to multilayered structures with various geometries, the elastic field predicted by the theoretical model would be compared with FE simulation results and some parametric studies would be conducted in this section.

5.3.1 Residual Stress in the Advanced Polymeric Solar Reflectors

As a multilayered structure, the advanced polymeric solar reflectors as shown in Fig. 5.2 has been widely applied in concentrated solar power systems [107; 104; 192; 175] due to their higher reflectance and lower cost for both manufacturing and installation compared with the traditional solar reflector design which utilizes silver painted on the back of glass [69; 107; 157; 78; 229].

These advanced polymeric reflectors are manufactured by depositing multiple thin metal oxide layers on the polymer substrates used both to impart abrasion resistance [107; 104; 175] or to improve the reflectance through thin-film interface [192]. However, under a temperature change, the surface layer would suffer premature damage due to OMF which cause the loss of its protective function and the reduction of the reflectance efficiency. In order to understand the fracture mechanism, the displacement and residual stress fields in the surface layer of the advanced polymeric solar reflectors driven by a temperature change are firstly obtained by applying the
Figure 5.2: Schematic reflector designs [107; 104; 229]

proposed model in Section 2. Then FE simulations are conducted using the commercial software ABAQUS 6.13 to verify the theoretical predictions. The material properties and geometric constants of the advanced polymeric solar reflector used in this FE analysis are generated from [229; 4] and provided in Table 5.1, where layer 1, 2, 3, and 4 represent the polymer substrate (here taken to be polyethylene terephthalate (PET)), bonding layer(copper), silver layer, and protective layer (titania), respectively. The temperature change is set to be 40°C in this simulation.

Table 5.1: Material properties and geometric constants used in the FE model [229; 4]

<table>
<thead>
<tr>
<th>Layers</th>
<th>Modulus (GPa)</th>
<th>Poisson’s Ratio</th>
<th>Thermal expansion coefficient (10^{-6}/°C)</th>
<th>Geometry (µ m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>PET</td>
<td>$E^1$</td>
<td>3.9</td>
<td>0.3</td>
<td>$\alpha_1$</td>
</tr>
<tr>
<td>Silver</td>
<td>$E^2$</td>
<td>110</td>
<td>0.34</td>
<td>$\alpha_2$</td>
</tr>
<tr>
<td>Copper</td>
<td>$E^3$</td>
<td>83</td>
<td>0.37</td>
<td>$\alpha_3$</td>
</tr>
<tr>
<td>Titania</td>
<td>$E^4$</td>
<td>230</td>
<td>0.27</td>
<td>$\alpha_4$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>$2\lambda$</td>
</tr>
</tbody>
</table>

Considering the symmetry, one quarter of the structure is simulated as shown in Fig. 5.3(a), where the symmetric boundary conditions are applied at both the left side face and the front side face while the displacement along the thickness direction at the bottom is fixed, the interfaces between layers are tied together to avoid any debonding or slipping. Fig. 5.3(b) shows the mesh of
the FE model in which the 3D stress 8 nodes linear brick elements are used to simulate the materials. In order to improve the computational efficiency and accuracy, a gradient mesh is applied along the length, width, and thickness directions. From the plane of symmetry to the side faces, the mesh size increases from 0.002 mm to 0.1 mm. Four layers of elements with uniform thickness are used to mesh the layers 2, layer 3, and layer 4 while the thickness of elements in layer 1 increases from 0.004 mm to 0.02 mm from the top to the bottom. In total, 131061 elements are used for the whole model. A temperature field of 0°C is defined in the initial step then modified to be 40°C in the following step, therefore, a temperature change of 40°C is applied.

The distribution of $u_x^4$ across the thickness of surface layer with different $y$-coordinates is shown in Fig. 5.4(a). As we assume $u_x^4$ is independent of $y$ coordinates in Eq. (5.11), only one distribution of $u_x^4$ is obtained from the theoretical model for different $y$-coordinates. Both the theoretical solutions and the FE analysis results show that $u_x^4$ will decrease from the interface to the top surface because the thermal expansion coefficient of surface layer is smaller than that of the lower layers, therefore, the lower layer would stretch the surface layer by applying a shearing stress at the interface and this shearing stress would decrease from the interface to the top surface. Although the FE analysis results show that $u_x^4$ will have minor changes with the change of $y$-coordinates, the theoretical model can still capture the distribution of $u_x^4$ across the thickness of the surface layer at different $y$-coordinates with a maximum difference smaller than 3%. The distribution of $u_x^4$ along
the width direction at different depths is presented in Fig. 5.4(b), both theoretical solutions and
FE analysis results show that $u_x^4$ would keep constant with the change of $y$ approximately, which
means our assumption in Eq. (5.11) is reasonable.

Fig. 5.5(a) shows the distribution of normal stress $\sigma_{xx}^4$ and indicates that the normal stress $\sigma_{xx}^4$
will not change with depth except at the very edge. A good agreement between the theoretical
predictions and the FE simulation results is observed as the maximum difference, which is reached
at the edge where $y = \lambda$, is smaller than 3%. Fig. 5.5(b) presents the distribution of $\sigma_{xx}^4$ across
the width, indicating that the normal stress would decrease from the center to the edge and the
difference between the simulation results and the theoretical prediction is within 2%, which denotes
the accuracy of our theoretical model.

5.3.2 Parametric Studies

Aimed to investigate the effect of geometry, particularly the thickness of each layer, on the accuracy
of the proposed model, some parametric studies are conducted and will be presented in this section.
As shown in last section, the maximum difference between theoretical predictions and FE simulation
results would be reached at the edge, therefore, only the displacement and residual stress at the
edge of the surface coating will be provided in this section.

The effect of $h_2$ on the distribution of displacement and residual stress at the corner of the
Figure 5.5: Comparison between the theoretical solutions and the FE simulation results for normal stress $\sigma_{xx}^4$

(a) Across thickness of coating at different $y$

(b) Along width direction at different depths

Figure 5.6: Comparison between theoretical solutions and FE simulation results for different $h_2$

(a) Comparison of $u_x^4(x = \lambda, y = \lambda, z)$

(b) Comparison of $\sigma_{xz}^4(x = 0, y = \lambda, z)$
surface layer is shown in Fig. 5.6. Based on Fig. 5.6(a), the theoretically predicted displacement would approach to the FE simulation results as \( h_2 \) increases, when \( h_2 \) is equal to \( h_1 \), the theoretical solutions would overlap with the FE simulation results. However, for the distribution of normal stress, the best agreement is gained when \( h_2 = 1 \mu m \). As \( h_2 \) increases or decreases, the difference between the theoretical solutions and FE simulation results would increase. When \( h_2 = h_1 \), the maximum difference can get to 15%. The reason is that with the increase of \( h_2 \), the edge effect or the singularity at the corner would become more and more significant. Fig. 5.7 shows the distribution of normal stress at locations far away from the edge (\( y = \frac{3A}{4} \) and \( y = \frac{A}{2} \)) for different \( h_2 \). It indicates that the theoretical model can predict a more accurate stress distribution for the inner area, when \( y = \frac{3A}{4} \), the maximum difference between the theoretical solution and FE simulation results is smaller than 5%. Note that, the calculation of fracture ERR, which used for fracture analysis based on energy model [26], uses the averaged normal stress, meanwhile, the maximum normal stress, which is used for fracture analysis based on strength model [49], is reached at \( y = 0 \) according to Fig. 5.5(b). Therefore, the inaccurate normal stress distribution at the edge has minor effect on the fracture analysis for either strength or energy model.

Fig. 5.8 and 5.9 shows the effect of \( h_3 \) and \( h_4 \) on the accuracy of the model, respectively. As similar, the developed model can predict a more accurate displacement distribution as the increase of \( h_3 \) and \( h_4 \). The prediction of normal stress at the edge would get worse with the increase of \( h_3 \)
Figure 5.8: Comparison between theoretical solutions and FE simulation results for different $h_3$ or $h_4$ due to the increase of edge effect or singularity at the corner, however, at locations away from the edge, the theoretical solutions still agree well with the FE simulations results which is similar as shown in Fig. 5.7.

Based on this parametric study, the presented model can predict the elastic distribution accurately in the surface layer of the multilayered structures with various thickness ratios when away from the edge. Although the difference between the theoretical predictions and FE simulation results is large at the edge due to edge effect or singularity, this error has minor effect on the fracture analysis.

### 5.4 Fracture Analysis

Consider the section with OMFs at each end in Fig. 5.1. When the temperature change reaches a critical value, a steady-state channeling straight crack will initiate at the middle edge of the section. There are two models for the fracture analysis, namely the strength model and energy model. The strength model is based on the maximum normal stress that fracture would initiate if the maximum normal stress is higher than the strength \[150\]. According to the results shown in Fig. 5.5(b), the maximum normal stress is reached at the center, where ($\lambda = 0$), therefore, the cracking pattern in the surface layer can be analyzed easily by comparing the normal stress at the
Figure 5.9: Comparison between theoretical solutions and FE simulation results for different $h_4$

center with the strength. The energy model is based on the fracture ERR during the process of cracking [26]. To recover an OMF, the normal stress along the central line just before the fracture initiates needs to be applied along the cracking surface to recover the crack opening displacement. As after cracking, the section is broken into four pieces, and the displacement field in each quarter can also be solved by replacing $\lambda$ with $\lambda/2$ in the new local coordinate system. Therefore, the crack opening displacement is solved. Refer to [26], the fracture ERR in surface layer of the advanced polymeric reflector, which is equivalent with the work done to close the crack opening displacement, can be obtained through Eq. (5.69). In the following the fracture ERR would be calculated and fracture analysis based on energy model would be conducted.

$$G = \frac{1}{\lambda h_4} \int_0^\lambda \int_{t_3}^{h} \sigma_{xx}^4 (0, y, z) [u_x^4(\lambda, t_3) - u_x^4(\lambda, z)] dzdy \quad (5.69)$$

Substitute the solved elastic field in Section 5.2 to Eq. (5.69), the fracture ERR in surface layer of the advanced polymeric solar reflector could be obtained. Fig. 5.10 presents the change of fracture ERR with respect to crack spacing and surface layer’s thickness. It shows that the fracture ERR would increase rapidly as the crack spacing increases until it reaches to 4mm. Beyond this point, the fracture ERR does not change any more although the crack spacing increases, indicating that under the temperature change ($\Delta T = 40^\circ C$), the potential crack spacing of the given geometry ($h_1 = 0.18mm, h_2 = 10nm, h_3 = 100nm, h_4 = 200nm$) will be smaller than 4mm. Fig. 5.10(b)
Figure 5.10: Variance of ERR with respect to crack spacing and surface layer’s thickness shows the variance of the fracture ERR with respect to the surface layer’s thickness with constant crack spacing $\lambda = 0.2\ mm$ under a temperature change of $40^\circ C$. The fracture ERR increases linearly as the surface layer’s thickness increases until it reaches a convex point. While after this point, the fracture ERR would decreases as the thickness increases. At this convex point ($h_4 = 45\mu m$), fracture saturation is reached, therefore, no more new crack will be developed.

