

**Predicting through-thickness
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coated system subject to
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ABSTRACT

Through-thickness cracking is one of the most important failure mechanisms for coatings, the consequences of which often lead to debonding of the interface and subsequent exposure of the underlying substrate to the environment. Whilst numerous test methods have been developed to measure through-thickness cracking there has been little detailed interpretation of the results in terms of fundamental properties, such as fracture energy. The main objective of this work was therefore to apply through-thickness cracking models to experimental data. The three test methods examined following industrial consultation were thermal, tensile and four-point bend. It has been concluded from the results that the most suitable test method for measuring through-thickness cracking appears to be the thermal fracture technique. This was experimentally the simplest technique to perform and as plastic deformation was not observed was also the least complicated to analyse.

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Approved on behalf of Managing Director, NPL by Dr C Lea,
Head of the NPL Materials Centre

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1. Introduction

Coatings are generally applied to engineering components in order to improve their performance and sometimes their appearance. Examples include hard coatings to prevent the wear of the substrate and thermal barrier coatings to enable metal components to operate safely in high temperature environments. For these examples, it is vital that the integrity of the coating is maintained throughout the normal service life of the engineering component. It is also vital that engineers have a proper understanding of the micro-mechanisms of coating failure.

One of the most important damage modes experienced by coatings is the debonding of the interface leading to spallation and the consequent exposure of the underlying substrate to the environment (either mechanical or chemical). Such debonding often arises because of prior through-thickness cracking of the coating, and the understanding of such cracking also becomes an important issue of practical importance.

Through-thickness cracking can occur due to the application of either tensile or bending loads, and can be predicted using the methods described in reference [1]. Continued loading of the system is expected to lead to progressive through-thickness cracking and then to the growth of interfacial debonds.

The objective of this report is to summarise the results of applying a through-thickness cracking model [1] to experimental data obtained from mechanical and thermal test methods used to characterise the fracture properties of chromium nitride coated stainless steel.

2. Experimental test methods

To determine the fracture behaviour of the coatings and enable the models to be validated a series of chromium nitride coated stainless steel specimens were tested using; thermal fracture, tensile, four-point bend techniques.

2.1 Test specimens

Test specimens were cut using spark erosion from a 3mm thick sheet of AISI 304 stainless steel into coupons $100 \times 10 \times 3$ mm. One side of each specimen was then coated with $5\mu\text{m}$ of PVD sputtered chromium nitride. The thickness of the coating measured at nine different positions along the surface using a Fischerscope X-RAY XDL.

2.2 Thermal fracture test

The thermal fracture experiments were conducted by placing the specimens into a high temperature oven and gradually increasing the temperature at a constant rate of $5^\circ\text{C} / \text{minute}$, whilst monitoring the temperature of the oven next to the specimen. A transducer for monitoring the acoustic emissions was spot welded to the coated side of the specimen, the area of the weld being cleaned prior to welding with the use of emery paper. Signals from a thermocouple and the acoustic emissions transducer were recorded throughout the experiment using a computer-controlled data-logger.

2.3 Tensile test

Tensile tests were performed using an INSTRON 5500R tensile test machine. The specimens were carefully aligned visually using a t-square and clamped within the Instron grips. Gauge-lines were attached approximately 10 mm apart across the width of the specimen. A video extensometer was then focused on to the gauge-lines in order to monitor the strain during the experiment. Acoustic emissions from fracture of the coatings were monitored using a transducer that was attached to the coated side of the specimens using a spring clip. A thin layer of Apiezon grease was used to ensure a good acoustic contact between the sensor and the coating. The tensile specimens were pre-tensioned to 10 N to remove slack in the load chain. The specimens were then loaded until the coating failed using a crosshead displacement rate of 1 mm/minute. Data from the video-extensometer, the Instron load cell and the acoustic emission sensor were collected simultaneously on a computerised data-logger.

2.4 Four-point bend test

The four-point bend tests were conducted using a bend jig with two inner rollers (8mm diameter) positioned 20 mm apart and two outer rollers 40 mm apart (Figure 1). An Instron 5565 test machine was used to apply a load. Gauge-lines were attached to the coated side of the specimen using two adhesive paper strips positioned approximately 10 mm apart. Specimens were placed in the jig so that the coated side was in tension during the test. A video extensometer was used to monitor the strain using the two gauge-lines on the specimen. A thin smear of Apiezon grease was applied to the coated side of the specimens so that an acoustic emission transducer could be attached using a spring clip. Prior to conducting the tests a 10 Newton pre-load was applied to remove slack in the system. The specimen were loaded until failure of the coating occurred at a crosshead displacement rate of 1 mm/minute. Load, strain and the acoustic emission signals were all recorded simultaneously during the experiment using a computer-controlled data-logger.

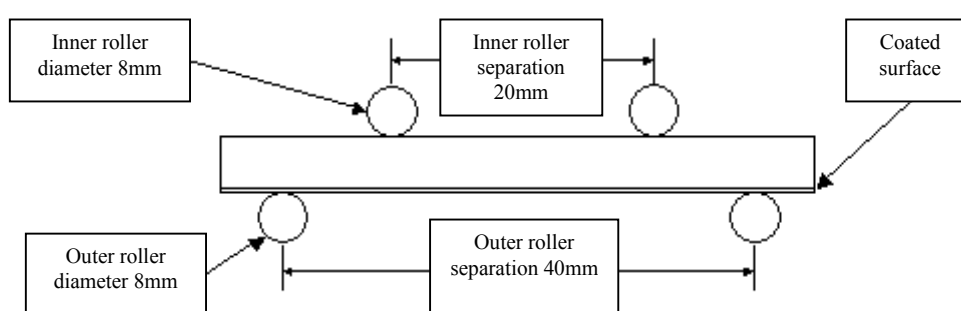


Figure 1 Schematic diagram of the four-point-bend apparatus used to determine the fracture stress of Chromium nitride coated stainless steel specimens

3. Experimental results

Graphs showing the acoustic emission signals and the cumulative counts obtained from the thermal fracture, tensile and four-point-bend test methods are shown in Figures 2 to 10. The

point at which fracture occurs in each case was determined using a cumulative plot of the acoustic emissions. In four-point bend tests where there is minimal background noise fracture is simply defined as the point at which the gradient of the cumulative acoustic emission graph first begins to increase (Figure 8). However, in the tensile and thermal fracture techniques where there is a background noise the point at which the coating fractures is determined by the intercept of the two linear portions of the graph either side of the point where the gradient begins to increase (Figure 2). Confirmation that the acoustic emissions were due to fracture of the coating was obtained by repeating the tests using uncoated specimens. In each case no signal other than the background was obtained with the uncoated specimens indicating that the acoustic signal came from the coating. As confirmation, a tensile test was conducted in which the load was increased in small steps to allow photographic images to be obtained of the coated surface. The results confirm that at the same point that acoustic emissions are first detected (320 MPa) the first cracks are observed in the coating (Figure 11). Visual inspection of the coatings after the experiments revealed that the coatings had not fractured at either the grips or the rollers but along the gauge length of the specimen. Significant plastic deformation of the substrate occurred in both the tensile and four-point-bend tests but not during the thermal fracture tests.

