Deformation, failure and removal mechanisms of thin film structures in abrasive machining

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Abstract Thin film structures are becoming increasingly more important for industrial applications such as the making of solar panels, microelectronic devices and micro systems. However, the challenges encountered in the machining of thin film structures have been a bottleneck that impedes further wide spread uses of such structures. The development of material removal processes that are capable of producing a damage free surface at high removal rates is critical for cost effective production. Such development relies highly on a comprehensive understanding of the deformation, failure and removal mechanisms of thin film structures involved in mechanical loading. In this paper, the current understanding of the deformation characteristics of thin film systems was reviewed to provide important insights into the interfacial failure under mechanical loading, with focuses on the interfacial failure mechanisms and existing problems in the machining of thin film structures. The key characterization techniques were outlined. In particular, the recent progress in the abrasive machining of a thin film multilayer structure was summarized. The potential research directions were also presented in the end of the review.

Keywords Abrasive machining · Thin film · Bilayer · Multilayer · Interface · Deformation · Failure

1 Introduction

Owing to the rapid development in nanotechnology and nanoscience, various nanomaterials or nano/micro-structured materials have been developed in the past two decades [1]. Among them, thin film materials have played a significant role in the development of nano-/micro-electronic devices. Thin films usually refer to a layer of material with thicknesses ranging from several nanometers to several micrometers [2]. Till now, different types of structures of dissimilar thin film materials, such as metal/ceramic, polymer/metal and ceramic/polymer have been fabricated for various purposes [3–10]. Those thin film materials or structures provide distinct advantages over conventional bulk counterparts in terms of cost efficiency, long lifespan, environmental friendliness and enhanced thickness-dependent properties [11, 12].

In the production of thin film based devices, for example, thin film solar panels, the side surfaces of the thin film structure must be machined before assembly. The manufacture of the side surfaces of a thin film structure is usually via abrasive machining. However, abrasive machining of such a thin film multilayer is very challenging, as ultrathin layers with very differing material properties need to be removed at the same time. Burrs on soft layers, chippings on brittle layers and delamination at interfaces often occur under mechanical loading. Such surface damages and structure failure will have significant negative effects on the connection between two thin film modules and eventually affect the performance of the devices [13, 14]. From the industrial point of view, machining efficiency is also required. Therefore, a practical high-quality machining process with a satisfactory removal rate for this special structure needs to be developed. To reduce or avoid surface damages in the process of machining, a comprehensive
understanding of the material removal and structure failure mechanisms is essential.

An in-depth investigation of deformation and structure failure mechanisms of thin film materials involved in a practical abrasive machining process is extremely difficult as the process is complex concerning a lot of uncertain effects from tooling and machining conditions. As a consequence, diverse characterization techniques for the quantifying of structure failure of thin film structures were developed, such as the tape peel test [15, 16], the pull-off test [17], and the three/four-point bending test [18], just to name a few. Nevertheless, as the sample requirements and testing environments differ greatly, the results from different testing approaches might be inconsistent.

Nanoindentation and nanoscratch have been widely used to characterize the mechanical properties of homogeneous materials at small scales, as well as the thin film adhesion [19–21]. They have shown great advantages in studying abrasive machining as penetration, and scratching processes are analogous to individual interaction between an abrasive grit and a workpiece. Also, the precision control of mechanical load and deformation magnitude in such simulated tests enables us to isolate the effects of key parameters, such as grit penetration depth and strain rate [22, 23]. The outcomes from such studies can thus provide important insights into the mechanisms of thin film deformation under mechanical loading [24, 25].

The structure failure of thin film system has been extensively investigated in the past two decades. Delamination at interfaces is a common failure mode during machining of thin film structures [13, 14, 26]. Nevertheless, some fundamental issues still remain unclear. For instance, the underlying mechanisms that induce interfacial failure are not well understood. The stress built-up at the interfaces between two thin film layers is believed to be responsible for interfacial delamination [27], but the effect of stress evolution during abrasive machining needs further investigation. Finite element method (FEM) has been a valuable tool for evaluating stress development and distribution in bulk materials [28–31]. This method is of particular value for analyzing interfacial delamination as the insights into stress distribution at the interfaces would provide a straightforward approach to revealing the underlying failure mechanisms of thin film systems involved in abrasive machining [26, 32]. Furthermore, FEM offers opportunities for parametrically investigating the effects of machining conditions on structural failure. Attempts to numerical investigation of the structure failure during nanoindentation and nanoscratch processes have been made in thin film systems over the years and will be critically reviewed in this paper.