Once the fracture ERR is obtained, energy model can be applied to conduct fracture analysis. The criteria used by the energy model is that new crack would nucleate once the fracture ERR reaches the critical fracture ERR as shown in Eq. (5.70):

$$ G \geq G_{cr} $$ (5.70)

where $G_{cr}$ is the critical fracture ERR of the surface layer and is set to be $0.277\ J/m^2$ based on [229].

Based on this criteria, the required temperature change to initiate new cracks in the surface layer of the advanced polymeric solar reflectors with different geometries can be obtained and presented in Fig. 5.11. Based on Fig. 5.11(a), the required temperature change to create new cracks increases as the crack spacing decreases. When $\lambda$ approaches $0.4\ mm$, the temperature change turns to infinity which means no new fractures will infill and the fracture saturation is arrived. For this specified
case \((h_1 = 0.18\, mm, h_2 = 10\, nm, h_3 = 100\, nm, h_4 = 200\, nm)\), the saturated crack spacing can be approximately evaluated as \(0.4\, mm\). Fig. 5.11(b) shows the variation of the required temperature change with respect to the surface layer's thickness at a constant crack spacing \((\lambda = 0.2\, mm)\) and indicates that the required temperature change to initiate a new crack in the surface layer will reduce as the coating thickness decreases until a critical thickness \(h_{4_{cr}}\) is reached. Under this critical thickness, the required temperature change to crack the surface layer increases to be infinite and the fracture saturation would be reached. For this study, the critical thickness is about \(2\mu m\) for a crack length of \(0.2\, mm\).

### 5.5 Summary and Conclusions

In this chapter, a 3D elastic model had been presented to study the residual stress in multilayered structures, consisting of arbitrary layers, under thermal loading. By employing a non-shearing assumption and the assumption of free normal stress in thickness direction, the explicit solutions of displacement and stress were obtained through solving the elastic boundary value problem. In order to verify the proposed model, the elastic field in the advanced polymeric solar reflector had been solved and compared with FE simulation results. The good agreement between the theoretical predictions and FE simulation results demonstrated the accuracy of the presented model.
In addition, the effect of the geometry, particularly the thickness of each layer, on the accuracy of the theoretical model was investigated by the parametric study. The results showed that the model can predict the displacement and stress fields in the inner area of multilayered structures with various thickness ratios between each layer accurately, although large differences between the theoretically predicted normal stress and FE simulated normal stress would be observed at the area very close to the edge due to the edge effect or singularity at the corner.

Based on the elastic solutions, the fracture ERR in the surface layer was calculated. It showed that the fracture ERR would increase rapidly as the crack spacing increased until a plateau stage was reached when the crack spacing approached 4\,mm. Therefore, under the temperature change of 40^{\circ}C, the potential crack spacing was smaller than 4\,mm. When the crack spacing was constant, the fracture ERR approximately increased linearly with the coating thickness until it reached the convex point, at which the fracture saturation was reached. In this case (\Delta T = 40^{\circ}C, \lambda = 0.2\,mm, h_1 = 0.18\,mm, h_2 = 10\,nm, h_3 = 100\,nm), the critical coating thickness was 45\,\mu m.

The fracture infilling and saturation were studied based on the calculated ERR and energy model. When the surface layer’s thickness remained constant, the temperature change required to form a new crack would increase as the crack spacing decreases and fracture saturation would be reached when the crack spacing approached 0.4\,mm. However, when the crack spacing was constant, the required temperature change to form a new crack would decrease as the surface layer’s thickness decreased, until a critical coating thickness was reached. Under this critical thickness the required temperature change would increase to be infinite which means the fracture saturation was obtained. For the crack spacing of 0.2\,mm, the critical coating thickness was about 2\,\mu m.

Overall, the presented model was able to capture the displacement and stress distributions in the multilayered structures accurately and predict the fracture initiation, infilling, and saturation of the surface layer successfully.
Chapter 6

The Effect of Aging on the Delamination Fracture Energy of Glass Solar Reflectors

Thin metal and metal oxide films deposited on glass has been widely used to manufacture front surfaced solar reflectors such as those used in the concentrated solar power (CSP) systems due to the facts that they are highly transparent, resistant to ultraviolet (UV) light, abrasion resistant, and chemically inert; However, the reliable operation over a long time of such solar reflectors depends on the adequate adhesion between each layer to prevent delamination and subsequent failures. In this chapter, the delamination fracture energy (DFE) of the weakest interface in both as-deposited and aged reflectors, where the reflector construction consists of a glass/copper/silver/oxide stack, are measured using a width-tapered beam peeling method. The test results show that the weakest interface of this solar reflector is the copper-glass interface, with a delamination fracture energy of approximately $4.4 J/m^2$. In order to verify the test results, finite element (FE) simulations are run using the commercial software package ABAQUS 6.14 based on the cohesive zone model (CZM). In the simulations, the DFE derived from the peeling measurement is treated as an input and the peeling forces from the FE simulations are compared to the experimental results. The good agreement between the tested and simulated peeling force indicates that this width-tapered beam method is accurate even for very small DFE, making it appropriate to test the DFE of
these front surfaced glass solar reflectors. Additionally, in order to study the aging effect on the DFE, accelerated aging tests are conducted using samples with different protective coatings, one group of samples with alumina ($Al_2O_3$) protective coating and the other group with titania ($TiO_2$) protective coating. The DFE after 50 hours of accelerated aging were measured. The tests results indicate that the copper-glass interface would still be the weakest interface for all samples after aging and the DFE for samples with $Al_2O_3$ protective coating is unchanged whereas it is found to undergo statistically significant decrease after 50 hours of aging for samples with $TiO_2$ protective coating.

6.1 Overview

The reflectors used in concentrated solar power (CSP) systems can be of various constructions, including traditional rear-surfaced glass mirrors [166], coated aluminum mirrors [67] and front surfaced silver mirrors on a variety of substrates [213]. Each type of reflector also can be produced out of various materials, such as glass or polymer as substrate, copper layers to act as adhesion promoters between silver and a substrate, silver to reflect the light and coatings such as silica, alumina or titania for reflectance tuning and protective purposes. Currently, most large CSP plants use reflectors with glass support because it is highly transparent, resistant to ultraviolet (UV) light, abrasion resistant, and chemically inert [61]. Fig. 6.1 shows a schematic front-surfaced glass reflector with a bonding layer between the silver and glass, and a protective layer atop the silver. The solar reflectors are important components in the CSP system because the ability to direct light to a target for heating directly impacts the operation efficiency of CSP plants. To reduce the cost associated with construction of the solar field of mirrors, reflector lifetime, weight and cost must be optimized to lower the levelized cost of energy of CSP plants. The exposure of solar reflectors to environmental conditions (humidity, dust), high radiation fluxes and elevated temperatures potentially causes stress and degradation due to the diffusion of oxygen and moisture into the system which further lead to loss in reflectance throughout the time [54; 65; 61]. As the reflectors are costly and cannot be replaced frequently [82], their reflectivity should be maintained as long as possible for any reflector that can be adopted for a CSP plant. Based on this consideration, a good bonding between each layer of the solar reflector is desired in order to slow down the aging
process and increase the service life. Hence, in this chapter we examine interlayer bonding as a route to understanding reflector degradation that may accompany delamination.

![Diagram of glass reflector designs](image)

**Figure 6.1: Schematic glass reflector designs [229]**

In order to quantify the bonding behavior between each layer of this glass reflector and study the effect of aging on the bonding quality, the delamination fracture energy (DFE), which is a material property and equal to the energy needed to delaminate a unit area, at the weakest interface of reflectors after different periods of accelerated aging tests would be measured in this chapter.

In this study, the DFE of glass reflectors were measured using the width-tapered beam testing method developed by [29]. This method employs an elastic width-tapered cantilever beam adhered to the top surface of the multi-layer structure, see Fig. 6.2. When the beam is loaded at its apex, delamination will initiate at the weakest interface and advance upon continued loading. The beauty of this method is that the differential of compliance and the width of this width-tapered cantilever beam would increase proportionally with the increase of crack length, therefore the peeling force becomes nearly constant when steady state of delamination occurs.

In the following, Section 6.2 presents the width-tapered beam testing procedures and the measured DFE of original glass reflectors with either alumina ($\text{Al}_2\text{O}_3$) or titania ($\text{TiO}_2$) protective coatings. Section 6.3 verifies the testing results presented in Section 6.2 through comparison to finite element (FE) simulations results based on a cohesive zone model (CZM) of delamination. The results of accelerated aging tests and studies about the effect of aging on DFE are given in
Section 6.4. Finally, some conclusions will be given in Section 6.5.

6.2 Width-Tapered Beam Tests

In this study, the reflectors were prepared by depositing a thin (10 nm) copper layer onto standard, 1/8 plate glass (green glass) to act as an adhesion layer between glass and a 100 nm layer of silver that acts as the solar reflector. Prior to deposition, the glass was cleaned with pumice, IPA, and a detergent solution (Billco #013-701). The silver reflective layer is coated with 200 nm of either alumina (Al$_2$O$_3$) or titania (TiO$_2$) layer as a protective layer. All layers were deposited with e-beam evaporation and the base pressure of the chamber was on the order of $3.0 \times 10^{-8}$ torr. The copper was deposited at a rate of $3.0 \AA/s$ from 99.999% copper source material, the silver was deposited at $5.0 \AA/s$ from 99.99% pure source material, the TiO$_2$ was evaporated from Ti$_3$O$_5$ source material (99.9%) at $5.0 \AA/s$ with an O$_2$ flow of 10 sccm, and the Al$_2$O$_3$ was evaporated from Al$_2$O$_3$ source material (99.99%) at $5.0 \AA/s$ with an O$_2$ flow of 10 sccm. Layers were deposited sequentially without removing the substrate from vacuum.

Based on the testing results, the DFE of this glass reflector is small, less than 10 $J/m^2$, so a flexible beam is required to allow continuous growth of the crack. (Too stiff beam can lead to sudden failure rather than a gradual peeling.) Hence, we used an acrylic beam with a thickness of 1.8 mm and the dimensions of this beam are given in Fig. 6.3. This beam was glued on the oxide top surface of the glass reflectors and pulled up with the peeling force continuously monitored. A handle was incorporated into the acrylic beam to provide a location for the attachment of a loading tab whose action could remain at the apex of the beam.
Figure 6.3: Dimensions of the width-tapered acrylic beam with an included angle $\theta = 20^\circ$ and thickness $1.8\,mm$ [29]

6.2.1 Sample Preparation

In order to glue the acrylic beam to the glass reflector well, the acrylic beam was polished using sandpaper in order to get a rough surface. Then the polished beam surface and the top surface of reflector were cleaned using isopropyl alcohol. After that, a volume of Epoxy (3M 8010) adequate to just cover the tapered acrylic beam was applied to its polished surface. The acrylic beam was then pressed to the protective layer of the glass reflectors and held secure for several seconds until the adhesive fully hardened. A sharp razor blade was then used to cut through the metal and metal oxide layers around the acrylic beam using the straight edge of the beam as a guide and a pre-crack was made using a sharp blade.