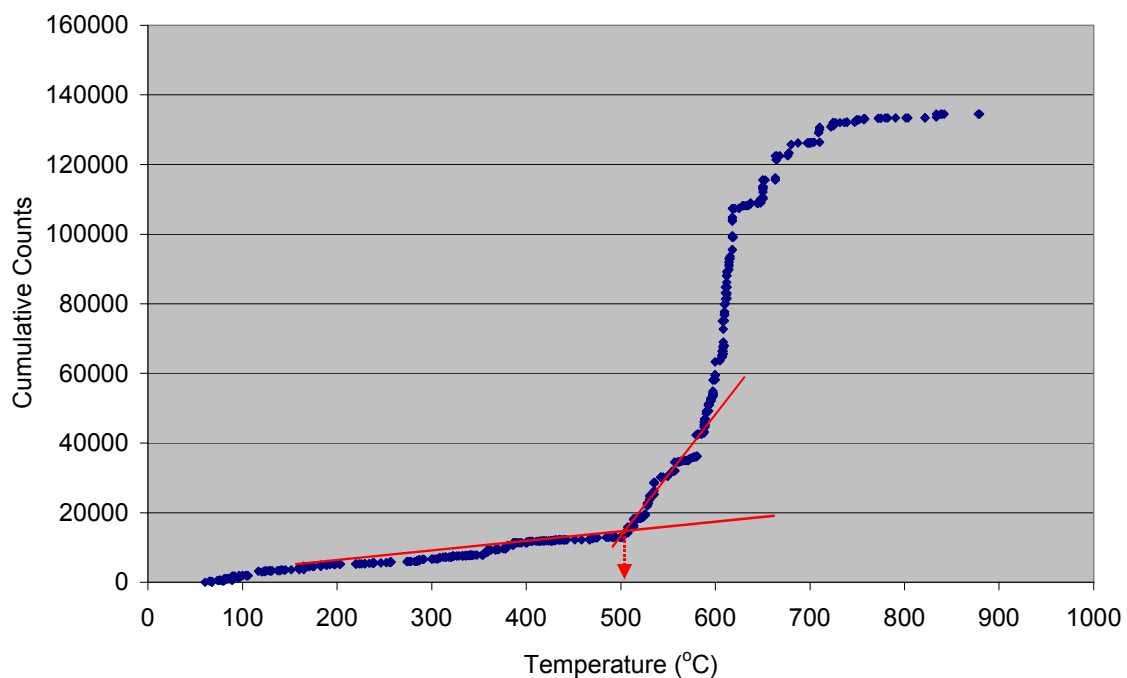


Figure 2 Cumulative acoustic emissions obtained from the fracture of a 5 μm thick CrN coating obtained during the thermal fracture test method.

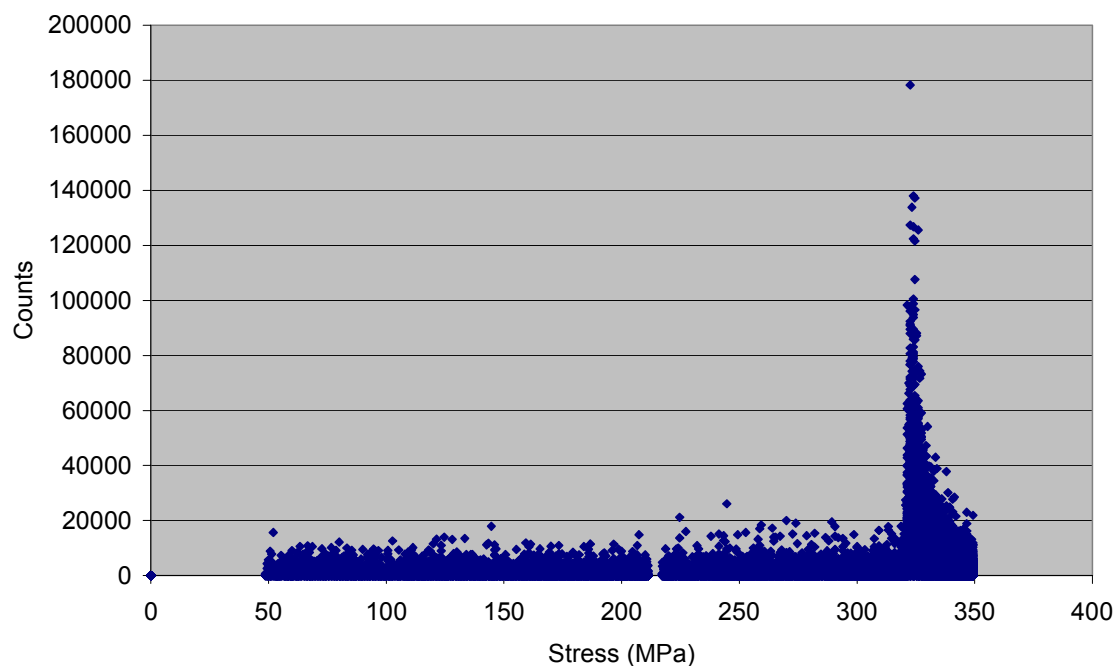


Figure 3 *Acoustic emissions obtained from the fracture of a 5 μm CrN coating during a uniaxial tensile test.*

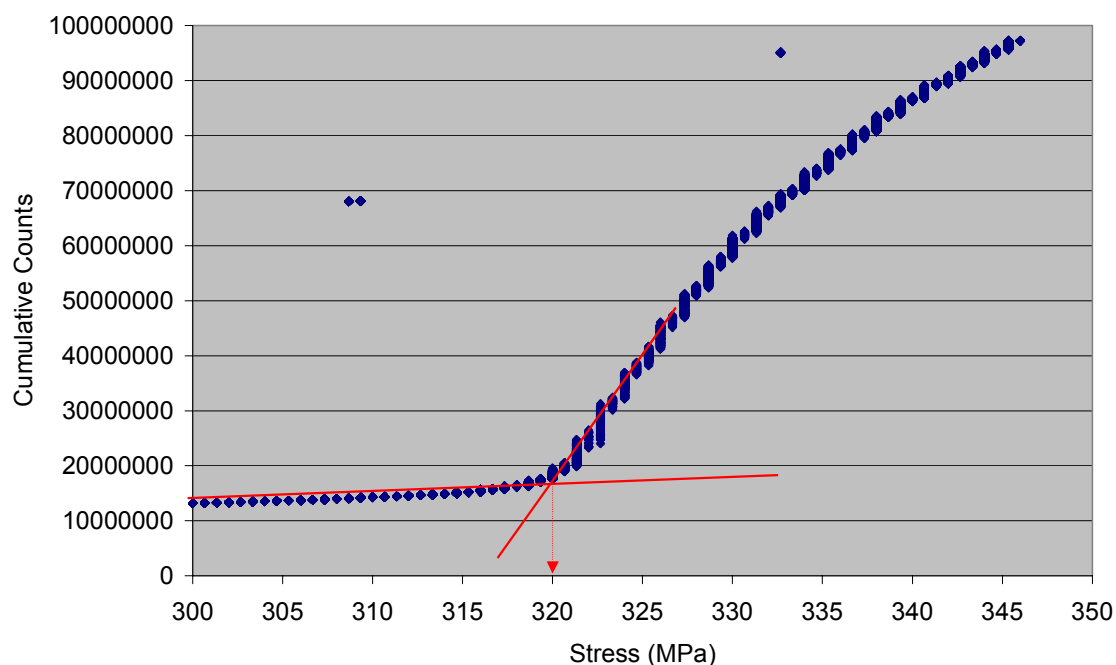


Figure 4 Fracture stress is obtained using a graph of the cumulative acoustic emissions obtained during the tensile test.