This paper first summarized the main structural failure modes of thin film structures under mechanical loading and discussed the critical issues involved in the characterization. An overview on the deformation mechanisms studied using nanoindentation and nanoscratch techniques was then presented. Further, recent studies on abrasive machining of a typical thin film multilayer structure were comprehensively reviewed. Suggestions on research directions in the future were provided in the end.

2 Deformation and failure of thin film structures under mechanical loading

2.1 Structural failure modes

The machining induced structure failure has become the main impediment of the wider application of thin film structures. In the past few decades, the mechanisms that control the structure failure of thin film systems have attracted great research interests. Many researches have been conducted to determine the mechanical behaviors of thin film structures under mechanical loading. Evans et al. [33] described the effects of material properties, layer thickness and yield strength on the cracking and decohesion of thin films. The typical failure modes for thin films on substrates governed by residual stress state and bonding strength were summarized in Table 1. It is obvious that three types of failure modes are commonly seen in the thin film structure: (i) films subject to residual compression are susceptible to buckling and spalling, where delamination would initiate at the interface; (ii) brittle films under residual tensile stress are liable to form cracks inside the layer; (iii) for ductile films subject to residual tension, film decohesion is usually triggered by substrate cracking that propagates to interfaces. The schematic illustrations of the three types of failure are shown in Fig. 1.

Apparently, the surface quality of the thin film structure is not only determined by the properties of individual layers, but also the “weak link” of the structure, which is normally the interface between two bonded thin film layers. It is obvious that the interfacial integrity is a key concern for improving the reliability of thin film structures. Therefore, understanding interfacial failure mechanisms is imperative.

2.2 Deformation and failure induced by nanoindentation

Nanoindentation is the most commonly used technique to measure highly localized mechanical properties of a material [34]. It involves impressing a sharp diamond tip into the surface of the sample being tested, while continuously measuring the imposed force and corresponding indentation depth. The load-displacement (P–h) curve obtained from nanoindentation can quickly provide insights into the
mechanical behavior. Using the Oliver-Pharr method [35], both hardness and elastic modulus of the specimen can be extracted from the $P-h$ curve [36]. Owing to its shallow indentation depth, which is as small as a few nanometers, this technique is also recognized as a nondestructive property testing method [37]. Nanoindentation is also a versatile tool for studying the interfacial strength of thin film structures [27, 38–40]. In comparison with other testing methods, nanoindentation can induce interfacial failure in a controlled manner [20]. However, interfacial toughness cannot be determined as easily as the hardness and elastic modulus because the failure behaviors depend on the indenter and specimen geometries, indentation load and depth, as well as the mechanical properties of both film and substrate. Failure may occur on the thin film systems during either loading or unloading [41]. The deformation and structure failure of thin film systems induced by nanoindentation will be summarized in terms of typical failure modes below.

### 2.2.1 Delamination initiated at interface

In a film/substrate system, the bonding strength between film and substrate contributes significantly to the occurrence of interfacial delamination and may cause various types of failure at the film/substrate interface. The failure mechanisms in a hard coating on a soft substrate were explained by Chen and Bull [40]. In the case of a thin film well bonded to a substrate shown in Fig. 2, the bilayer structure remained intact during indenting. Tension at the interface was generated when the tip was withdrawn from the substrate. Once the interfacial tensile stress exceeded the threshold value, the hard coating would be torn apart from the substrate, as can be seen in Fig. 2b.

If the bonding between a hard film and a substrate is poor, the mechanism of the interfacial failure is somehow different. In this case, with the indenter penetrated deeper, the film deflected into the plastically deformed impression on the substrate. At this point, high bending stress was

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Table 1: Modes of thin film decohesion [33]

| Residual stress | Film/substrate      | Interface bonding | Decohesion mechanisms                  |
|----------------|---------------------|-------------------|----------------------------------------|
| Tensile        | Brittle/ductile     | Good              | Film cracking (no decohesion)          |
|                | Poor                |                   | Film cracking (interface decohesion)    |
| Ductile/brittle| Good                |                   | Edge decohesion at interface           |
|                | Poor                |                   | Film/substrate splitting (substrate decohesion) |
| Ductile/ductile| Poor                |                   | Film cracking (interface decohesion)    |
| Brittle/brittle| Good                |                   | Edge decohesion at interface           |
|                | Poor                |                   | Film cracking (interface decohesion)    |
| Compressive    | Brittle/ductile     | Good              | Buckle propagation in film              |
|                | Poor                |                   | Buckle propagation at interface        |
| Ductile/brittle| Good                |                   | Substrate splitting                    |
|                | Poor                |                   | Buckle propagation at interface        |
| Ductile/ductile| Good                |                   | No decohesion                          |
|                | Poor                |                   | Buckle propagation at interface        |