After the samples were prepared, a small load tab was attached to the handle at the apex of the acrylic beam and connected to the tensile machine. Then the testing was conducted at a constant displacement rate of $10\,\mu m/s$, the load and load-line displacement were recorded. The test configuration is presented in Fig. 6.4(a). After testing, the sample was unloaded and removed from the loading frame. The crack tip was marked and the crack length was measured using a caliper. Fig. 6.4(b) presents one tested sample with $Al_2O_3$ protective coating and shows that the delaminated interface is the interface between the copper layer and glass, which denotes that the copper-glass
Figure 6.4: (a) Test configuration, and (b) peeled sample.

Figure 6.5: Tested load-displacement curve
interface is the weakest interface. Fig. 6.5 presents the corresponding load-displacement curve which includes the unloading process.

6.2.2 Data Analysis

For this width-tapered beam testing method, the material property of interest, the DFE, is related to the measured parameters as described by Eq. (1.2), where $P_c$ is the critical load to extend the debond, $a_i$ is the crack length under a load-line displacement $\Delta_i$, $\theta$ is the apex angle of the width-tapered beam. From Eq. (1.2), the DFE can be calculated based on the tested peeling force and the measured crack length with a load-line displacement.

Based on the load-displacement curve as shown in Fig. 6.5, the peeling force is not perfect constant. In order to get a better estimation, the DFE at every point in the section where the force is approximately constant (section where the load-line displacement is between 2 mm and 4.4 mm for this test) was calculated using Eq. (1.2) based on the measured final crack length and the corresponding peeling force and load-line displacement. Then the average value was used to represent the DFE of this sample. For this specific sample, the calculated DFE is 3.9339 $J/m^2$. 

Figure 6.6: (a) Two beams glued on each sample, and (b) crack tips after three pulls.
6.2.3 Testing Results of Unaged Samples

The tested DFEs for samples with either $\text{Al}_2\text{O}_3$ or $\text{TiO}_2$ protective coating are summarized in Table (6.1). For each type of protective coating, 2 samples were prepared and 2 beams were glued on each sample as shown in Fig. 6.6(a). In order to investigate the DFE at different locations, 3 pulls were conducted for each beam, the marked crack tips for each beam were shown in Fig. 6.6(b) (the marker most close to the apex of the beam indicates the pre-crack tip). Therefore, 6 DFE values can be obtained for each sample. The samples in the Table (6.1) is named in this way: $\text{Al}_2\text{O}_3$ or $\text{TiO}_2$ indicates the type of protective coating of sample, the followed number denotes the first or second sample with same type of protective coating, the second number denotes the first or second beam glued on this sample, and the last number denotes the pull number for this beam. For example, sample $\text{Al}_2\text{O}_3$-1-1-2 denotes the second pull on the first beam on the first alumina coated reflector.

The testing results show that the tested DFEs for samples with $\text{Al}_2\text{O}_3$ protective coating seem lower than that of samples with $\text{TiO}_2$ protective coating (the average DFE of samples with $\text{Al}_2\text{O}_3$ is 3.9639$J/m^2$, which is lower than the average DFE of samples with $\text{TiO}_2$ (4.8974$J/m^2$) from Table 6.2), however, the DFEs for all samples have a large uncertainty. The measured DFEs for samples with $\text{Al}_2\text{O}_3$ protective coating range from 2.5705 to 5.8804$J/m^2$, with a standard deviation (SD) of 1.2244$J/m^2$, and from 3.0834 to 6.8978$J/m^2$, with a SD of 1.4899$J/m^2$ for samples with $\text{TiO}_2$ protective coating as shown in Table 6.2. The large heterogeneity found in the DFE values indicates that despite the identical cleaning and deposition procedures, the binding between copper and glass is not uniform over several mm or cm. The lower SD and standard deviation of the mean (SDM) for samples with $\text{Al}_2\text{O}_3$ coating suggests that the copper/glass interface is more uniform compared with samples with $\text{TiO}_2$ coating.

In order to estimate ranges of DFE for each sample type, two-tailed Student’s t-tests (with 11 degrees of freedom (DOF)) were performed. The results from the two-tailed t-tests show that, with 95% confidence, the DFE of samples with $\text{Al}_2\text{O}_3$ coating would be in the range of 3.1858–4.7420$J/m^2$, while the range for samples with $\text{TiO}_2$ coating would be 3.9507–5.8441$J/m^2$. Theoretically, there should no big different for the DFE between samples with $\text{Al}_2\text{O}_3$ and $\text{TiO}_2$ coatings, because the weakest interface is the copper-glass interface and the protective coating would be expected to have a minor effect on the DFE of copper-glass interface for these original
Table 6.1: Tested DFE for original glass reflector without aging

<table>
<thead>
<tr>
<th>Samples</th>
<th>DFE (J/m$^2$)</th>
<th>Samples</th>
<th>DFE (J/m$^2$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Al$_2$O$_3$-1-1-1</td>
<td>5.8804</td>
<td>TiO$_2$-1-1-1</td>
<td>5.9743</td>
</tr>
<tr>
<td>Al$_2$O$_3$-1-1-2</td>
<td>5.4713</td>
<td>TiO$_2$-1-1-2</td>
<td>3.2683</td>
</tr>
<tr>
<td>Al$_2$O$_3$-1-1-3</td>
<td>5.6339</td>
<td>TiO$_2$-1-1-3</td>
<td>6.7623</td>
</tr>
<tr>
<td>Al$_2$O$_3$-1-2-1</td>
<td>3.1248</td>
<td>TiO$_2$-1-2-1</td>
<td>6.7729</td>
</tr>
<tr>
<td>Al$_2$O$_3$-1-2-2</td>
<td>2.6127</td>
<td>TiO$_2$-1-2-2</td>
<td>6.8978</td>
</tr>
<tr>
<td>Al$_2$O$_3$-1-2-3</td>
<td>3.1555</td>
<td>TiO$_2$-1-2-3</td>
<td>3.4601</td>
</tr>
<tr>
<td>Al$_2$O$_3$-2-1-1</td>
<td>3.1276</td>
<td>TiO$_2$-2-1-1</td>
<td>5.3908</td>
</tr>
<tr>
<td>Al$_2$O$_3$-2-1-2</td>
<td>2.5705</td>
<td>TiO$_2$-2-1-2</td>
<td>5.6308</td>
</tr>
<tr>
<td>Al$_2$O$_3$-2-1-3</td>
<td>3.3628</td>
<td>TiO$_2$-2-1-3</td>
<td>4.1204</td>
</tr>
<tr>
<td>Al$_2$O$_3$-2-2-1</td>
<td>3.9339</td>
<td>TiO$_2$-2-2-1</td>
<td>3.7959</td>
</tr>
<tr>
<td>Al$_2$O$_3$-2-2-2</td>
<td>5.1461</td>
<td>TiO$_2$-2-2-2</td>
<td>3.6114</td>
</tr>
<tr>
<td>Al$_2$O$_3$-2-2-3</td>
<td>3.5471</td>
<td>TiO$_2$-2-2-3</td>
<td>3.0834</td>
</tr>
</tbody>
</table>

Table 6.2: Statistical properties of the measured DFE of unaged reflectors.

<table>
<thead>
<tr>
<th>Protective Coating types</th>
<th>Mean</th>
<th>SD</th>
<th>SDM</th>
</tr>
</thead>
<tbody>
<tr>
<td>Al$_2$O$_3$</td>
<td>3.9639</td>
<td>1.2244</td>
<td>0.3535</td>
</tr>
<tr>
<td>TiO$_2$</td>
<td>4.8974</td>
<td>1.4899</td>
<td>0.4301</td>
</tr>
</tbody>
</table>

samples without any aging, and the overlap of the 95% confidence intervals is consistent with this idea. Therefore, we also can treat these un-aged samples as a single set with 23 DOF. For the combined set, the mean value for all samples would be $4.4306 J/m^2$ with a SD of $1.4164 J/m^2$ and SDM of $0.2891 J/m^2$. The two-tailed t-test gives a range for the DFE of $3.8325 - 5.0287 J/m^2$ with 95% confidence.

6.3 Verification using FE Simulations

In this section, the testing results would be verified using FE simulation. As we have known the delaminated interface (the copper-glass interface), the CZM was used to enable the delamination simulation and cohesive elements were inserted between the copper and glass layers. The consti-
tutive behavior of the cohesive elements was simulated using the bilinear traction-separation law whose response is shown in Fig. 6.7, where $K$ is the initial stiffness, $T$ is the strength, $G_c$ is the critical DFE, $\Delta^c$ is the separation when delamination is initiated, and $\Delta^{fail}$ is the separation at damage. For this bilinear traction-separation law, the initial response of the cohesive elements is assumed to be linear until the damage initiation criterion is met when the stress reaches the strength $T$. After this point, the stress in cohesive elements would be released linearly until the damage evolution property is reached when the fracture energy release rate is equal to $G_c$, and the cohesive elements would be damaged.

![Figure 6.7: Bilinear traction-separation response of the cohesive element](image)

### 6.3.1 Determination of Parameters for Cohesive Elements

In order to run the simulations, the parameters characterizing the bilinear traction-separation law must be specified, including the initial stiffness ($K$), damage initiation threshold ($T$), and damage evolution properties ($G_c$).

As stated before, interface strength determines the damage initiation point; beyond this point damage begins to develop in the cohesive zone leading to reduction in the traction [173]. For a bilinear traction-separation law, the interfacial strength can be obtained by applying Eq. (6.1).

$$T = \frac{2G_c}{\Delta^{fail}}$$  \hspace{1cm} (6.1)
For elastic double cantilever beam analysis Diehl found that a good match with the analytical solution is obtained when $\Delta_{\text{fail}}$ is taken as 0.05 of the cohesive element length [52].

As for the initial stiffness, Diehl [50; 51; 52; 53] proposed an approach to estimate the elastic stiffness of the cohesive element based on classical fracture mechanics and numerical stability considerations. For a bilinear traction-separation relationship, the stiffness is defined in terms of fracture energy ($G_c$), separation at final failure ($\Delta_{\text{fail}}$), and the damage initiation ratio ($\Delta_{\text{ratio}} = \Delta_c / \Delta_{\text{fail}}$) as:

$$K = \frac{2G_cT_0}{\Delta_{\text{ratio}}(\Delta_{\text{fail}})^2} \quad (6.2)$$

where $T_0$ is the specified initial constitutive thickness of the cohesive element (typically specified as 1.0). Diehl [52] has parametrically studied the effects of $\Delta_{\text{ratio}}$ on various mode I fracture characteristics of elastic double cantilever beam. The results of his parametric studies reveal that $\Delta_{\text{ratio}}$ does not significantly affect the overall load-displacement response of the specimen when compared with the benchmark solution; he recommends a value of 0.5 ($\Delta_{\text{ratio}} = 0.5$).

For the damage evolution, the energy criterion was used. Once the fracture energy is higher than the measured DFE (3.9339 J/m$^2$), the fracture would propagate.