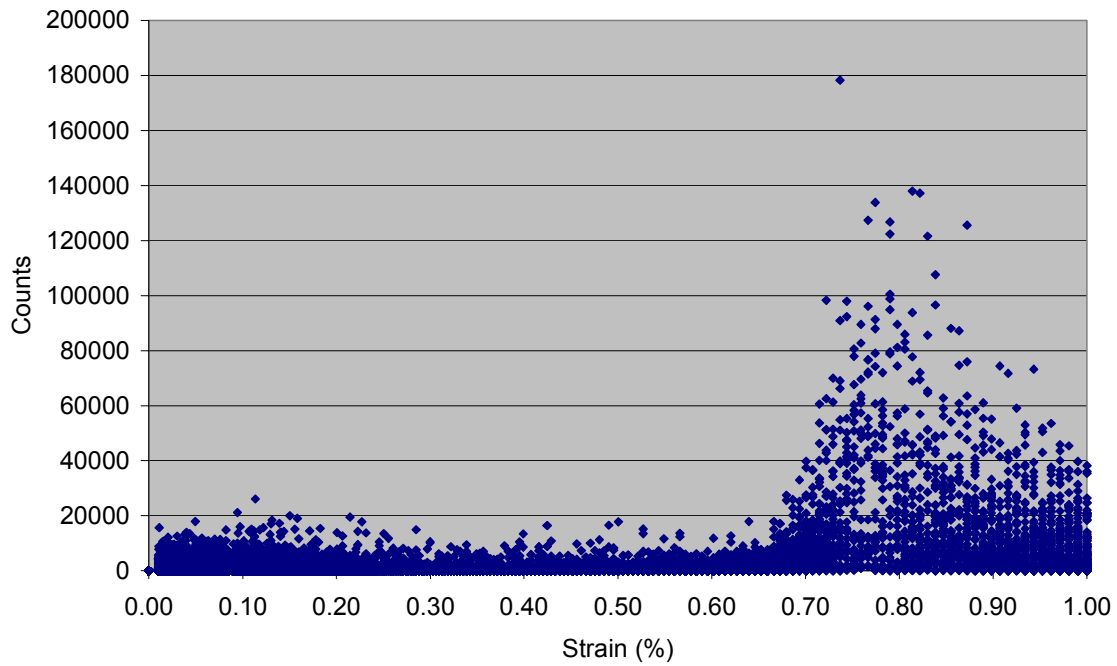


Figure 5 Acoustic emissions obtained during the tensile test as a function of percentage strain.

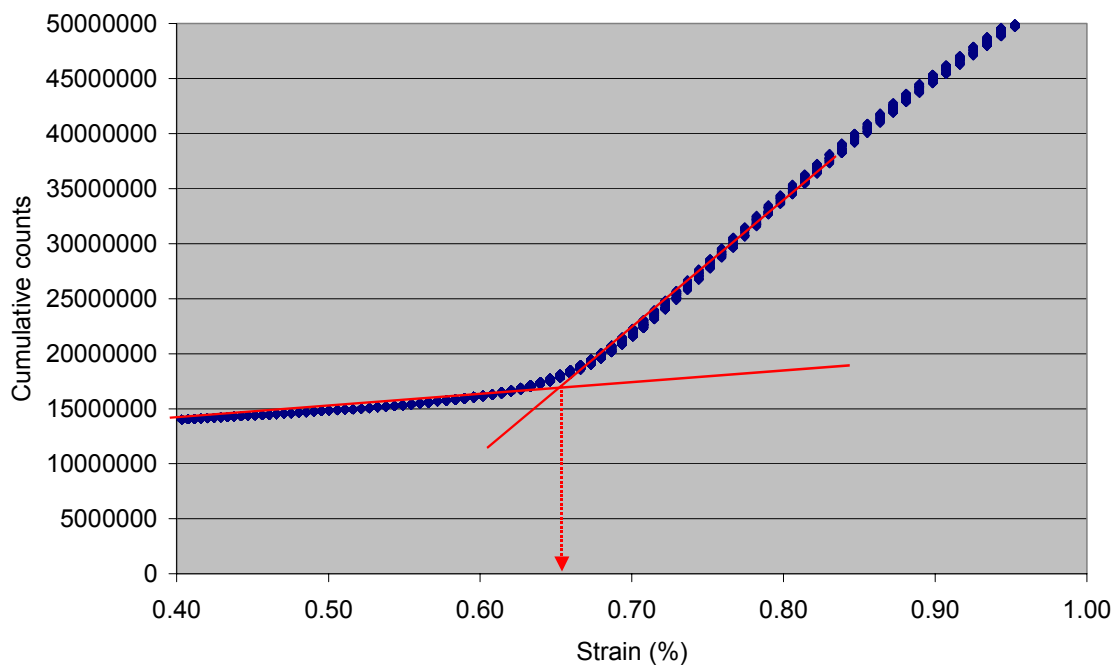


Figure 6 The fracture strain of the coating in the tensile test is obtained from a graph of the cumulative acoustic emissions using a similar technique as is used for fracture stress.

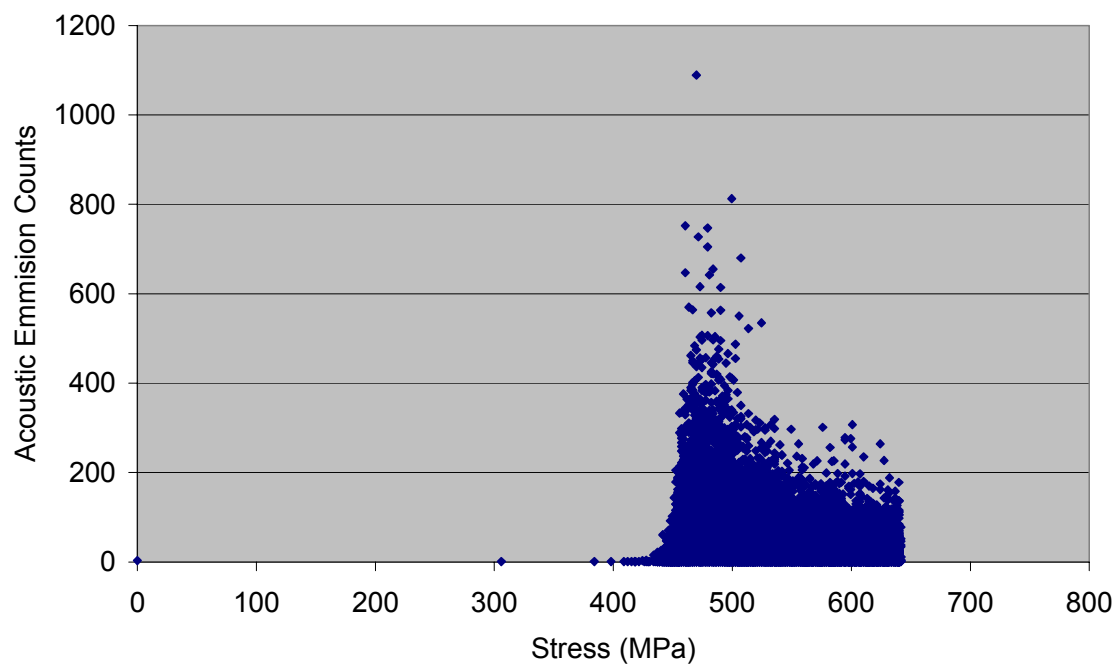


Figure 7 The acoustic emissions obtained from the fracture of a 5 μm CrN coating during a four-point bend test.