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Fig. 1 Schematics of typical failure modes in a bi-layer thin film structure [41]

Fig. 2 Interfacial status of a bi-layer structure with strong adhesion during indentation [40]
generated at the contact edges, driving the thin film detach from the substrate. When the interfacial crack length reached its critical buckling length, double buckling could be formed during indentation [42]. After the indenter withdrew, the interfacial cracks would propagate toward the middle of the indent as the thin film was no longer under constraint. Therefore, the double buckling failure outside the contact area could be developed into single buckling upon tip removal [40]. Figure 3 schematically shows the rebound of the debonded thin film with poor adhesion during unloading.

It is apparent that for a bilayer structure, in which the thin film possesses higher yield stress, the softer substrate is likely to yield first during indenting and deform plastically, while elastic deformation is still predominant in thin films [40, 43, 44]. As a consequence, the mismatch in elastic recoveries during unloading would build up interfacial stresses and hence significantly influence the deformation characteristics. Lu et al. [27] comprehensively investigated the deformation behavior of a bilayer structure with SiN thin film was coated on GaAs substrate using nanoindentation. Both pop-in and pop-out events were observed from the $P-h$ curve when the normal load applied was sufficiently high, as shown in Fig. 4 [27]. The pop-in event was attributed to the plane slip occurred in the GaAs substrate, and the appearance of the pop-out was identified as a sign of interfacial delamination during tip withdrawal.

The characterization of interfacial failure was also carried out via FEM simulation [27]. FEM was used in this study to investigate the underlying mechanisms of thin film deformation and decohesion by analyzing the stress distribution and evolution during indenting [27]. The tangential and normal responses were achieved using a coupled constitutive law and the delamination occurrence at the weakest link of the structure was realized through embedding cohesive zone elements into the model. The results demonstrated that mechanical load induced tensile stress was the main contributor to interfacial delamination. The residual stress at the interface was likely to alter the energy release rate during delamination and consequently affect the mechanical response of thin film layers.

Interfacial failure could occur at both loading and unloading stages with different delamination types [27, 45, 46]. Different crack initiation modes were observed in the model and analyzed using the linear elastic fracture mechanics (LEFM), as shown in Fig. 5 [47]. A tangential or sliding mode crack, as shown in Fig. 5a, in which the relative movement of the film was in parallel to the substrate surface, was likely to be generated during indenting. At this mode, the crack was found to be initiated at a radial distance of 2–3 times of the contact radius. Shear stress attained at the interface was believed to attribute to this type of failure. During unloading, tensile stress was built up significantly underneath the contact region and tended to lift the film from the substrate. Once the stress exceeded the interfacial bonding strength, delamination was triggered and left an opening mode crack at the interface, as shown in Fig. 5b. Figure 6 shows the results from an FEM study, demonstrating that tensile stress was built up during unloading of indentation and the delamination was thus induced [27]. Abdul-Baqi A and

![Fig. 3](image-url) Interfacial status of a bi-layer structure with poor adhesion during indentation [40]

![Fig. 4](image-url) Schematic illustration of indentation induced interfacial failure: a slip bands occurred in GaAs substrate during loading and formed a pop-in event in the $P-h$ curve; b tension was built up between SiN film and GaAs substrate at the unloading stage and c the pop-out event in $P-h$ curve reflected the occurrence of delamination at the interface [27]
Van der Giessen E [48] also carried out an FEM study and emphasized that tangential cracks were normally formed earlier and easier than normal cracks. In turn, if the interfacial strength was sufficiently high to prevent tensile cracks, tangential delamination would be possibly avoided. The sample used in the study was a bilayer structure and the material properties of the film were assumed to be linear elastic. Cracking inside the layer was not taken into account.

### 2.2.2 Through-thickness cracking

Apart from the interfacial cracks occurring, through thickness fracture or cracking inside a thin film layer is another type of failure that may occur during indenting. Such failure might be caused if a brittle thin film layer was bent into the plastically impressed substrate or the piling-up of substrate material around the indenting area [49]. In fact, for most brittle thin films under mechanical loading, through-thickness cracks are formed in conjunction with interfacial failure. The mechanisms of the failure are very complex and have been extensively studied [46, 49–51]. Li et al. [51] established a simplified three-stage fracture mechanism through performing nanoindentation on a bilayer structure, which consisted of a silicon substrate and a hard coating of amorphous carbon, as shown in Fig. 7. In their test, a ring-shape through-thickness crack was first formed in the hard coating due to the layer toughness being insufficient to withstand the high stress formed at the contact edge. With the progress of indentation, a second ring-like through-thickness crack was formed, in the periphery of which delamination and buckling could be found. The occurrence of delamination was coincident with the discontinuities in the $P$-$h$ curves obtained from indentation. In the final stage of indentation, chipping and partial spalling occurred as a result of propagation of the secondary through-thickness crack.