### 6.3.2 FE Model

The FE model and mesh are shown in Fig. 6.8(a). Totally 16476 uniformly sized elements with a size of 1 mm were employed to mesh the structure. In order to simulate the delamination between the copper and glass interface, a layer of cohesive element (COH3D8) was introduced between copper and glass. The thickness of the cohesive layer was 10 nm, the DFE was 3.9339 J/m$^2$. The
### Table 6.3: Thickness and Material Properties of Each Layer

<table>
<thead>
<tr>
<th>Layers</th>
<th>Thickness</th>
<th>Young’s Modulus (GPa)</th>
<th>Poisson’s Ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>Acrylic Beam</td>
<td>1.8 mm</td>
<td>3.2</td>
<td>0.35</td>
</tr>
<tr>
<td>$TiO_2$</td>
<td>200 nm</td>
<td>230</td>
<td>0.27</td>
</tr>
<tr>
<td>Ag</td>
<td>100 nm</td>
<td>83</td>
<td>0.37</td>
</tr>
<tr>
<td>Cu</td>
<td>10 nm</td>
<td>110</td>
<td>0.34</td>
</tr>
<tr>
<td>Glass</td>
<td>3.175 mm</td>
<td>50</td>
<td>0.22</td>
</tr>
</tbody>
</table>

The thickness and material properties these layers are summarized in Tab. (6.3).

The boundary conditions of the FE model are presented in Fig. 6.8(b), where the bottom of the glass and the end of all layer were fixed to ensure the cantilever beam condition. A velocity boundary condition was applied at the hole near the apex.

### 6.3.3 Simulation Results

The deformed shape of the sample is presented in Fig. 6.9(a). The stresses in the beam and glass substrate were small compared with that in the metal layer. The reason is that the stiffness of the metal layer is much larger than that of the acrylic beam, therefore, the metal layer would carry more stress. Also the delamination limited the stress transferred to the glass substrate.
After simulation, the reaction force at the hole changing with delamination process was recorded and compared with the tested peeling force in Fig. 6.9(b). It shows that the FE simulation can capture the increase of force before delamination and the peeling force is near constant during the peeling process. This is consistent with the theoretical prediction. In contrast to the expectation of a constant peeling force after onset of delamination, in general the tested peeling force decreases with the increase of crack length. This can be caused by many factors such as non-uniform bonding across the interface such that the DFE varies with respect to crack length.

### 6.4 Effects of Aging on DFE

In order to investigate the effect of aging on the bonding of each interface of the glass reflectors, accelerated aging tests were conducted and the DFE at the weakest interface were measured after 50 hrs of aging using the width-tapered beam method.

#### 6.4.1 Accelerated Aging of Oxide-Coated Front-Surfaced Reflectors

In these tests, customized aging conditions of temperature, humidity and irradiance were applied using an Atlas Ci5000 weatherometer. The Ci5000 is a 12000 W xenon arc lamp environmental chamber with temperature and humidity control. Irradiance from the xenon lamp is filtered to simulate the terrestrial solar spectrum with a Right Light inner filter and a CIRA (coated infrared absorbing) quartz outer filter. Irradiance is controlled to a 340 nm set point. In addition to chamber temperature and humidity control, an uninsulated black panel sensor is used to monitor and control the maximum rack temperature. The exposure conditions used to stress specimens are listed in Table 6.4.

Meanwhile, in order to prevent the penetration of oxygen and humidity to the sample through the edge, 3M weather resistant film tape 838 was used to cover the edge of coatings during the acceleated aging tests.

#### 6.4.2 Testing Results

After aging for 50 hrs, the samples were removed from the chamber and the DFE were measured using the width-tapered beam method as described above. The results show that as for the un-aged
<table>
<thead>
<tr>
<th>Parameter</th>
<th>Set Point</th>
</tr>
</thead>
<tbody>
<tr>
<td>Irradiance (340 nm)</td>
<td>0.7 $Wm^{-2}$</td>
</tr>
<tr>
<td>Chamber Temperature</td>
<td>45°C</td>
</tr>
<tr>
<td>Relative Humidity</td>
<td>40% RH</td>
</tr>
<tr>
<td>Rack Temperature</td>
<td>45°C</td>
</tr>
</tbody>
</table>

Table 6.4: Accelerated exposure conditions

samples described in Section 6.2, delamination initiated at the interface of copper and glass for all aged samples, with either $Al_2O_3$ or $TiO_2$ protective coating. Hence, the copper-glass interface was still the weakest interface after 50 hrs of aging.

The measured DFEs for all samples after 50 hrs of aging are summarized in Table 6.5. Similarly as the tests for un-aged samples, 2 samples were prepared for each type of protective coating for each aging period, 2 beams were glued on each sample, and 3 pulls were conducted for each beam. The samples are named using the same rule as that in Section 6.2.2.

Results of statistical analysis of the testing results for samples with $Al_2O_3$ or $TiO_2$ protective coatings are presented in Table 6.6 and 6.7, respectively. Meanwhile, the mean measured DFE after different aging periods are plotted in Fig. 6.10 with error bars indicating plus or minus one SDM. One can see that after aging there is a large uncertainty for the measured DFE, with a SD is higher than 0.5 $J/m^2$ for both types of samples after both aging periods.

Two-tailed Student’s t-tests were conducted in order to obtain confidence intervals for DFE. The obtained 95% confidence intervals are summarized in Tables 6.6 and 6.7 and compared with the statistic analysis results for samples without any aging (Recall that for unaged reflectors, samples with different protective coatings were treated as the same for the statistical analysis.)

Based on the statistical analysis, the DFE for samples with $Al_2O_3$ protective coating are found to decrease slightly, but in a non-statistically significant amount upon aging: The mean of DFE decreases by about 8.3% after 50 hrs of aging. In view of the large uncertainty of the measured DFE for all aging conditions, the reduction DFE with aging period is negligible with an $Al_2O_3$ coating. Therefore, we can state that the aging has very minor effect on the DFE of samples with $Al_2O_3$ protective coating. This result is consistent with the finding that the reflector with a protective alumina coating represents an advancement in solar reflector durability as samples of
Figure 6.10: Plot of the mean of measured DFE after different aging periods with SDM error bar for samples with: (a) $\text{Al}_2\text{O}_3$ protective coating; and (b) $\text{TiO}_2$ protective coating.

The reflector have shown an initial solar-weighted hemispherical reflectance of 95% and outstanding optical performance in both accelerated and outdoor (Colorado) exposure testing [106].

In contrast to what happens with alumina protection, the DFE for $\text{TiO}_2$ coated samples shows large and significant decrease upon aging. After 50 hours, the mean DFE has decreased more than 30%, with the 95% confidence intervals at 0 and 50 hours of aging not overlapping at all. This suggests that $\text{TiO}_2$ coatings do not provide sufficient encapsulation to prevent modifications occurring at the copper/glass interface; this is consistent with the larger changes in reflectance we have found for $\text{TiO}_2$-coated reflectors constructed and aged the same way as reported here.

6.5 Conclusions

In this study, the width-tapered single cantilever beam method was applied to test the DFE of the glass reflectors with either $\text{Al}_2\text{O}_3$ or $\text{TiO}_2$ protective coating. The DFE measured in our tests showed substantial variation even for different pulls on the same sample, suggesting perhaps that the surface interaction at the copper/glass interface varies widely at different positions of each sample. In other words, the delaminated interface may not be homogeneous and the DFE would depend on both the crack length and the location of the delaminated region. We found that for both as-deposited and aged reflectors, the copper-glass interface was the weakest. The measured DFE of samples with $\text{Al}_2\text{O}_3$ protective coating was slightly lower and with a smaller variance
### Table 6.5: Tested DFE for glass reflector 50 hrs of aging

<table>
<thead>
<tr>
<th>Aging period (hrs)</th>
<th>Samples</th>
<th>DFE (J/m²)</th>
<th>Samples</th>
<th>DFE (J/m²)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>$Al_2O_3$-1-1-1</td>
<td>4.6690</td>
<td>$TiO_2$-1-1-1</td>
<td>3.5400</td>
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<td>2.4988</td>
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<td>3.4436</td>
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<td>2.0773</td>
</tr>
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Table 6.6: Statistical analysis of testing results for samples with $Al_2O_3$ protective coating

<table>
<thead>
<tr>
<th>Aging period (hrs)</th>
<th>Mean</th>
<th>SD</th>
<th>SDM</th>
<th>Range of DFE (95%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>4.4306</td>
<td>1.4164</td>
<td>0.2891</td>
<td>[3.8325 5.0287]</td>
</tr>
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<td>0.2061</td>
<td>[3.6077 4.5149]</td>
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Table 6.7: Statistical analysis of testing results for samples with $TiO_2$ protective coating

<table>
<thead>
<tr>
<th>Aging period (hrs)</th>
<th>Mean</th>
<th>SD</th>
<th>SDM</th>
<th>Range of DFE (95%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>4.4306</td>
<td>1.4164</td>
<td>0.2891</td>
<td>[3.8325 5.0287]</td>
</tr>
<tr>
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<td>0.7139</td>
<td>0.1655</td>
<td>[2.4536 3.1822]</td>
</tr>
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</table>
than for samples with $TiO_2$ protective coating, but that unaged samples with both coatings have overlapping confidence intervals. Hence, our statistical analysis of the DFE of unaged reflectors combined the results from both protective coatings. An averaged DFE was obtained as $4.4306 J/m^2$ to represent the DFE of original samples.

The results of the width-tapered beam pull tests were verified by FE simulation in ABAQUS using CZM with parameters for cohesive elements obtained based on literature. The peeling force generated from the FE simulation was compared with the test results and it was shown that the simulated peeling force did become nearly constant, with a plateau value that agreed well with the testing results, on average. This good agreement denoted that the width-tapered beam testing method provided an accurate way to measure the DFE of this glass reflector. A decrease of the peeling force following the initial fracture was observed for most tests, suggesting that the wide range of DFE values measured is based on in-sample inhomogeneity, rather than on variations between the different members of our sample sets.

In addition, the effect of aging on the DFE was investigated by measuring the change of DFE in samples after 50 hrs of accelerated aging. The results showed that the DFE of samples with $Al_2O_3$ protective coating would slightly decrease with the increase of aging period; however, this decrease was within the statistical uncertainty of our data. Therefore, we concluded that the aging had minor effect on the DFE of samples with $Al_2O_3$ samples. However, for the samples with $TiO_2$ protective coating, the DFE was found to decrease after 50 hrs’ aging significantly. This result denotes $Al_2O_3$ coating would be a good protective coating to be used in the glass solar reflectors.
Chapter 7

Conclusions and Future Work

7.1 Summary

This dissertation studied the fracture mechanics of multilayered structures and the degradation behavior of asphalt binders.

A two-dimensional (2D) elastoplastic fracture model was developed to study the opening-mode fractures (OMFs) in the protective alumina coating fully bonded to an aluminum plate or wire substrate under tensile loading considering large yielding in the substrate. The displacement and stress field were solved explicitly and verified using the finite element (FE) results. Based on the solved displacement and stress field, the fracture energy release rate (ERR) was obtained and used to predict the fracture initiation, infilling, and saturation successfully. Experiments were run to verify the fracture analysis. The good agreement between the theoretical predictions and FE and experimental results denote that the proposed model can capture the displacement and stress distribution in the coating/substrate system and predicts the fracture behavior in the coating accurately.