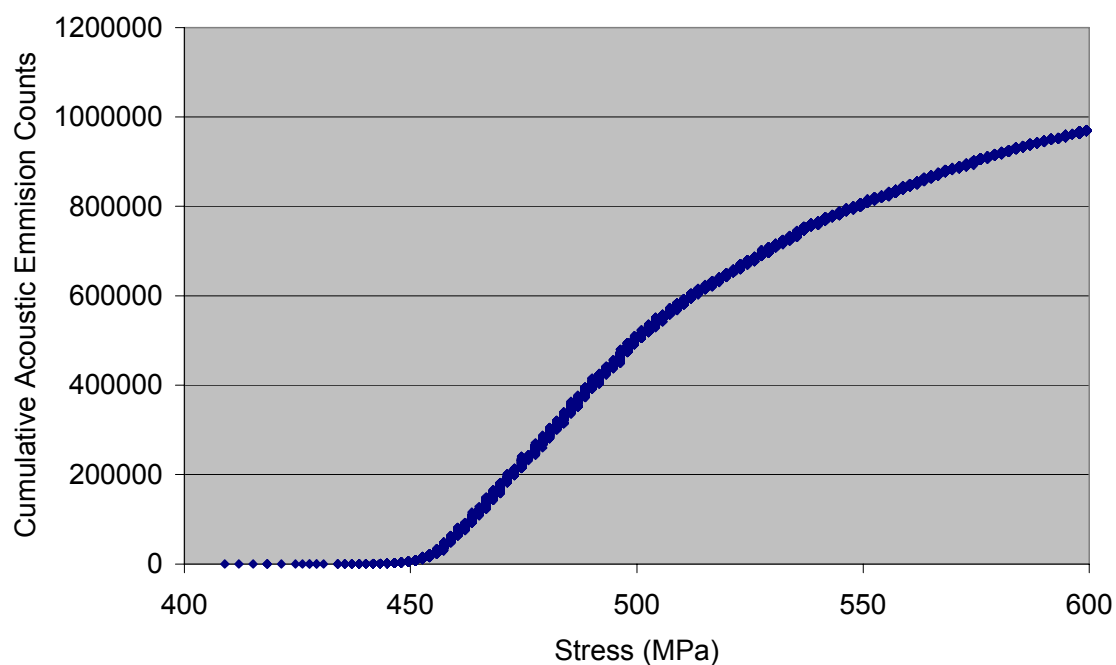


Figure 8 The fracture stress of the coating is easily identified from the four-point bend data using a graph of cumulative acoustic emissions against stress.

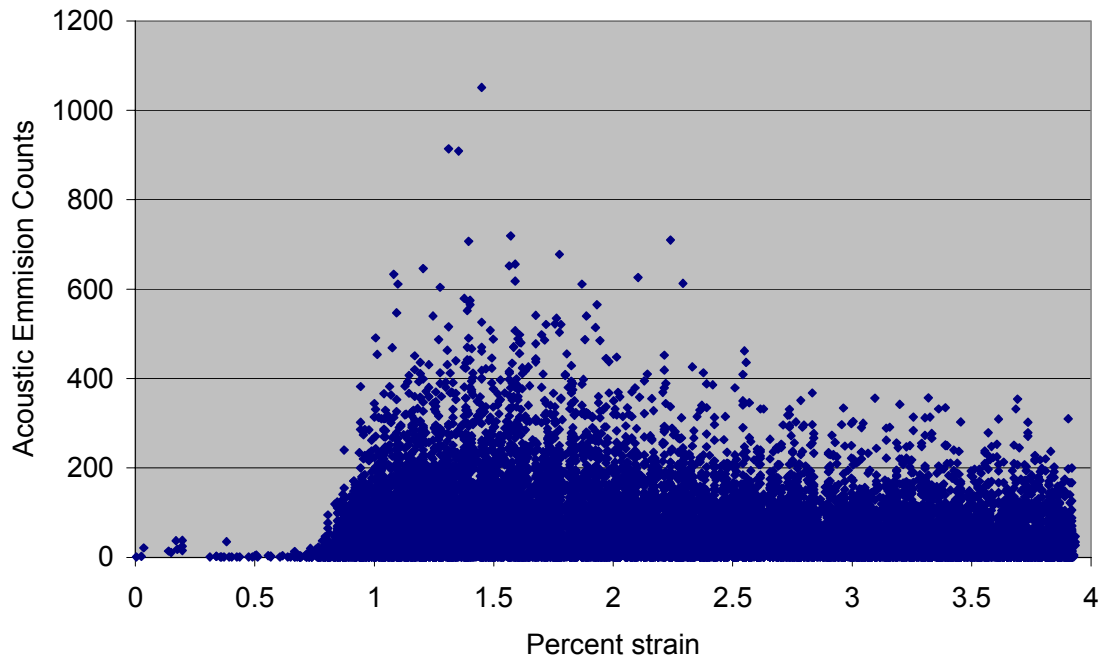


Figure 9 *Acoustic emissions obtained during the four-point bend test as a function of percentage strain.*

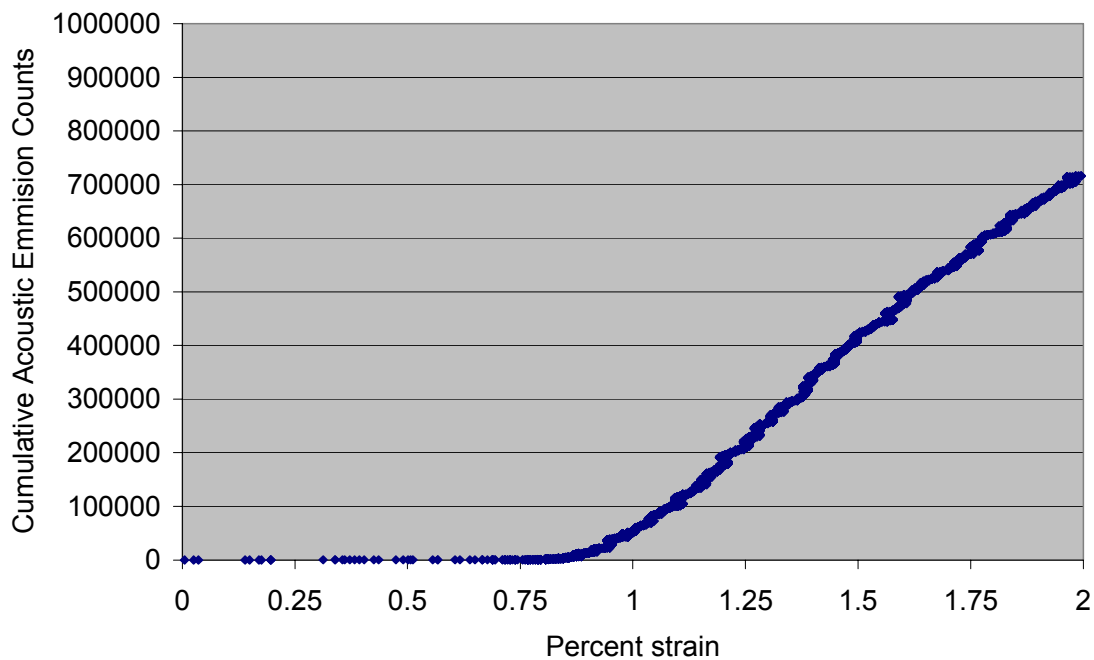


Figure 10 *The fracture strain of the coating is also easily identified from the four-point bend data using a graph of cumulative acoustic emissions against strain.*