So far, most of the previous studies focused on bi-layer structures, which had only one layer of thin film or coating.

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**Fig. 5** Interfacial crack initiation modes observed during indentation: a tangential and b normal, modified from the fracture crack separation modes by Hudson and Harrison [47]

**Fig. 6** Cross sectional view of the tensile stress distribution during nanoindentation of a SiN/GaAs bi-layer system (the interfacial delamination, as indicated by arrows) [27]

**Fig. 7** The three stages of nanoindentation induced fracture of a brittle coating bi-layer [51]
deposited on a substrate. So the structure failure was observed at the interface between film and substrate or inside a brittle thin film layer. Liao et al. [52] performed a series of indentations on a Cu/Ta/Black Diamond™/Si substrate film stack structure and found that interfacial delamination would be first initiated at the weakest link of the structure, i.e., the interface between Cu and Ta thin films in this case. When the indentation load was increased to a critical value, through-thickness cracks were formed inside the Black Diamond™ (BD) layer and then propagated to the interface between the BD layer and Si substrate. Figure 8 shows the cross-sectional surfaces of the damaged structures after indentation. The results suggest that the combined failure modes including both interfacial delamination and through-thickness cracks are more likely to occur in complex thin film structures.

Failure in a multilayer structure is more complicated than that in a bilayer system. The FEM simulation carried out by Chen and Bull [45] shows that the stress field and distribution that determine the interfacial failure not only rely on the mechanical properties and thickness of an individual layer, but also highly depend on the penetration depth of the indenter. As shown in Fig. 9, a deeper penetration would impose more plastic deformation in soft film layers, thus affecting the bending effect of neighboring layers. The mechanisms revealed in this work applied for other similar multilayer structures [45].

In the FEM simulation of the nanoindentation on a multilayer system that consisted of a number of bulk and film layers, Zhao et al. [53] confirmed that the introduction of multilayer structure would evidently alter the stress field underneath the indentation contact area. Figure 10 shows the stress contours of the indented multilayer captured at the moment when the shear stress maximized. The maximum shear stress formed during indentation was located slightly underneath the contact edge in both cases. However, the overall stress level was reduced significantly in the layered structure. For more direct comparison purposes, the shear stress variation below the edge of contact was plotted. A reduction of about 35% in maximum shear stress was achieved. Given that the lateral cracking was governed by shear stresses, the study clearly demonstrated that the use of a multilayer structure could significantly increase the shear strength of a structure [53, 54].

### 2.2.3 Interfacial failure induced by substrate cracking

The cross-sectional nanoindentation (CSN) technique was developed by Sanchez et al. [55] to characterize the interfacial adhesion strength of film/substrate systems.
CSN was designed specifically for intuitional observation of the delamination formed in a thin film multilayer structure. Figure 11 schematically illustrates how CSN works when a multilayer structure of silicon nitride and silicon oxide thin films deposited on a silicon substrate is tested. In this approach, an indentation was placed on the Si substrate, but very near to the film/substrate interface, aiming to produce interfacial cracking. Prior to test, the tip was well calibrated, so one side of the triangular indentation impression was parallel to the interface, as shown in Fig. 11a. During indenting, radial cracks were generated at two corners of the Berkovich indenter if the indentation load was sufficiently high, and then propagated to the interface. When the cracks approached to the interface between the substrate and the film, they would normally change the direction and keep propagating along the interface, hence formed interfacial delamination, as shown in Fig. 11b. In this case, chipping-off also occurred in the substrate and hence further enlarged the interfacial crack. A jump-in observed in the load-displacement curve was associated with the interfacial cracking. Based on the linear elastic fracture mechanics and plate theory, the interfacial critical energy release rate was calculated [55, 56]. CSN was often used for identifying the weakest interface in multilayer structures and for characterizing interfacial adhesion [13, 56–58]. Compared with conventional testing methods, CSN presents some advantages. First, interfacial crack paths can be handily formed and directly examined using SEM or optical microscopy. Second, it is applicable to variety types of multilayer structures as it can induce interfacial delamination in a controlled manner. A disadvantage of using CSN is that the method is not suitable for...
those substrates that do not have orientated cleavage preferential planes, as for such materials the propagation of the cracks in the substrate is hard to control.