As an extension of the proposed 2D elastoplastic fracture model, a three-dimensional (3D) elastic fracture model was then developed to study the fracture behavior of the protective coating in the multilayered advanced polymeric reflectors under thermal loading as the plain strain or plane stress assumptions can not be applied. In this study, the advanced polymeric solar reflector was simplified and simulated with a two layers structure as the bonding layer and silver layer are
much thinner. The displacement and stress field were solved and verified using the FE simulation. Then the fracture behavior including fracture initiation, infilling, and saturation were analyzed and validated using a cohesive zone model (CZM) and experimental data from literature. Later on, this simplified model was extended to study multilayered structures consisting of arbitrary number of layers. By applying this model, the displacement and stress in each layer of the advanced polymeric solar reflector was solved explicitly and used for fracture analysis.

As another common fracture type, the delamination of the glass solar reflectors with different protective coating was studied by measuring the delamination fracture energy using the width-tapered beam method. FE simulations were conducted based on CZM to simulate the delamination test. The good agreement between the simulated and testing results denoted the accuracy of the width-tapered beam method. Additionally, the effect of aging on the delamination fracture energy of this glass solar reflectors was investigated.

Besides the fracture mechanics, another failure mechanism, material degradation and aging, was studied by aging three types of asphalt binders extracted from reclaimed asphalt pavements (RAPs) and one extracted from fresh Hot Mix Asphalt (HMA) under continuous UV exposure and UV/moisture/condensation exposure. After the accelerated aging process, the weight percentage of oxygen (WPO) in the samples were measured and fitted using two classic aging models: the fast-rate - constant-rate (FRCR) model and the nonlinear differential dynamic (NDD) model. By comparing the WPO in the samples after continuous UV aging and UV/moisture/condensation aging, the effect of moisture and condensation was investigated.

7.2 Key Results

7.2.1 2D Elastoplastic Fracture Model in Cartesian Coordinates

In Chapter 2, an elastoplastic fracture model was developed to study the OMF in coating layered structures undergoing large-scale yielding. Because of the fracture pattern with an approximately uniform fracture spacing, the stress field in the coating system was described by one section between two adjacent cracks. As the coating layer is much thinner and more brittle than the substrate, a plane strain formulation was used to analyze the elastic field in the coating. A one-dimensional (1D) linear hardening plastic model was applied to account for the large plastic deformations in
the substrate under substantial yielding, and an elastoplastic shear lag model was established to transfer the tensile stress in the substrate to the coating. With the increase of the tensile load, three stress phases were induced: linear elastic behavior, yielding of the substrate and interface, and OMF in the coating. The general formulation and explicit elastic/elastoplastic solutions of the coating/substrate system under different loading stages were developed.

The elastic field predictions were compared with FE results, the good agreement between the present solution and the FE simulation demonstrates the accuracy of the present elastic solutions. Using the periodic condition, the ERR was calculated, through which crack initiation, infilling, and saturation in the coating were successfully captured. To validate the elastoplastic solution, experimental tests were further conducted to explore the OMFs developed in the coating layer, where the crack spacing and critical coating thickness were investigated and compared with the predictions made by the present model. From the analytical solutions and experimental results, the following conclusions were reached:

(1) Under the same applied load, the crack spacing proportionally decreases as the coating thickness decreases until a critical coating thickness is reached, below which no more fractures will be developed.

(2) The saturated crack spacing can be approximately evaluated as $\lambda_{cr} = 3.8h_1$ for a constant coating thickness, while the critical coating thickness can be approximated as $h_{1cr} = \lambda/4.2$ for a constant crack spacing.

(3) The critical coating thickness decreases as the applied load (strain) increases.

Overall, the theoretical prediction is able to effectively capture the varying trend of the crack spacing with respect to the coating thickness. Due to the discontinuous coating thickness available from experimental tests, the exact critical coating thickness cannot be determined at different applied loads. Thus, to better characterize the critical coating thickness, more accessible coating thicknesses from more samples are desirable for future studies. Nevertheless, good agreement between the experimental observations and the theoretical predictions validate the presented elastoplastic fracture model. When the stiffness of the substrate in the elastic stage $E_{s1}$ is assumed to be infinite, the employed bi-linear elastoplastic model will become a linear hardening model; when the linear hardening rate $E_{s2}$ is assumed to be zero, a linear elastic - perfectly plastic model will be recovered. In this respect, the present formulation is general and can be applicable to other types
of coating/thin film ductile substrate systems and layered material/structures.

7.2.2 2D Elastoplastic Fracture Model in Cartesian Coordinate

Chapter 3 extends the proposed 2D elastoplastic model in Cartesian coordinates to polar coordinates and studies the fracture behavior of alumina coating fully bonded to an aluminum wire considering the axial symmetry. As the applied tensile load increases, the system undergoes three different stress stages: elastic stage, elastoplastic stage, and OMF stage. The displacement and stress distributions in the coating/substrate were firstly solved at the elastic stages and been verified by FE solutions. Elastoplastic solutions were further provided for the coating/substrate system as large deformation develops with an increased applied load. Based on the elastoplastic solutions, the ERR at different loading stages were calculated and fracture analysis was conducted. Simulation results show that, when the coating thickness remains constant, the load required to form a new crack increases as the crack spacing decreases, and fracture saturation is reached when the cracking spacing approaches 1.2 times of the coating thickness.

Experimental characterization is conducted to validate the present elastoplastic solution when the substrate or interlayer undergoes large deformation. Both experimental and theoretical results indicate that the crack spacing decreases linearly as the thin film thickness decreases until a critical film thickness is reached, while below this critical thickness, no new cracks will be developed. Overall, the varying trend of the crack spacing with respect to the coating thickness revealed by the test results can be effectively captured by the theoretical prediction, which demonstrates that the present model is able to accurately capture the stress and strain distribution in the coated structure and predict the fracture initiation, infilling, and saturation in the thin coating layer. The present formulation is general and can be applicable to other types of coating ductile substrate systems.

7.2.3 3D Elastic Fracture Analysis for Coating/Substrate System

In Chapter 4, a 3D elastic fracture model has been presented to simulate block cracking in the multilayered advanced polymeric solar reflectors based on a simplified bilayer structure comprising PET and TiO2. The displacement and stress fields in the system under temperature change are obtained theoretically which show that the displacement along the x-direction is nearly constant
across the width. Then the obtained elastic fields are verified with FE simulations. The good agreement between theoretical predictions and simulation results (maximum difference within 4%) reveals the accuracy of the presented fracture model.

Based on the elastic solutions, the ERR is calculated. It shows that the ERR would increase rapidly as the crack spacing increases until a plateau stage is reached when crack spacing approaches 6 times of the substrate’s thickness indicating that under the temperature change of $40^\circ C$, coating thickness $100\mu m$, and substrate thickness $4.2\; mm$, the potential crack spacing is smaller than $25.2\; mm$. When the crack spacing is constant, the ERR approximately increases linearly with the coating thickness until it reaches the convex point, at which the fracture saturation is reached. In this case ($\Delta T = 40^\circ C, \lambda = 21\; mm, h_s = 4.2\; mm$), the critical coating thickness is $120\; \mu m$.

The fracture infilling and saturation are then studied based on the calculated ERR. The results show that the temperature change required to form a new crack would increase with respect to the decrease of crack spacing when the coating thickness remains constant, and that fracture saturation would be reached when the cracking spacing approaches 0.5 times of the substrate thickness. However, when the crack spacing is constant, the required temperature change to form a new crack would decrease as the coating thickness decreases, until a critical coating thickness is reached. Under this critical thickness the required temperature change would increase to be infinite which means the fracture saturation is obtained. For the crack spacing of $21\; mm$, the critical coating thickness is about $5\mu m$. Furthermore, the saturated crack spacing decreases linearly as the thin film thickness decreases until a critical film thickness is reached, while below this critical thickness ($70\mu m$), no new cracks will be developed. In order to verify the theoretical fracture analysis, FE simulations based on CZM with the bilinear traction-separation constitutive behavior are conducted. The simulated temperature changes to initiate a new crack in coating with different crack spacings but constant coating thickness are compared with the theoretical predictions. The good agreement between simulation results and theoretical solutions indicates the accuracy of the proposed fracture model.

### 7.2.4 3D Elastic Fracture Analysis for Multilayered Structures

In Chapter 5, a 3D elastic model has been developed to study the residual stress in multilayered structures, consisting of arbitrary layers, under thermal loading. By employing a non-shearing
assumption and the assumption of free normal stress in thickness direction, the explicit solutions of displacement and stress are obtained through solving the elastic boundary value problem. In order to verify the proposed model, the elastic field in the advanced polymeric solar reflector has been solved and compared with FE simulation results. The good agreement between the theoretical predictions and FE simulation results demonstrates the accuracy of the presented model. In addition, the effect of the geometry, particularly the thickness of each layer, on the accuracy of the theoretical model is investigated by the parametric study. The results show that the model can predict the displacement and stress fields in the inner area of multilayered structures with various thickness ratios between each layer accurately, although large difference between the theoretically predicted normal stress and FE simulated normal stress would be observed at the area very close to the edge due to the edge effect or singularity at the corner.

Based on the elastic solutions, the fracture ERR in the surface layer is calculated. It shows that the fracture ERR would increase rapidly as the crack spacing increases until a plateau stage is reached when the crack spacing approaches 4\( \text{mm} \). Therefore, under the temperature change of 40\(^\circ\text{C} \), the potential crack spacing is smaller than 4\( \text{mm} \). When the crack spacing is constant, the fracture ERR approximately increases linearly with the coating thickness until it reaches the convex point, at which the fracture saturation is reached. In this case (\( \Delta T = 40^\circ\text{C}, \lambda = 0.2\text{mm}, h_1 = 0.18\text{mm}, h_2 = 10\text{nm}, h_3 = 100\text{nm} \)), the critical coating thickness is 45\( \mu\text{m} \).

The fracture infilling and saturation are studied based on the calculated ERR and energy model. When the surface layer’s thickness remains constant, the temperature change required to form a new crack would increase as the crack spacing decreases and fracture saturation would be reached when the crack spacing approaches 0.4\( \text{mm} \). However, when the crack spacing is constant, the required temperature change to form a new crack would decrease as the surface layer’s thickness decreases, until a critical coating thickness is reached. Under this critical thickness the required temperature change would increase to be infinite which means the fracture saturation is obtained. For the crack spacing of 0.2\( \text{mm} \), the critical coating thickness is about 2\( \mu\text{m} \).

Overall, the presented model is able to capture the displacement and stress distributions in the multilayered structures accurately and predict the fracture initiation, infilling, and saturation of the surface layer successfully.
7.2.5 The Effect of Aging on the Delamination Fracture Energy of Glass Solar Reflectors

In Chapter 6, in order to investigate the bonding performance of the multilayered solar reflectors with different protective coating, namely alumina ($Al_2O_3$) coating and titania ($TiO_2$) coating, a width-tapered beam method is employed to measure the delamination fracture energy at the weakest interface. As for the original glass reflectors without any aging, the weakest interface would be the copper-glass interface. The measured delamination fracture energy of samples with $Al_2O_3$ protective coating is lower but more consistent compared with that of samples with $TiO_2$ protective coating. As the delaminated interface is the copper-glass interface which should not be affected by the type of protective coating significantly, therefore, we assume the DFEs for samples with both protective coating are coincident and an averaged DFE is obtained as $4.4306J/m^2$ to represent the delamination fracture energy of original samples.