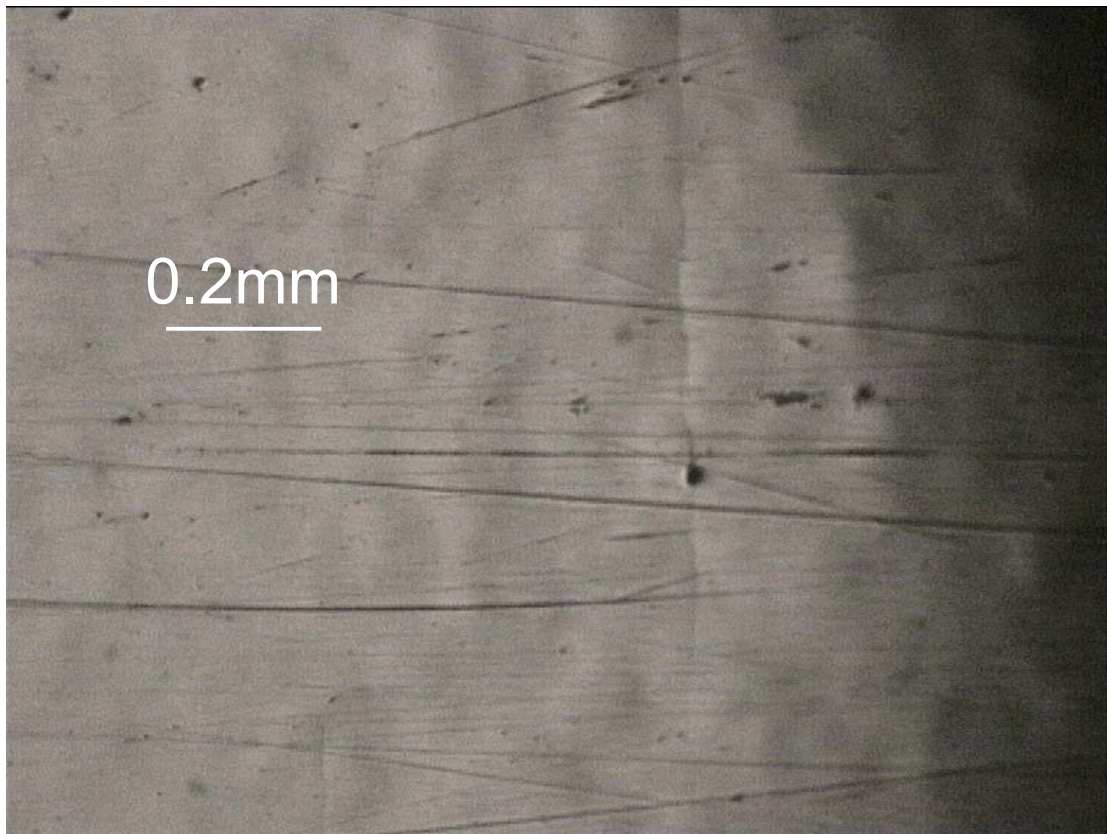


Figure 11 Image of a 5 μm thick CrN coating on a 304 stainless steel substrate subject to an applied stress of 320 MPa. Fracture of the coating is observed at the centre of the specimen midway between the inner supports.

Table 1 Temperature of coating fracture in thermal experiments.

Specimen Number	Temperature
JDV127	502
JDV128	492
Average	497

Table 2 Stress and strain of coating fracture obtained in the tensile experiments.

Specimen Number	Strain (%)	Stress (MPa)
JDV120	0.57	318
JDV121	0.67	320
JDV122	0.62	323
Average	0.62	320

Table 3 Stress and strain of coating fracture obtained in the 4-point bend experiments.

Specimen Number	Strain (%)	Stress (MPa)
JDV125	0.66	451
JDV126	0.89	420
JDV130	0.59	485
Average	0.71	452

4. Geometry assumed for modelling of through-thickness cracking

A two-layer coated system of length $2L$, width $2W$ and total thickness h consisting of two perfectly bonded isotropic layers is considered. The system is located within a Cartesian coordinate system such that the x -axis is in the through-thickness direction; the y -axis is in the axial direction and the z -axis is in the in-plane transverse direction (see Figure 12 showing the location of the through-thickness crack in the coating). The origin is selected to lie on the free surface of the substrate. The thickness of the coating is denoted by h_2 , x_2 , x_1 and the thickness of the substrate is denoted by h_1 , x_1 , x_0 , where x_0 is taken to be zero.

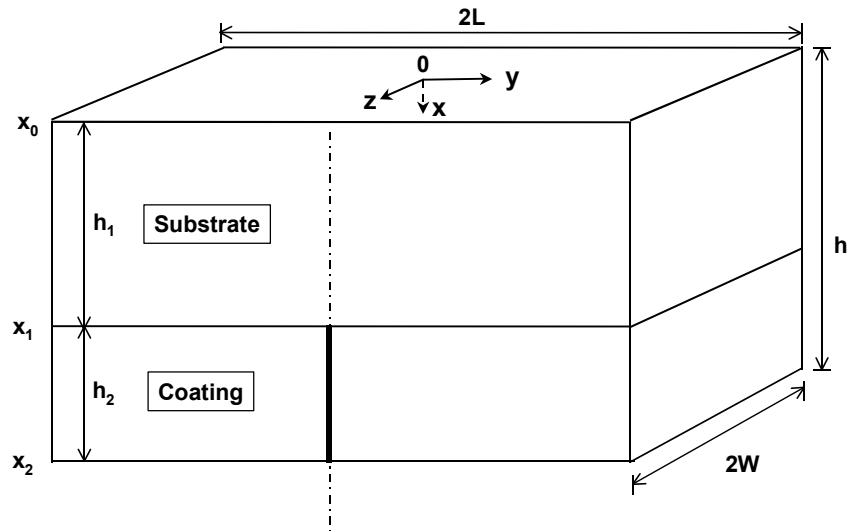


Figure 12 Schematic diagram of the geometry and coordinate system for the coated system showing the through-thickness crack in the coating.

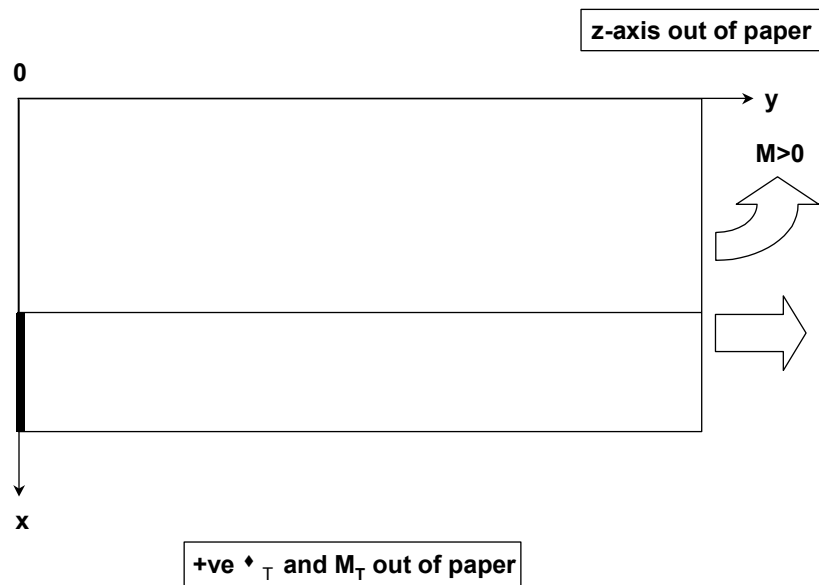


Figure 13 Schematic diagram of the loading conditions applied to the coated system.

An isolated through-thickness crack is assumed to have formed in the coating normal to the free surface. The through-thickness crack lies in the plane $y = 0$. Symmetry is assumed about the mid-plane ($y=0$) of the coated system, which is subjected to biaxial loading such that the effective applied stress in the axial direction is σ and that in the transverse direction is σ_T . Bending moments M and M_T are also applied oriented in the axial and transverse directions respectively. The directions of action of positive applied bending moments per unit area are shown in Figure 13.

5. Use of the software tools

During the project various software systems have been developed for use when predicting through-thickness cracking in coatings. The first system known as COAT (which has now been extended to multi-layer coatings as part of the MMS3 project) may be used to predict the tensile stress at which a coating is expected to crack during the in-plane biaxial loading of the system, assuming that the fracture energy of the coating is known. The software allows continued loading beyond the first cracking stress and the progressive development of an array of parallel through-thickness cracks. The cracking behaviour is governed by the fracture energy of the coating and the major problem that arises is the development of methods to estimate the fracture energy from experiments conducted on coated samples. As it is not possible to test macroscopic samples of coating material, which will have properties that differ from bulk properties, there is no alternative but to test coatings that are attached to a substrate. Thus, the model, and associated software, that has been developed to understand through-thickness cracking of a coating, needs to be used to estimate the coating fracture energy. The methodology that has been developed assumes that the coating and substrate deform as elastic materials. For such cases the model can indeed be used to estimate reliably the coating fracture energy when it is attached to the substrate. The model enables the extraction of the coating fracture energy from the behaviour of a composite system involving both the coating and substrate.