2.3 Deformation and failure induced by nanoscratch

2.3.1 Top surface nanoscratching

Scratching was first used in 1950s to assess the adhesion properties of a range of metal/ceramic coatings at microscale [59], but the scratching depth was reduced dramatically to nanoscale nowadays [60–62]. Nanoscratching is one of the most established mechanical characterization methods to study ductile-brittle deformation transition of a material [63], wear under the effect of sliding contact [64], tribological behavior in asperity contact [65], and material removal mechanisms in abrasive machining [66].

Similar to nanoindentation, nanoscratching was valuable for investigating the failure mechanisms of thin film structures [67, 68]. During scratching, if a ramping load is applied on the moving tip, the critical load that induces adhesion failure can be measured. Normally, the minimum load that triggers the first crack in the coating is regarded as the lower critical load \( \left( L_{c1} \right) \) which is also termed as “scratch toughness” and widely used to directly predict the crack resistance in thin film structures [50, 69–72]. The load corresponding to complete peeling of the film is named as the higher critical load \( \left( L_{c2} \right) \) [50]. Roy et al. [28] characterized the interfacial adhesion of amorphous SiCN thin film on Cu/Si substrates using nanoscratching with a Berkovich tip. During testing, both reactive force and penetration depths were recorded. As shown in Fig. 12a, the rupture of the film/substrate interface was related to the normal load applied. Before reaching the critical load \( L_{c1} \), pile-ups were found along the edges of the scratching groove and became clearer with the increased load. At this stage, both reactive force and penetration depth increased linearly with the scratch distance, indicating that plastic deformation occurred in the thin film without cracking. Figure 12b shows that cracks and flakes are formed on both sides of the scratching path when the normal load is over the threshold value. The occurrence of structure failure was reflected by the discontinuities appeared on both measured scratching depth and force. Tang et al. [73] experimentally studied the interfacial delamination behaviors of a Au/NiCr multilayer structure under nanoscratching and found three stages of failure process. At the first stage, plastic deformation was dominant in films when the normal load was small; at the second stage, the plastic/total deformation ratio decreased significantly with the evolution of the normal load and at the final stage interfacial failure occurred when the normal load reached the critical value. It was interesting to note that plastic deformation was dominant over the elastic deformation prior to the failure of structure.

Recent nanoscratch studies revealed that film thickness had great effect on the critical normal load that induced interfacial failure [67, 74–76]. Beake et al. [74] characterized the nanoscratch induced surface damages in Ta-C films of different thicknesses deposited on a Si substrate. The scratching results shown in Fig. 13 clearly revealed that the critical load for inducing lateral cracking in the thin film was considerably higher in thicker Ta-C films. The thinner the film was, the more easily through-thickness cracks occurred. This might be attributed to the higher stresses generated at the interface during scratching as thinner films provided less protection. In contrast, a thicker
Film would provide more support in scratching and hence more resistance to the deformation in the substrate, which in turn delayed the occurrence of interfacial delamination. This work also suggested that tangential loading promoted the formation of lateral cracks, so structure failure in nanoscratching took place at much lower load than that in nanoindentation.

Favache et al. [10] investigated the scratch resistance of a functional multilayer structure that consisted of a brittle coating of CrN, a soft interlayer of polyimide and a silicon substrate. In their study, brittle fractures on the hard film were found to be dominant during scratching, but the high elastic mismatch between two films significantly influenced the crack energy release rate and hence determined the crack density, as shown in Fig. 14.

2.3.2 Cross-sectional surface nanoscratching

Nanoscratching was used to simulate an individual abrasive grit penetrating and sliding on the thin film layer surface in abrasive machining [24, 66]. Sumitomo et al. [13] performed a series of nanoscratching tests on the cross-sectional surface of a thin film multilayer solar panel. The structure of the multilayer being investigated is shown in Fig. 15a. By judiciously selecting the scratching parameters, ductile mode material removal was achieved in brittle layers, as shown in Fig. 15b and the ductile-brittle transition was found to be related to the scratching depth. Below the critical depth, plastic deformation was dominant in the thin film layers as clear pile-ups were observed without cracks. Evident fractures were observed when the scratching depth was above the threshold value, as shown in Fig. 15c. The indenter shape was an important factor that determined the threshold depth as the tip with smaller included angle resulted in the greatest scratching depth under the ductile regime.