Aimed to verify the test results, FE simulations are done using the CZM, in which the tested delamination fracture energy is treated as an input and the returned peeling force form simulations are compared with the test results. The good agreement between the FE simulation and test results indicates that the width-tapered beam method is accurate and can be applied to measure the delamination fracture energy of this multilayered glass solar reflector.

The effect of aging on the delamination fracture energy is investigated by measuring the change of delamination fracture energy in samples after 50 hrs of accelerated aging. The results show that, the delamination fracture energy of samples with $Al_2O_3$ protective coating would slightly decrease; however, this decrease is within the uncertainty of this measurement. Therefore, we simply conclude that the aging has minor effect on the delamination fracture energy of samples with $Al_2O_3$ samples. As for the samples with $TiO_2$ protective coating, the delamination fracture energy would decrease significantly after 50 hrs’ aging. This result denotes that $Al_2O_3$ coating would be a good protective coating to be used in the glass solar reflectors.
7.2.6 Accelerated Aging of Asphalt by UV Photo-oxidation Considering Moisture and Condensation Effects

A combined experimental and analytical approach is presented in Appendix A that investigates the aging behavior of asphalt binder under different aging conditions. Two different UV aging tests, the continuous UV aging test and the UV/moisture/condensation aging test, are conducted on four different asphalt binders to study the kinematics of asphalt UV photo-oxidation and the effect of condensation and moisture on UV photo-oxidation. Among the four different binders, three are extracted from RAP and one is extracted from fresh HMA. The aging cycle for the UV/moisture/condensation aging test were conducted based on ASTM D4799.

The WPO in asphalt binder samples after aging is measured using EDX. Test results for continuous UV are then fitted using the NDD model. The fitting results show that the continuous UV aging follows the NDD model very well with all the R square values being larger than 99%. Test results for UV/moisture/condensation are fitted using both the NDD model and the FRCR model. The fitting results show that, overall, both the FRCR model and the NDD model are able to predict the UV/moisture/condensation aging very well with the R square values larger than 95%. While the FRCR model provides slightly more accurate predictions for the transition and final part of the aging process. After the continuous aging and UV/moisture/condensation aging, it is found that the WPO in T-Fresh samples is the lowest among different binders while the P-RAP samples have the highest WPO. In addition, the WPO in T-RAP samples are lower than that in P-RAP samples but higher than that in S-RAP samples. In addition, the aging rates of T-FRESH in continuous UV aging is 1.32 times, 1.35 times, and 1.40 times larger than that of T-RAP, S-RAP and P-RAP respectively, while it is 1.42 times, 1.05 times, and 1.32 times larger than that of T-RAP, S-RAP, and P-RAP respectively in UV/moisture/condensation aging.

Additionally, the effects of condensation and moisture on UV aging are evaluated by comparing the change in the WPO caused by UV radiation during the continuous UV aging with that during the UV/moisture/condensation aging tests. It is found that the increase in the WPO caused by the UV radiation during the UV/moisture/condensation aging test is lower than that during the continuous UV aging test, which indicates that condensation and moisture effectively reduces the UV aging rate.
7.3 Future Work

The proposed 2D elastoplastic fracture model in Chapters 2 and 3 simplify the substrate as 1D, which would be fine for the case when the thickness of the coating is much smaller than that of the substrate. However, for the case when the coating thickness is comparable to that of the substrate, the effect of the coating on the substrate should be considered and the substrate cannot be simplified as a 1D bar. In this sense, we would like to extend the 2D fracture model proposed in this dissertation to be more general by considering the variance of stress across the thickness of the substrate and simulate the substrate as a 2D structure.

The 3D residual stress analysis in Chapter 4 and 5 consider the polymer substrate as elastic which is fine under lower temperature change. However, significant plastic deformation would be developed in the polymer layer when the temperature change is high. Based on this consideration, a 3D elastoplastic model is desired to predict the residual stress and cracking pattern more accurately.

In Chapter 6, the delamination fracture energy of glass solar reflector is tested using the width-tapered beam method. This tested fracture energy is pure mode I fracture energy. However, during the service period the thermal loading would introduce both normal and shear residual stress. Therefore, the delamination in glass solar reflectors should be a mixed-mode fracture behavior. Based on this consideration, the mixed-mode delamination fracture energy of this glass solar reflector would be measured and the aging effect would also be investigated.
Part I

Bibliography
Bibliography


Part II

Appendix
Accelerated Aging of Asphalt by UV Photo-oxidation Considering Moisture and Condensation Effects

In order to understand the long-term performance degradation of asphalt, ultraviolet (UV) photo-oxidation was used to accelerate the aging process. Three types of asphalt binders extracted from reclaimed asphalt pavements (RAPs) and one extracted from fresh Hot Mix Asphalt (HMA) were aged under continuous UV exposure and UV/moisture/condensation exposure. After accelerated aging tests, the weight percentage of oxygen (WPO) in all samples were measured using energy-dispersive X-ray (EDX) spectroscopy. The testing results indicate that the aging rates of the asphalt binder under both the UV and UV/moisture/condensation exposures are fast at the beginning and stabilize after a certain period of time. Experimental results were also modeled using two classic asphalt aging models, namely the fast-rate constant-rate (FRCR) model [103] and the nonlinear differential dynamic (NDD) model [120]. Although the NDD model exhibits acceptable agreement with the experimental results for both the UV aging and the UV/moisture/condensation aging samples, the FRCR model fits the UV/moisture/condensation aging better and thus is recommended for future UV/moisture/condensation aging performance prediction. Additionally, although exposed under UV for the same time, the WPO in samples after UV/moisture/condensation aging was lower than those in samples after continuous UV aging, indicating that condensation and moisture reduce the UV-induced photo-oxidative aging rate.
1 Overview

From a review of the literature, it was found that most relevant studies on the UV degradation of asphalt binder have mainly focused on new asphalt binders considering the effects of temperature, sample thickness, and UV radiation intensity. However, no relevant study has been conducted on the aging process of asphalt extracted from RAP and also considering the effects of condensation and moisture. Moreover, no UV irradiation has been applied in those studies in which mathematical aging models were used, and no quantitative analysis on the aging process has been conducted in those studies in which the UV degradation was involved. To fill this need, a quantitative analysis has been performed using two aging models to study the behavior of asphalt binder extract from RAP that have been exposed to different aging conditions. The objective of this study is utilizing an accurate asphalt aging model to explore the accelerated aging behavior of binder extracted from RAP. Using this type of model, the long-term aging behavior can be predicted by conducting a short-term accelerated aging test. The aging index used in this study is the WPO, which has a linear relationship with the carbonyl area \([30;126]\). Therefore, the FRCR and NDD models, which can be expressed in terms of the carbonyl area, are fit to the test data and used for further data analysis. By comparing the aging rate of asphalt binders under these two different aging conditions, the effects of condensation and moisture on UV aging are investigated for both the new asphalt binder and the binder samples extracted from RAPs.

2 Experiments

2.1 Sample Preparation

In this study, three different types of RAP and one freshly mixed HMA loose mix sample were collected from various sources throughout the State of New Jersey (NJ) and denoted as P-RAP, S-RAP, T-RAP, and T-FRESH depending on the sources from which they were obtained (P-RAP from Pierson, S-RAP from Stavola, T-RAP and T-FRESH from Tilcon).

The gradations for different RAPs are presented in Fig. 1, where the straight line is the maximum density line. T-Fresh is a fresh mix in which the fines are clumped together because of the existence of the binder, thus preventing sieve analysis from providing accurate results. For
Table 1: Binder content in RAP and fresh HMA mix samples

<table>
<thead>
<tr>
<th>Specimen</th>
<th>Asphalt Binder Content (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>P-RAP</td>
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</tr>
<tr>
<td>S-RAP</td>
<td>3.50</td>
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<tr>
<td>T-RAP</td>
<td>4.45</td>
</tr>
<tr>
<td>T-Fresh</td>
<td>4.17</td>
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</table>

AASHTO T319 Standard Method of Test for Quantitative Extraction and Recovery of Asphalt Binder from Asphalt Mixtures was followed to extract and recover binder samples from the collected RAP samples. n-propyl bromide was used as the solvent to extract the binder from the RAP samples.
samples. To prepare each asphalt binder sample for the aging test, a layer of masking tape was first applied to an aluminum plate while three 0.5” × 0.25” sections were left bare. A small amount of extracted and recovered asphalt binder was then attached to the bare sections and pressure was applied until a thickness of 0.025” was reached. Thereafter, the masking tape was removed and three 0.5” × 0.25” × 0.025” asphalt binder samples were obtained on each plate, which is shown in Fig. 2(a). Once the samples were trimmed, tape was reapplied around each sample to prevent the binder from running because of the elevated temperatures during aging. The prepared asphalt binder samples were then named based on the source from where they were extracted. For example, the P-RAP sample is the asphalt binder sample extracted from P-RAP and the T-FRESH sample is the one extracted from fresh HMA. Therefore, P-RAP, T-RAP, S-RAP, and T-FRESH presented in the following part represent asphalt binder samples extracted from different RAPs.

2.2 Aging Tests

The four different asphalt binder types were conditioned in a QUV accelerated weathering tester, which is shown in Fig. 2(b). The QUV tester reproduces the damage caused by sunlight, rain, and dew. In a few days or weeks, the QUV can reproduce the long-term outdoor degradation that occurs over months or years [7]. It tests materials by exposing them to alternating cycles of UV light and moisture at controlled, elevated temperatures. The effect of sunlight is simulated with fluorescent UV lamps (UVA 340 nm) whose spectral irradiance is in a close match to the
ultraviolet-A (UVA) portion of sunlight and gives an excellent simulation of sunlight in the critical short wavelength region from 365 nm down to the solar cut-off of 295 nm where most of the damage in durable materials occurs.

The two aging tests used in this study, a continuous UV aging test and a UV/moisture/condensation aging test, were performed using a QUV machine. The aging conditions are described in the following subsections. The cyclic exposure conditions for both test methods were based on ASTM D4799 Standard Practice for Accelerated Weathering Tests Conditions and Procedures for Bituminous Materials - Cycle D.

2.2.1 Continuous UV aging

Prepared samples were placed at the bottom of the QUV machine under continuous UV with a radiation intensity of 0.89 $W/m^2 \cdot nm$ and a temperature of 113 °F (45 °C) as shown in Fig. 2(b). In order to study the effects of UV radiation only, the water spray and condensation steps were omitted. Additionally, the temperature was lowered to 45 °C because Zeng et al. [228] have reported that the influence of temperature can be ignored below 50 °C and also because 45 °C is the minimum temperature that the QUV can maintain during UV exposure. The sample conditions were interrupted at 10, 30, 50, and 100 hours of UV exposure so that one sample for each type of asphalt binder could be taken out for analysis.

2.2.2 UV/moisture/condensation aging

In the tests, fourteen samples of each of the four different types of asphalt binders were placed at the bottom of the QUV machine and exposed to the following conditions:

- 4 hours of UV at 45 °C with a radiation intensity of 0.89 $W/m^2 \cdot nm$.
- 15 minutes of water spray.
- 3 hours and 45 minutes of condensation at 40 °C.