For a coated system subject to the pure bending that arises during a four-point bend test, a software system ENERGY is used to predict the applied bending moment per unit cross-sectional area at which it is energetically favourable for through-thickness cracks in the coating to form. The methodology also assumes that the coating and substrate deform as linear thermoelastic solids.

When the substrate is a metal, the fracture energy predicted by the model will be a function of both the coating and substrate properties as through-thickness crack formation will also lead to localized plastic flow in the region of the crack tips that lie on the interface between coating and substrate. Such plastic flow will increase the apparent fracture energy of the coating due to the energy dissipation as heat that arises during the localized plastic deformation (see Appendix for further discussion).

When coatings are relatively thin, energy balance principles demand that they become more difficult to crack, leading to applied stress levels that cause macroscopic plastic deformations in the substrate. For combined biaxial in-plane loading and bending, in the presence of thermal residual stresses an application BIAXIAL has been developed from an analysis described in the Appendix that predicts approximately, the stress and strain distributions in coating and substrate provided there are no through-thickness cracks and interface cracks.

The system has been extended to deal with multi-layered systems as part of the MMS3 project [2]. When applied to a single coating system subject to combined uniaxial loading and bending in the absence of thermal residual stresses, the application has been shown to give accurate predictions by comparing them with the results of an equivalent FEA (see Appendix).

6. Accounting for residual stresses

In order to estimate the fracture energy for through-thickness cracking of the coating, the parameters needed by the model are the thicknesses of the coating and substrate, the thermoelastic constants of coating and substrate, and most importantly the stress-free temperature of the coated system. At this temperature, the coating and substrate, when in an externally unloaded state, are entirely stress free. At other temperatures, including room temperature, internal thermal residual stresses are present that can easily be modelled for the case of elastic deformations. For the coating system being studied, X-ray diffraction methods have been used at NPL to measure the residual stress of -1.97 GPa in a chromium nitride (CrN) coating having thickness $5\text{ }\mu\text{m}$ applied to a 304 stainless steel substrate. The thermoelastic constants assumed for the coating and substrate are given in Table 4. Two values of the coating modulus are given in order to investigate the sensitivity of predictions to the properties of the coating. The first value of 244 GPa is thought to be realistic while the second value 400 GPa is thought to be appropriate only for CrN in bulk form.

Table 4 Coating (CrN) and substrate (304 stainless steel) property data.

	E (GPa)	ν	α ($^{\circ}\text{C}^{-1}$)
CrN	244 / 400	0.2	0.7×10^{-6}
304 Stainless Steel	220	0.3	17.3×10^{-6}

If the CrN coating modulus is assumed to be 244 GPa then the stress free temperature T_0 that would generate the measured residual stress in the coating is $412\text{ }^{\circ}\text{C}$. The temperature difference $\Delta T = T - T_0$ applied in the software, where T is the test temperature (i.e. room temperature), then has the value $-392\text{ }^{\circ}\text{C}$. If the CrN coating modulus is assumed to be 400 GPa (a likely bulk value) then the stress free temperature T_0 that would generate the measured residual stress in the coating is $260\text{ }^{\circ}\text{C}$. The temperature difference $\Delta T = T - T_0$ applied in the software, where T is the test temperature, then has the value $-240\text{ }^{\circ}\text{C}$.

7. Assessment of theoretical model

The coated system modelled consists of a $5\text{ }\mu\text{m}$ thick CrN coating perfectly bonded to a 3.00 mm thick 304 stainless steel substrate. The assumed moduli, Poisson's ratios and thermal expansion coefficients for CrN and steel are shown in Table 4.

7.1 Thermal fracture test

The first test to be analysed involved the thermal heating of the system to the point where the first through-thickness crack formed, which was experimentally determined using an acoustic emission technique (section 2.2). The expansion coefficient for the substrate is assumed to exceed that of the coating. Following coating deposition, large biaxial compressive stresses build up in the coating during cooling while the much thicker substrate is slightly in biaxial tension. If the coated system is heated sufficiently then tensile stresses will occur in the coating and it becomes energetically favourable for through-thickness cracks to form. The software application COAT may be used to analyse this situation and carry out the necessary energy balance calculations. The predicted values for the through-thickness cracking energy are given in Table 5. For a coating modulus 244 GPa the fracture energy for through-thickness cracking is estimated to be 7.66 J/m^2 that corresponds to values of relatively brittle materials. For this case the BIAXIAL application leads to an equi-biaxial coating stress of 0.44 GPa. When a coating modulus of 400 GPa is used, a much larger fracture energy of 117 J/m^2 is obtained. For this case the BIAXIAL application leads to an equi-biaxial coating stress of 1.97 GPa. It is clear that the choice of coating modulus has a very large effect on estimates of the fracture energy, and that a method is urgently needed to measure accurately the in-situ properties of coatings (see [3] for details concerning one possible approach).

Table 5 Predicted fracture energies for through-thickness cracking in a $5 \mu\text{m}$ CrN coating on a 304 stainless steel substrate. (Thermal loading)

Coating material	E (GPa)	Through-thickness cracking temperature ($^{\circ}\text{C}$)	Estimated fracture energy (J/m^2)
CrN	244	500	7.66
CrN	400	500	117

It is worth noting that during the thermal test, the application of an approximate elastic-plastic model [2], that agrees very well with FEA, to the prediction of the deformation and stress fields in a two layer uncracked coating system, indicates that the response of the substrate remains in the elastic regime of deformation. This type of behaviour was also confirmed by experiment, since after the thermal test the coating system did not exhibit any permanent deformation. Thus the through-thickness cracking model based on linear elasticity theory is expected to be valid. The application of the model has, however, ignored the effects of temperature on the thermoelastic constants of both coating and substrate, and this technique depends on the expansion coefficient of the coating being less than that of the substrate. There may also be temperature dependence of the fracture energy for through-thickness cracking. Strictly speaking, the values given in Table 5 correspond to a temperature of 500°C .

7.2 Tensile test

Having determined the fracture energy for through-thickness cracking using the thermal test, as described above, it is now useful to attempt to test the model by making predictions of the applied tensile stress at which the first through-thickness crack would form during tensile loading at room temperature. This is achieved using the software application COAT that neglects any bending that might occur due to the presence of the coating. Such bending will be exceedingly small as the coating is very thin ($5 \mu\text{m}$) when compared to the thickness of the

substrate (3.00 mm). The temperature difference $-392\text{ }^{\circ}\text{C}$ relevant for a coating Young's modulus of 244 GPa, between the test temperature ($20\text{ }^{\circ}\text{C}$) and the stress-free temperature of the system ($412\text{ }^{\circ}\text{C}$) is applied so that before loading the coating has a compressive residual stress of -1.97 GPa . The predicted applied stress in a tensile test for the formation of the first through-thickness crack in the coating is 2.23 GPa . At this applied stress, the maximum tensile stress in the coating is 0.45 GPa , almost the same value as that for the thermal test. For this case the coating stress field is biaxial but not equi-biaxial. In the substrate, however, the maximum tensile stress has the value 2.25 GPa indicating that plastic deformation is certain to have occurred leading to a re-distribution of the stresses.