Multiple nanoscratches were also made on the cross-sectional surface of such a thin film multilayer to examine the effect of neighboring scratches on the surface finish [26]. The comparison of single and multi-scratched cross-sectional surfaces is shown in Fig. 16, demonstrating that neighboring scratches could have significant influence on the deformation characteristics and interfacial failure. Under the same experimental conditions, more severe brittle fractures and interfacial delaminations were generated on the multi-scratched surfaces. To understand the interfacial failure mechanisms, the interaction of neighboring scratches and its influence on the severity of interfacial failure was systematically investigated [26]. This was done by repeating the scratching at the same location for several times. Figure 17a shows the single-scratched cross-sectional surface of the multilayer, where brittle fractures were found on the thinner layers of ZnO and α-Si but the thicker layer of SnO₂ remained intact. Further scratching produced the interfacial delamination at the interface between SnO₂ and α-Si, as can be seen in Fig. 17b. Thin films of α-Si, ZnO and Al were severely chipped off after performing 4 scratches and the interfacial cracks were exaggerated and

![Fig. 13 Optical micrographs of nanoscratched thin film structures with different coating thicknesses (A ramping normal load from 0–300 mN is used and the onset of lateral cracking is marked by an asterisk) [74]](image-url)
further propagated across the α-Si layer under the loading of the following scratches (see Fig. 17c). After carrying out 6 scratches, as shown in Fig. 17d, catastrophic failure was observed as all the layers outside of the SnO₂ layer were removed along the interfacial crack, forming a large chipping-off area. The results also demonstrated that the interaction between neighboring scratches would crush the fractured debris produced by previous scratches and hence exaggerated the interfacial failure.

2.3.3 FEM modeling of nanoscratching

FEM studies of nanoscratching on thin film structures were conducted by Li and Beres [77], aiming to explain the failure modes in scratched thin film systems. Their model used in the simulation is shown in Fig. 18a. A bilinear elastic-plastic model with isotropic strain was used to characterize the material deformation. Figure 18b shows the representation of the constitutive law. In their simulation study, a ramping normal load was applied on the top of the indenter. Stress distribution was recorded during scratching and three stages were found at the film-indenter interface. The stages were found to be well matched with the contact modes obtained by Holmberg et al. [78], namely static, sliding and plowing. The evolution of stress distribution showed that significant shear stress was generated during scratching at the film/substrate interface and contributed to interfacial delamination. Tensile stress was formed behind the moving tip and was responsible for the transverse damages observed in the experiments. Compressive stress, which was the cause of film buckling, was found at the head area of the indenter. It is clear that the stress field under the indenter can be enhanced notably in the sliding process than penetration.

In the thin film multilayer structure, interfaces between dissimilar materials are susceptible to delamination or debonding when sufficient mechanically induced shear stress or tensile stress is experienced [79, 80]. It is thus crucial to understand the stress distribution induced by scratching and how the distribution affects the interfacial failure in multilayers. Nevertheless, till now little has been reported on such understanding. An FEM simulation was carried out to predict the stress evolution under scratching.
In this study, a 3D symmetrical FEM model was established to simulate the scratching process. During simulation, the input normal loads on the tip were the critical forces that induced interfacial delamination at different interfaces measured from nanoscratching tests. Although both tensile and shear stresses formed at the interface are the potential causes for delamination, the simulation results indicated that shear stress played a more dominant role than tensile stress. Figure 19 shows the shear stress distribution contours captured at the moment when the shear stress value at the delaminated interface was maximized. The maximum shear stress region was located slightly underneath the contact surface between the indenter and the specimen and the critical stresses that induce interfacial failure obtained at the respective interface of \( \alpha \)-Si/ZnO, SnO\(_2\)/\( \alpha \)-Si and glass/SnO\(_2\) were 452 MPa, 525 MPa and 616 MPa, respectively. The outcomes achieved offered valuable guidances for developing a high efficiency machining technology for thin film multilayer structures.

3 Response of thin film structures to abrasive machining

3.1 Lapping and polishing

Although being widely used in the understanding of deformation and removal mechanisms involved in abrasive
machining, nanoscratching has its limitations in simulating the practical machining process. This is because the lateral speed of the indenter is much lower than the working speed of abrasive grits during lapping, polishing or grinding. Also, nanoscratching does not take the thermal effect into account. In abrasive machining, temperature rise at the contacting area between abrasives and workpiece could be significant, which might affect interfacial delamination.

Polishing and lapping were performed to study the removal characteristics of the thin film multilayer shown in Fig. 15a [26, 81]. During polishing, surface damages in the glass substrate and thin films reduced with the decreased grit size. The polished surfaces shown in Fig. 20 demonstrated that fracture and delamination were obvious in between the layers when the abrasives used were larger than 3 μm, while the thin films became intact after polishing with the abrasives smaller than 1 μm [81]. By using fine abrasives, the surface roughness values in the brittle layers of glass, SnO₂ and α-Si decreased to the order of 1 nm. Crack-free surfaces indicated that ductile mode material removal was dominant during polishing. Nevertheless, the material removal rate in polishing was too low to be applied in practical application [81].