One sample of each type of asphalt binder was removed for further analysis at the following number of cycles: 1, 2, 3, 4, 5, 6, 7, 9, 11, 13, 15, 18, 21, and 25.
2.3 Aging Index Evaluation

It is noted that most studies on asphalt aging are based on the measurement of the carbonyl area using Fourier Transform Infrared Spectroscopy (FTIR) \([103; 125; 216]\). However, mixtures of multiple materials tend to confuse the library search function in FTIR due to the complexity of overlapping spectral fingerprints. Thus, FTIR works well only when the sample matrix is either homogeneous or composed of only a few materials. For this reason, alternative methods such as Energy-dispersive X-ray (EDX) have been explored to investigate the material degradation. EDX is an analytical technique used for the elemental analysis or chemical characterization of a sample, which uses the X-ray spectrum emitted by a solid sample that has been bombarded with a focused beam of electrons to obtain a localized elemental or chemical analysis \([75]\). Compared with FTIR, EDX can determine the element types and concentrations in both homogeneous and composite materials. Thus, it has been widely used to quantitatively characterize the degradation process of polymer or rubber materials \([47; 111; 133]\), the level of mixing between the aged and virgin binder by tracking the blending \([117; 174]\), the micro-structure of porous asphalt \([163]\), the adhesion between aggregates and bitumen \([46; 85]\), and the effect of mica and aging on asphalt binder \([194]\). In this study, the WPO measured by EDX, is going to be used to calculate the aging index of the asphalt binder in this study.

The FRCR model is usually expressed in terms of carbonyl area. In order to employ this model to predict the aging behavior, a relationship between carbonyl area and WPO is required. According to current findings \([30; 126]\), there is a relationship between the carbonyl area and WPO. Using Attenuated Total Reflection Fourier Transform Infrared Spectroscopy (ATR FTIR), Liu et al. \([126]\) found that the carbonyl area measured in the infrared spectrum as the absorbance peak area above the range of 1650 to 1820/cm is linearly related to the amount of oxygen which has reacted with asphalt. Also, Boysen and Schabron \([30]\) demonstrated that both the WPO and the carbonyl area can be related to the asphaltene determinator aging index ratio at 500 nm (500nm Asphaltene Determinator Aging Index Ratios (ADAIR)) as

\[
CA(t) = 0.01257O(t) + 0.000446
\]

(1)

where \(CA(t)\) is the carbonyl area and \(O(t)\) is the WPO at time \(t\). Therefore, by considering the
linear relationship between the carbonyl area and WPO, the latter is used as an appropriate aging index to characterize the asphalt aging process in this study.

After the accelerated aging tests, the WPO in the aged asphalt binders was measured through EDX using a scanning electron microscope. Although EDX is surface-sensitive (the testing field is about 1 2 micrometers in depth), it can still be used to test the aging process as most of the oxidation reaction occurs at the surface of asphalt binder and the WPO in this area can be used to quantify the aging effect. Because asphalt binders are non-conductive, all the aged samples were first coated using a sputter coater before the EDX analysis was performed. With a coating time of 20 seconds, a uniform 10 nm layer of gold/palladium is obtained on the surface. Through the EDX analysis, it was found that the primary elements in the samples were oxygen, sulfur and carbon. Certain amounts of gold and palladium are present as well because of the coating, while nitrogen was found in smaller quantities.

3 Test Results and Data Analysis

3.1 EDX Test Results

3.1.1 Continuous UV aging

The EDX test results show that the WPO in the same asphalt binder sample after continuous UV aging varies from location to location due to the testing area of one EDX shot being quite small (about 1 micrometer across). Therefore, an averaged WPO of four to six random points on the sample surface is used as the overall WPO in all subsequent analyses.

The EDX test results for different types of asphalt binder samples corresponding to different amounts of continuous UV aging and the coefficient of variation (COV) are summarized in Table 2 to Table 5. The results clearly show that the WPO in aged asphalt increases quickly at the beginning at a rate that decreases significantly after about 30 hours, which is consistent with the overall trend of both the FRCR model and the NDD model.
<table>
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<th>30</th>
<th>50</th>
<th>100</th>
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<tbody>
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<td>WPO (%)</td>
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<td></td>
<td></td>
<td></td>
<td></td>
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Table 2: WPO in T-RAP after continuous UV aging

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Table 3: WPO in S-RAP after continuous UV aging
### Table 4: WPO in P-RAP after continuous UV aging

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### Table 5: WPO in T-Fresh after continuous UV aging

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Table 6: WPO in P-RAP after UV/moisture/condensation aging

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</tr>
<tr>
<td>Ave. (%)</td>
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<tr>
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Table 7: WPO in S-RAP after UV/moisture/condensation aging

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<td>2.1</td>
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</table>

3.1.2 UV/moisture/condensation aging

Similar to that in the binder samples after continuous UV aging, the WPO in each sample after UV/moisture/condensation aging also varies from location to location. The average value of the test results from four different locations for each sample is used as the WPO. The EDX test results for UV/moisture/condensation aging are included in Table 6 to Table 9.

3.2 Aging Models

The FRCR and NDD models used to conduct the data analysis in this study are presented in this section.

Table 8: WPO in T-RAP after UV/moisture/condensation aging

<table>
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<tr>
<th>Cycle Number</th>
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<tr>
<td></td>
<td>4.0</td>
<td>7.3</td>
<td>8.4</td>
<td>9.4</td>
<td>9.9</td>
<td>9.4</td>
<td>10.5</td>
<td>10.9</td>
<td>10.8</td>
<td>10.6</td>
<td>11.0</td>
<td>11.4</td>
<td>12.1</td>
<td>12.53</td>
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<tr>
<td></td>
<td>4.0</td>
<td>7.7</td>
<td>8.3</td>
<td>9.1</td>
<td>9.2</td>
<td>10.2</td>
<td>10.3</td>
<td>10.4</td>
<td>10.7</td>
<td>10.9</td>
<td>10.8</td>
<td>11.1</td>
<td>12.4</td>
<td>12.54</td>
</tr>
<tr>
<td>WPO (%)</td>
<td>4.2</td>
<td>7.2</td>
<td>8.3</td>
<td>9.3</td>
<td>10.3</td>
<td>10.4</td>
<td>10.2</td>
<td>10.6</td>
<td>11.2</td>
<td>11.7</td>
<td>12.0</td>
<td>11.5</td>
<td>12.53</td>
<td></td>
</tr>
<tr>
<td>Ave. (%)</td>
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<td>7.5</td>
<td>8.3</td>
<td>9.3</td>
<td>10.6</td>
<td>10.7</td>
<td>11.0</td>
<td>10.9</td>
<td>11.3</td>
<td>11.1</td>
<td>11.1</td>
<td>11.9</td>
<td>12.53</td>
<td></td>
</tr>
<tr>
<td>COV (%)</td>
<td>3.4</td>
<td>3.2</td>
<td>0.6</td>
<td>1.3</td>
<td>5.6</td>
<td>5.4</td>
<td>1.6</td>
<td>3.9</td>
<td>1.1</td>
<td>2.9</td>
<td>3.6</td>
<td>3.8</td>
<td>3.2</td>
<td>0.12</td>
</tr>
</tbody>
</table>

Table 9: WPO in T-Fresh after UV/moisture/condensation aging

### 3.2.1 FRCR model

Jin [102] proposed an asphalt oxidation kinematics model in terms of carbonyl formation, as shown in Eq. (2) to Eq. (5).

\[
CA = CA_{tank} + M(1 - e^{-k_ft}) + k_ct \tag{2}
\]

where

\[
k_f = A_f e^{-E_a f / RT} \tag{3}
\]

\[
k_c = A_c e^{-E_a c / RT} \tag{4}
\]

\[
M = CA_0 - CA_{tank} \tag{5}
\]

and \(CA_{tank}\) is the carbonyl area of the un-aged tank asphalt, \(CA_0\) is the intercept of the constant-rate line, \(k_f\) and \(k_c\) are two reaction constants that are temperature dependent according to Eqs. (3) and (4). \(M\) is a constant that depends on both the source of the asphalt and the oxygen partial pressure. \(A_f\) and \(A_c\) are pre-exponential factors for \(k_c\) and \(k_f\), \(E_a f\) and \(E_a c\) are the apparent activation energies for \(k_f\) and \(k_c\), \(R\) is the gas constant \((8.314 \text{ J/(mol} \cdot \text{K})\), and \(T\) is the absolute temperature \((K)\).

Recall that there is a linear relationship exists between carbonyl area and WPO; therefore, Eq. (6) is proposed to have a similar correlation between the carbonyl area and the WPO as that in Eq. (2):

\[
CA(t) = aO(t) + b \tag{6}
\]

where \(a\) and \(b\) are constants which correlate with the type of binder and \(O(t)\) is the WPO in the aged asphalt.
By substituting Eqs. \((3)\) to \((6)\) into Eq. \((2)\), the FRCR model proposed by Jin [102] is rewritten in terms of WPO as:

\[
a \times O(t) = a \times O(t)_{\text{tank}} + [O(t)_0 - a \times O(t)_{\text{tank}} - b](1 - e^{-\frac{A_f e^{-E_{af}/RT}}{t}}) + A_ce^{-\frac{E_{ac}/RT}{t}}
\]  

\[(7)\]

3.2.2 NDD model

According to the study in [120], the NDD model can be written as:

\[
x(t) = \frac{Lx_0}{[1 + (L - 1)e^{-rt}]}
\]

where \(x(t)\) is the property of asphalt binder at time \(t\) while \(x_0\) is the value of \(x(t)\) when \(t\) is equal to zero. The parameter \(r\) is the aging rate and \(L\) is the ratio between the maximum and the initial values of \(x\). In other words, \(L\) is a measurement of the maximum increase in \(x\) (this is demonstrated by substituting \(t = \infty\) in the equation). These two parameters can be used to compare both the magnitude and the rate of aging for different types of asphalt binder.

4 Data Analysis

4.1 Continuous UV Aging

For the FRCR model shown in Eq. \((7)\), there are seven parameters that need to be determined using nonlinear curve fitting; however, only five different aging times were applied in this continuous UV aging test. Therefore, the test results from the continuous UV aging cannot be fitted by the FRCR model, but can be fitted by the NDD model, where only two parameters need to be determined through curve fitting.

Fig. 3 plots the test data of all types of asphalt samples with error bars and the fitted curves using the NDD model. The error bars indicate the variance of WPO between different locations in same asphalt sample. The determined constants \(L\) and \(r\) are summarized in Table 10. The \(R^2\) for all of the four types of asphalt binder are larger than 99%, which indicates that the continuous UV aging follows the prediction of the NND model with very little deviation. Meanwhile, the value of the aging rate, \(r\), for T-FRESH is higher than that of the RAP binders, which denotes that the aging rate of T-FRESH is faster than that of the RAP binder during the continuous UV aging
Figure 3: EDX test results and fitted curves using NDD model for all asphalt binder types after continuous UV aging with error bars.