For the case of tensile loading, experiments have shown that, following the formation of the first through-thickness crack, the substrate has yielded during the loading, as shown by permanent deformations that remain after unloading. The yielding is macroscopic affecting the entire length of the substrate, although localised additional plasticity will occur near the tips of through-thickness cracks, as already discussed in Section 3. The macroscopic plastic deformation, that must occur before the first through-thickness crack forms, will lead to a redistribution of the stresses in the coating and substrate. It is useful to investigate the effects of plasticity on stress-redistribution by making use of an approximate model (see Appendix and [2]) and the associated software BIAxIAL, that has been shown by means of FEA to provide accurate predictions for a coated system subject to combined uniaxial tension and bending.

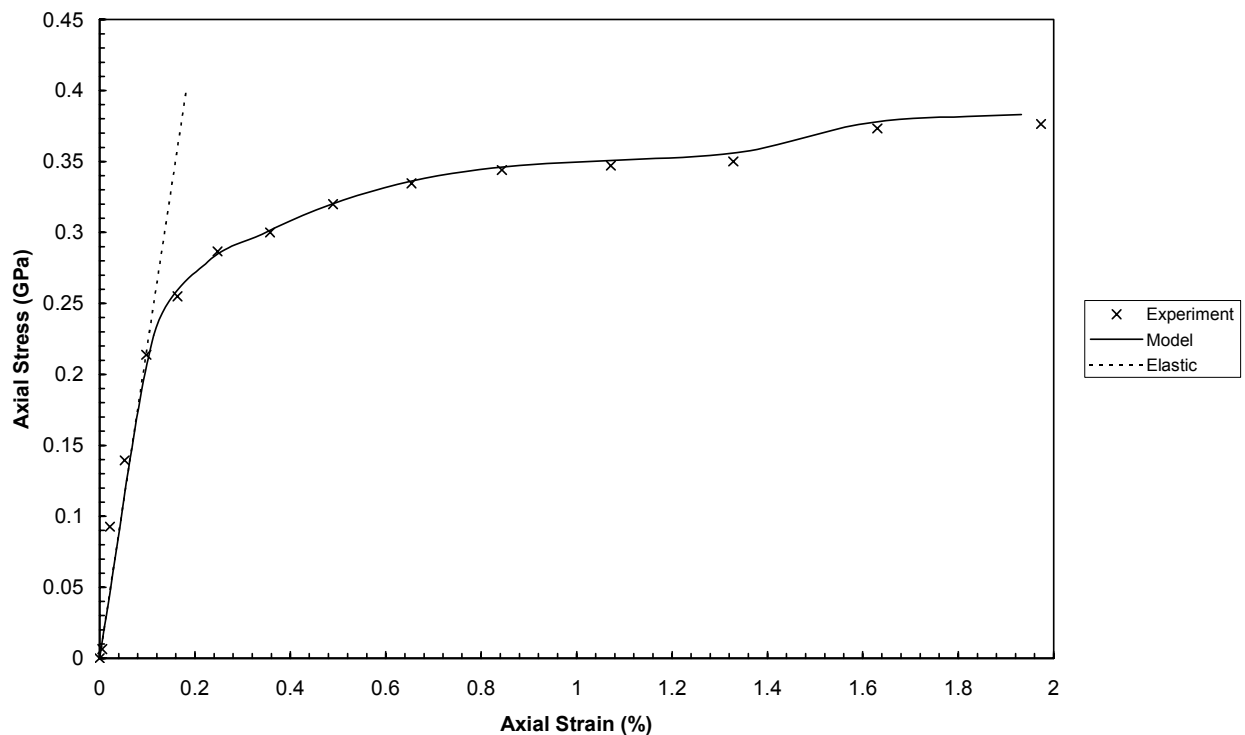


Figure 14 Stress strain curve for tension test on 304 stainless steel coated with CrN.

In order to model the effects of plastic deformation, the experimental stress-strain curve shown as discrete points in Figure 14 was used to define the plasticity data needed by the software system BIAxIAL (see Appendix and [2] for details of plasticity modelling). While the discrete points shown in Figure 14 were obtained during a tensile test for a $5\text{ }\mu\text{m}$ coating

on CrN on a 304 stainless steel substrate of thickness 3.00 mm, the stress-strain response will be almost identical to that for a homogeneous sample of substrate material. The dotted straight line in Figure 14 represents the linear elastic response based on a substrate Young's modulus of 220 GPa. By assuming that the discrete data in Figure 14 is valid for the substrate material alone, it is possible to estimate the plasticity curves for the substrate by the application of the software system BIAXIAL (using linear interpolation between discrete values). The yield stress assumed is 0.22 GPa. On using plasticity data obtained by this method it is then possible to predict the stress-strain response of the coated system. The prediction is shown as a continuous line in Figure 14 that follows very closely the experimental data, as to be expected.

An attempt will now be made to compensate for the effects of plastic flow in the substrate during tensile loading that leads to the formation of through-thickness cracks during a tensile test. The applied strains, that correspond to the applied stress 2.23 GPa predicted by COAT to be sufficient to form the first through thickness crack in the coating, are used as input values for the elastic-plastic model (see Appendix and [2]) that predicts the stresses and deformation in the coated system assuming that there are no cracks present. This calculation is achieved using the software application BIAXIAL that takes account of the combined effect of in-plane biaxial loading and out-of-plane bending about orthogonal axes. On applying the elastic strains it is found that in the corresponding elastic-plastic calculation the applied stress would have reached the value 0.34 GPa. This is comparable with the average applied stress 0.32 GPa that was observed in experiments to be the stress at which through-thickness cracks first formed (see Figure 11). The model indicates that at this value of the applied stress the axial stress in the coating has the value 0.90 GPa, almost the same value as for the tensile test when a plasticity correction has been made. It should be noted that Figure 14 shows there has been some localised interface debonding. It is emphasised that such debonding has not been modelled.

7.3 Four-point bend test

It is now useful to attempt to test the model for through-thickness cracking by making predictions of the applied bending moment per unit cross-sectional area at which the first through-thickness crack would form during a four-point bend test. This is achieved using the software application ENERGY. The temperature difference $-392\text{ }^{\circ}\text{C}$, relevant for a coating Young's modulus of 244 GPa, between the test temperature ($20\text{ }^{\circ}\text{C}$) and the stress-free temperature of the system ($412\text{ }^{\circ}\text{C}$) is applied, so that before loading the coating has a compressive residual stress of -1.97 GPa . The predicted applied bending moment per unit area in a four-point test for the formation of the first through-thickness crack in the coating is 1.115 MN/m . For this loading, the maximum tensile stress in the coating is 0.45 GPa , almost the same value that was found in the uniaxial tension and thermal fracture cases. However, the tensile yield strength of the stainless steel substrate is 0.22 GPa (Figure 14) indicating that plastic deformation must have occurred in the substrate.

It is again useful to investigate the effects of plasticity on stress-redistribution by making use of an approximate model (see Appendix and [2] and the associated software BIAXIAL. On using substrate plasticity data obtained by the method described for tensile loading, it is possible to predict the stress-strain response of the coated system during 4-point bending using BIAXIAL the elastic-plastic model that predicts the stresses and deformation in the coated system assuming that there are no cracks present. The applied biaxial and bending strains used for input correspond to the value 1.115 MN/m of the applied bending moment

per unit cross-sectional area predicted by ENERGY to be sufficient to form the first through-thickness crack in the coating. It is found that in the corresponding elastic-plastic calculation the applied bending moment per unit area would have reached the value 0.247 MN/m. This is comparable with the average applied bending moment per unit area 0.258 GPa that was observed in experiments to be equivalent to the stress at which through-thickness cracks first formed. The corresponding maximum coating stress is 0.89 GPa, which is almost the same value found in the uniaxial tensile loading case.