Figure 21 shows the AFM and SEM images of the thin film solar panel multilayer after lapped with different diamond abrasive sizes of 6 μm, 3 μm, 0.5 μm and 0.1 μm [26]. The results demonstrated that the grit size of lapping films had the most significant effect on surface finish, comparing to other lapping parameters, such as lapping speed and normal force. In Fig. 21a, when 6 μm lapping grits were used, apparent streaks were observed on the glass substrate. Both AFM and SEM images indicated that the surfaces of the thin film layers were significantly rougher comparing to the glass substrate. Figure 21b shows the surface of the specimen lapped by a smaller grits of 3 μm diameter. In this case, lapping grooves on the substrate became more continuous. However, thin film layers were hard to be distinguished due to the significant cracking and chipping occurred in the layers. Interesting to note that no fatal disruption was found at the interface between the substrate and SnO₂ layer when relatively coarse grits were used, indicating a strong adhesion between these two layers. Significant improvements in surface finish were made when the grit size reduced to 0.5 μm, as shown in Fig. 21c. Chipping or fracture was barely seen on the glass substrate. The glass/
SnO$_2$ interface and SnO$_2$ layer were intact and could be clearly distinguished from both AFM and SEM images, although there were still some shallow pits near the interfaces. The defects were successfully improved through applying finer abrasives. It is evident in Fig. 21d that the use of diamond lapping film with 0.1 $\mu$m abrasives was able to obtain excellent surface finishes on glass, SnO$_2$ and $\alpha$-Si layers with no cracks or other brittle damages, but a small crack was still formed at the interface between $\alpha$-Si and ZnO.

It was noteworthy that the deformation characteristics of the lapped thin film multilayer solar panels generated in the lapping process indeed exhibited similar characteristics to those obtained from the nanoscratching tests reviewed in Sect. 2.3. It appeared that delamination occurred in the
same sequence in both nanoscratching and lapping tests. Good agreements between nanoscratching and lapping were also found when plotting the roughness values of individual layers measured from both tests as a function of grit penetration depth. As shown in Fig. 22, all the roughness data fell on one common trend line. Interestingly, there existed threshold depths that marked a transition between two distinct removal regimes for the thin films of SnO₂ and α-Si. Below the threshold depth the thin film materials could be removed in a ductile mode whereby the scratched surfaces were relatively smooth and an increase in penetration depth only led to slight increase in roughness. Above the threshold depth, brittle fracture occurred and an increased penetration depth significantly increased surface roughness. It is also noted that the scratched surfaces appears slightly better than the lapped ones, which is likely because the lapping is a process with uneven protrusion height of diamond grits when compared to the controlled conditions in nanoscratching. Nevertheless, the results still strongly suggest that the material deformation and removal characteristics of thin film structures involved in abrasive machining can be well understood by using nanoscratching.

3.2 Grinding

There has been increasing interests in the application of coating/substrate bilayer or multilayer materials [82]. In some cases, the surface of coated materials needs to be ground as a finishing operation [83, 84]. The effect of grinding on the deformation and removal characteristics was investigated in a number of studies [82, 83, 85–89]. Liu et al. [88, 89] performed grinding tests on nanostructured WC/12Co and Al₂O₃/13TiO₂ coatings and

![Fig. 21 AFM images (left column) and SEM micrographs (center and right columns) of the surfaces after lapping with diamond films of a 6 µm, b 3 µm, c 0.5 µm and d 0.1 µm [26]](image-url)
comprehensively explored the relationship between grinding conditions and surface topographies. The results revealed that increasing grinding feed rate or depth of cut led to rougher surfaces on both coatings. Larger abrasive grits and harder wheel bond would increase actual grit cutting depth and hence had negative effects on the surface finish. Both ductile and brittle mode removal were observed in two ground coatings but more severe damages were observed in the Al₂O₃/13TiO₂ coating under the same grinding condition. As shown in Fig. 23a, clear grinding marks could be seen on the top surface of the WC/12Co coating, but the ground Al₂O₃/13TiO₂ coating was overwhelmed by chippings and microcracks as it possessed higher brittleness, though the grinding conditions remained the same [89]. The depths of subsurface damage in the two coatings were close if the grinding cutting depth was relatively small. However, if the depth of cut was over a critical value the depth of subsurface damage in the relatively soft WC/12Co coating was worsened more dramatically. This phenomenon could also be explained by the different brittleness in two coatings as most grinding energy was consumed by the formation of new cracks rather than developing new cracks in more brittle materials [88].