<table>
<thead>
<tr>
<th>Binder Type</th>
<th>$L$</th>
<th>$r (day^{-1})$</th>
<th>$R^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>P-RAP</td>
<td>3.503</td>
<td>2.598</td>
<td>0.99</td>
</tr>
<tr>
<td>S-RAP</td>
<td>3.323</td>
<td>2.706</td>
<td>0.99</td>
</tr>
<tr>
<td>T-FRESH</td>
<td>3.458</td>
<td>3.655</td>
<td>0.99</td>
</tr>
<tr>
<td>T-RAP</td>
<td>3.308</td>
<td>2.767</td>
<td>0.99</td>
</tr>
</tbody>
</table>

Table 10: Determined parameters for the NDD model (continuous UV aging)

process (The aging rate of T-FRESH samples during continuous aging is 1.32 times, 1.35 times, and 1.40 times larger than that of T-RAP, S-RAP, and P-RAP, respectively). It is also seen from Fig. 3 that the T-FRESH samples have the lowest final WPO, while the P-RAP samples have the highest final WPO, the WPO in the T-RAP samples are lower than that in P-RAP samples but higher than the S-RAP samples.

4.2 UV/moisture/condensation Aging

Fig. 4 shows the EDX test results for all four types of asphalt binder samples and the fitted results using the NDD and FRCR models. It is seen from Fig. 4 that the T-FRESH samples have the
lowest WPO while the P-RAP have highest WPO, which is consistent with the result shown in Fig. 3 for the continuous UV aging.

Table 11 summarizes the curve fitting parameters for both the NDD and FRCR models and shows that both the NDD and the FRCR aging models can predict the UV/moisture/condensation aging very well, which is demonstrated by the high $R^2$ square value (>95%). By comparing the values of the aging rate $r$ between Tables 10 and 11, the value of $r$ for each type of asphalt binder in Table 11 is much smaller than the corresponding value in Table 10. Recall that $r$ is a measurement of the rate of increase in WPO; thus, the UV/moisture/condensation aging is much slower than the continuous UV aging (the aging rate in the UV/moisture/condensation aging is only 0.58 times of that in the continuous UV aging for S-RAP, 0.42 for T-RAP, 0.48 for P-RAP, and 0.45 for T-FRESH). Additionally, similar to the continuous UV results shown in Table 10, the value of $r$ for T-FRESH is largest in Table 11. Therefore, the T-FRESH sample also has the fastest aging rate during the UV/moisture/condensation aging test, which is 1.42 times, 1.05 times, and 1.32 times larger than that of T-RAP, S-RAP, and P-RAP, respectively.

Using the results shown in Table 11, both the fast-rate activation energy and the constant-rate activation energy of P-RAP are the largest among the different binders which means that the P-RAP has the slowest aging rate [102]. This is consistent with the fitting results from the continuous UV aging as shown in Table 10 (the value of $r$ for P-RAP is lowest). However, for
the UV/moisture/condensation aging, the aging rate of P-RAP is greater than that of T-RAP (as the value of \( r \) for P-RAP is larger than that for T-RAP in Table 11). This error may result from the poor fitting of the NDD model to the UV/moisture/condensation aging results. Also shown in Table 11, the fast-rate activation energy of T-FRESH is the smallest, which indicates that the aging rate of T-FRESH during the fast-rate aging period is the fastest, whereas the constant-rate activation energy of T-FRESH is larger than those of S-RAP and T-RAP. This indicates that the faster aging rate of T-FRESH is mainly caused by the high aging rate during the fast-rate aging period.

In order to investigate which classic aging model can better predict the aging under UV/moisture/condensation, Fig. 5 compares the fitted results of the two aging models for each type of asphalt binder. It shows that both the NDD and FRCR models are able to capture the aging process very well as the \( R^2 \) for all types of binder samples are greater than or equal to 95% as shown in Table 11. During the initial aging period both models are in close agreement with the data. However, as the initial fast-rate aging transitions to the later constant-rate aging, the NDD model increases at a high rate and overestimates the WPO. After about 8 cycles, the NDD model begins to level off and underestimates the WPO while the FRCR model continues to rise with the EDX results. In this

<table>
<thead>
<tr>
<th>Binder Type</th>
<th>S-RAP</th>
<th>T-RAP</th>
<th>P-RAP</th>
<th>T-FRESH</th>
</tr>
</thead>
<tbody>
<tr>
<td>NDD Model</td>
<td>( L )</td>
<td>3.041</td>
<td>3.112</td>
<td>3.139</td>
</tr>
<tr>
<td>Fitting</td>
<td>( r(\text{days}^{-1}) )</td>
<td>1.567</td>
<td>1.163</td>
<td>1.254</td>
</tr>
<tr>
<td></td>
<td>( R^2 )</td>
<td>0.97</td>
<td>0.96</td>
<td>0.96</td>
</tr>
<tr>
<td>FRCR Model</td>
<td>( a )</td>
<td>0.04431</td>
<td>0.03718</td>
<td>0.04932</td>
</tr>
<tr>
<td>Fitting</td>
<td>( b )</td>
<td>0.0007783</td>
<td>0.0005748</td>
<td>0.0009133</td>
</tr>
<tr>
<td></td>
<td>( A_e(\text{days}^{-1}) )</td>
<td>( 1.005 \times 10^8 )</td>
<td>( 1.454 \times 10^8 )</td>
<td>( 1.066 \times 10^8 )</td>
</tr>
<tr>
<td></td>
<td>( A_f(\text{days}^{-1}) )</td>
<td>( 1.801 \times 10^8 )</td>
<td>( 1.5 \times 10^8 )</td>
<td>( 1.506 \times 10^8 )</td>
</tr>
<tr>
<td></td>
<td>( E_{ac}(\text{J/mol}) )</td>
<td>( 6.012 \times 10^4 )</td>
<td>( 6.091 \times 10^4 )</td>
<td>( 8.929 \times 10^4 )</td>
</tr>
<tr>
<td></td>
<td>( E_{cc}(\text{J/mol}) )</td>
<td>( 4.962 \times 10^4 )</td>
<td>( 5.014 \times 10^4 )</td>
<td>( 5.035 \times 10^4 )</td>
</tr>
<tr>
<td></td>
<td>( O(t)_0 )</td>
<td>0.5201</td>
<td>0.4689</td>
<td>0.7722</td>
</tr>
<tr>
<td></td>
<td>( R^2 )</td>
<td>0.98</td>
<td>0.98</td>
<td>0.97</td>
</tr>
</tbody>
</table>

Table 11: Fitted parameters of UV/moisture/condensation aging test
Figure 5: Comparison between NDD model fitting and FRCR model fitting for UV/moisture/condensation aging
respect, the NDD model can only be used to simulate the short-term UV/moisture/condensation aging process, while the FRCR model can capture the entire UV/moisture/condensation aging process.

4.3 Effect of Condensation and Moisture on UV Photo-oxidative Aging

The effect of moisture and condensation on UV aging can be evaluated by comparing the increase in the WPO caused by UV radiation during the continuous UV aging tests with that in the UV/moisture/condensation aging tests. In the continuous UV aging test, only UV was used to condition the asphalt binder. However, for the UV/moisture/condensation aging test, continuous UV was only applied for the first 4 hours of the aging cycle that lasted for 8 hours, and then moisture was introduced by 15 minutes of water spray, which was followed by a condensation period that lasted 3 hours and 45 minutes. Therefore, the WPO caused by UV radiation during UV/moisture/condensation aging needs to be determined first. An extreme case will be considered by assuming that the asphalt binder samples were only aged during the UV radiation period. Based on this assumption, the data shown in Table 6 to Table 9 are the aging results of the UV radiation only and the effective aging time should be half of the total aging time.

Fig. 6 presents the WPO in the asphalt samples after both the continuous UV aging tests (fitted using the NDD model) and the UV/moisture/condensation aging tests (fitted using the FRCR model) as a function of the effective aging time (equal to the elapsed time for continuous UV and half of the elapsed time for UV/moisture/condensation). It clearly shows that under the same UV radiation, the WPO in asphalt binders after the continuous UV aging is larger than that in binders after the UV/moisture/condensation aging for all types of binder samples. In reality, the condensation and moisture during the second half of a UV/moisture/condensation aging cycle could also cause the increase in the WPO. Therefore, the increase in the WPO that results from only the UV radiation in the UV/moisture/condensation tests should be smaller than that used in Fig. 6 indicating that the condensation and moisture in the UV/moisture/condensation aging tests actually decreases the UV aging rate. One possible explanation is that the water vapor formed in the QUV during the condensation step remains during a portion of the UV step. This water vapor then absorbs some of the UV radiation, effectively reducing the intensity of the UV radiation incident on the surface of the asphalt binder. Based on Wu et al. [216], the UV degradation rate
Figure 6: Comparison of UV aging in continuous UV aging and UV/moisture/condensation aging test
decreases as the intensity of UV radiation reduces.

5 Discussion and Conclusions

This study presents a combined experimental and analytical approach to investigate the aging behavior of RAP binder under different aging conditions and compare this behavior with that of virgin asphalt. Two different UV aging tests, the continuous UV aging test and the UV/moisture/condensation aging test, were conducted on four different asphalt binders to study the kinematics of asphalt UV photo-oxidation and the effect of condensation and moisture on UV photo-oxidation. Among the four different binders, three were extracted from RAP and one was extracted from fresh HMA. The aging cycle for the UV/moisture/condensation aging test was conducted based on ASTM D4799.

The WPO in the asphalt binder samples after aging was measured using EDX. Test results for samples after continuous UV aging were then fitted using the NDD model. The fitting results show that the continuous UV aging follows the NDD model very well with all the $R^2$ being larger than 99%. Test results for samples after UV/moisture/condensation aging were fitted using both the NDD model and the FRCR model. The fitting results show that, overall, both the FRCR model and the NDD model are able to predict the UV/moisture/condensation aging very well with the $R^2$ larger than 95%, although the FRCR model seems to provide slightly more accurate predictions for the transition and final part of the aging process. After the continuous aging and UV/moisture/condensation aging, it was found that the WPO in T-Fresh samples is the lowest among different binders, while the P-RAP samples have the highest WPO, the WPO in the T-RAP samples is lower than that in P-RAP samples but higher than that in S-RAP samples. In addition, the aging rates of T-FRESH in the continuous UV aging is 1.32 times, 1.35 times, and 1.40 times of those in T-RAP, S-RAP and P-RAP respectively, while it is 1.42 times, 1.05 times, and 1.32 times of those in T-RAP, S-RAP, and P-RAP respectively in the UV/moisture/condensation aging.

Additionally, the effects of condensation and moisture on UV aging were evaluated by comparing the change in the WPO caused by UV radiation during the continuous UV aging with that during the UV/moisture/condensation aging tests. The test results show that the increase in the WPO caused by the UV radiation during the UV/moisture/condensation aging was lower than that during
the continuous UV aging, which indicates that condensation and moisture effectively reduces the UV aging rate.

Note that the chemical properties of different binders might slightly change after various aging conditions. In this sense, tracing the change of chemical and mechanical behaviors of the asphalt samples in the course of the aging process would help better understand the aging behavior of asphalt binder. Such information would require a multidisciplinary team to work together for a longer period. Due to the limited amount of aged material and research funding period, these tests and information are not currently included. However, the current exploratory study has provided us very encouraging results, which may stimulate a new research area in our research community to comprehensively understand the complex aging behavior of asphalt binder through chemical and mechanical characterization.