The grinding of the cross-sectional surface of a thin film multilayer shows more complicated characteristics of deformation and failure. Sumitomo et al. [14] aimed at investigating the abrasive machining performance and material removal mode of the thin film multilayer solar panel shown in Fig. 15a. The grinding tests were carefully conditioned in order to achieve ductile mode removal. Nevertheless, their results revealed that fractures were still observed on the thin film layers even though the measured grinding streak depth was smaller than the ductile-brittle transition cutting depth calculated by the Bifano model [90], which was likely because the crack initiated at interfaces propagated into the neighboring layers. Apparently, the material removal mechanisms of thin film structures involved in abrasive machining were different from bulk materials. Delamination at interfaces was found to be more easily to occur than fracture on the brittle layers for this multilayer structure. Either reducing the grit size or feedrate during grinding would improve the interfacial quality. Obviously, the improvements were achieved through decreasing the aggression level of machining, but the trade-off was the sacrifice of productivity.

High speed grinding, in contrast to conventional speed grinding, has great advantages in achieving favorable surface quality combined with high productivity [91, 92]. The application of high speed grinding in the machining of thin film structures was carried out [93]. Figure 24 shows the surface characteristics of the thin film multilayer ground by different grinding wheels and speeds. When the coarsest diamond grits of 17 μm used, the increase in grinding speed had limited improvement on surface finish as severe brittle damages were overwhelming on both substrate and thin film layers, though slightly better surface finish was achieved when the greatest speed of 120 m/s was used, as shown in Fig. 24c. When the grit size was decreased to 7 μm, the grinding speed started to play a more dominant role in surface quality. Figure 24d shows the ground surface at the conventional grinding speed of 40 m/s, where severe fractures were observed at the thin film interface, while surface fractures were significantly reduced at higher wheel speed. At the highest wheel speed, as shown in Fig. 24f, no significant brittle damage was observed and distinct grinding grooves could be seen on both substrate and thin film layers. When using the finest grit size of 2 μm and maintaining the other grinding parameters the same, both substrate and thin films appeared to be smooth for all
the wheel speeds used, but the increase in wheel speed led to a better surface finish, as shown in Figs. 24g–i. This study apparently demonstrated the advantage of high speed grinding in the manufacture of thin film multilayer structures.

4 Potential research direction and future work

The previous studies on the deformation and interfacial failure mechanism of thin film multilayer structures demonstrated some common removal characteristics in nanoscratching and abrasive machining. However, thermal effect is expected to have much more significant impact in abrasive machining than that in nanoscratching. In the future work, nanoscratching should be performed at elevated temperatures, so the role of thermal effect in the interfacial delamination of thin film multilayer structures can be clarified.

Through thickness cracks were observed inside thin film layers after nanoscratching and abrasive machining. Such cracks are expected to alter the material removal mechanism during machining, as stress distribution would be varied. However, in most of the modelling works published, the effect of stress status at the interface on crack formation and propagation was not taken into consideration due to the limitation of modelling. It is documented that the use of cohesive zone models can be an effective method to simulate material fracture [94, 95]. The application of such models would not only give the interpretation of crack initiation, but provide detailed insight into the evolution of stress during interfacial debonding.

5 Conclusions

The deformation characteristics and failure modes in thin film bilayer and multilayer structures induced by nanindentation and nanoscratch were systematically reviewed. Under such mechanical loads, three typical failure modes could be identified, namely interfacial delamination, through-thickness cracking and interfacial failure induced by substrate cracking. Among the three failure modes, interfacial delamination is the failure mode occurred most frequently as interfaces between thin films are likely the weakest link in most of the bilayer and multilayer structures.

Nanoscratch appears a viable tool to understand the deformation characteristics and removal mechanism involved in the abrasive machining of thin film multilayer structures, whose results agree well with those obtained from lapping and grinding. The previous studies on abrasive machining of thin film structures showed that so called “ductile” mode machining conditions must be satisfied in order to achieve the required surface integrity. However, the requirement on ductile mode machining is somehow different from that for bulk materials as interfacial failure is the most likely failure mode in abrasive machining and
the conditions for eliminating interfacial failure is more stringent than those for avoiding brittle damages in bulk materials. Both shear and tensile stresses generated in abrasive machining are attributed to the cause of interfacial failure in thin film multilayers, but shear stress seems playing a more significant role. Recent studies also showed that high speed grinding had certain advantages over conventional grinding as the high wheel speed could reduce the grinding force induced, hence, the stress at interfaces, which would help improve the machined surface integrity of thin film multilayers without sacrificing machining efficiency.

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