8. Conclusions

1. The thermal test for measuring fracture energies of coatings for through-thickness cracking, is the preferred method of testing, as plastic deformation is unlikely, thus avoiding a complicated analysis to interpret experimental measurements. This method is suitable only for coatings and substrates for which there is a sufficiently large difference in the values of the thermal expansion coefficients. The technique will measure the fracture energy corresponding to the temperature at which the coating first cracks.
2. If the fracture energy measured in a thermal test is used to predict the loading conditions for the formation of the first through-thickness crack in the coating for a tensile and four-point test, then there is reasonable agreement between the predictions and measurements.
3. Plasticity corrections need to be applied when thin coatings are examined using either the tensile or the four-point-bend techniques.
4. It is recommended that the coating to substrate thickness ratio should be as large as possible. This should avoid, in some situations, the need to consider corrections to measurements in order to account for plastic deformation.
5. It is recommended, when performing fracture tests, that a substrate should be used having as large a yield stress as possible, in order to reduce the plastic deformation that occurs locally at the crack tip, and macroscopically.
6. When testing thin coatings using tensile and four-point bend tests, it is recommended that uncoated samples are also tested in order to obtain high quality data that can be used to model the plasticity that occurs when coated samples are tested.

Acknowledgement

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APPENDIX 1

APPENDIX: Plasticity model of coated system for uniaxial tension and bending

A1 Introduction

There is a need to understand the elastic-plastic deformations that arise during the fracture testing of coated systems. The first objective of this technical note is to describe an approximate method of predicting the axial stress and axial strain distributions in a coated system subject to combined uniaxial tension and bending in the absence of thermal residual stresses. The second objective is to investigate the performance of the approximation by comparing predictions with FEA solutions.

A2 Geometry

Consider first of all a multiple layered system made of n different materials labelled $i = 1 \dots n$ as shown in Figure A1, some or all of which can behave as elastic-plastic materials. The x -coordinate is defined in the through-thickness direction and the y -coordinate is defined in the axial direction of the system. The upper and lower surfaces are at the locations $x = x_0$ and $x = x_n$, while the interfaces between the various materials are at $x = x_1, x_2, \dots, x_{n-1}$. The total thickness of the system is $h = x_n - x_0$.

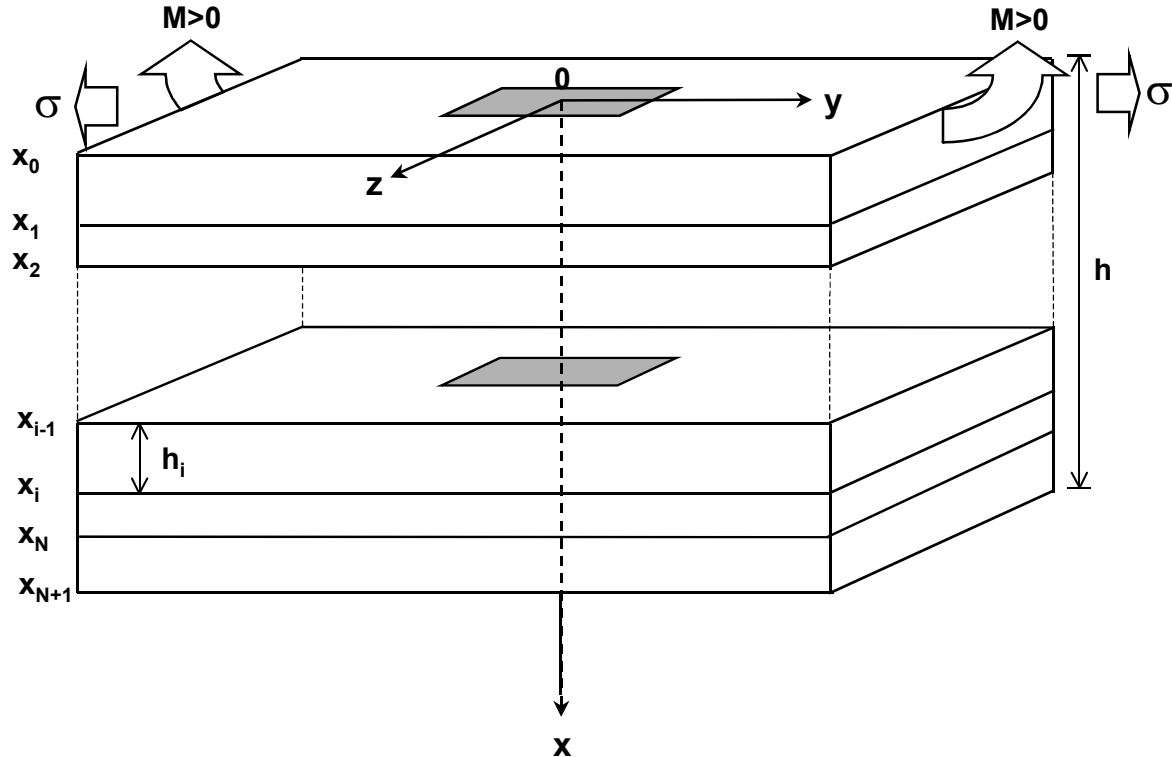


Figure A1 Schematic diagram of the geometry and coordinate system for the layered system.

A3 Elastic-plastic deformation

The layered system is subjected to a state of combined uniaxial tensile force per unit width F in the axial direction and bending moment per unit area M , leading to the displacement distribution

$$v_i = (\varepsilon + \hat{\varepsilon} x) y, \quad i = 1 \dots n, \quad (A1)$$

where v_i is the displacement component for the i^{th} layer in the y -direction, and where ε and $\hat{\varepsilon}$ are the axial strain and curvature of the laminate when subject to combined uniaxial tension and pure bending. The x -coordinate is selected so that the origin is on the lower surface of the system. The parameter ε then denotes the axial strain on $x = 0$ and $\hat{\varepsilon} = 1/\rho$ where ρ is the radius of curvature of the lower surface. Denoting the axial stresses experienced by the i^{th} layer to be $\sigma_i(x)$, the uniaxial stress-strain relation of the i^{th} layer of the system is assumed to be of the general form (assuming that Poisson ratio effects can be ignored)

$$\sigma_i(x) = E_i[\varepsilon_i(x) - \alpha_i \Delta T] - \phi_i(\varepsilon_i(x)), \quad (A2)$$

defined for both positive and negative values of the axial strain $\varepsilon_i(x)$ in the i^{th} layer which has the form

$$\varepsilon_i(x) \equiv \frac{\partial v_i}{\partial y} = \varepsilon + \hat{\varepsilon} x. \quad (A3)$$

When writing (A2) it has been assumed that the other stress components (transverse and through-thickness) are negligible. The parameter ΔT denotes the temperature difference between the current temperature of the layered system (assumed uniform) and the stress-free temperature. The Young's modulus and thermal expansion coefficient for the i^{th} layer in the axial direction are denoted by E_i and α_i respectively. The function $\phi_i(\varepsilon)$ denotes the effect on the stress-strain curve of plastic flow in the i^{th} layer. The function will be zero when $\varepsilon < \varepsilon_Y^i$ where ε_Y^i is the yield strain for the i^{th} layer.

From (A3) the axial strain is linear in x so that for $x_{i-1} \leq x \leq x_i$, $i = 1 \dots n$

$$\sigma_i(x) = \Phi_i(\varepsilon + \hat{\varepsilon} x) = E_i[\varepsilon + \hat{\varepsilon} x - \alpha_i \Delta T] - \phi_i(\varepsilon + \hat{\varepsilon} x). \quad (A4)$$

Ignoring Poisson's ratio terms, it is assumed that stresses within the laminate can arise from any combination of mismatched thermal expansion coefficients, an applied in-plane loading that is equivalent to an applied axial force F acting at the mid-point between the upper and lower surfaces of the laminate, and an applied bending moment per unit area of laminate M . From mechanical equilibrium

$$F = h \sigma = \sum_{i=1}^n \int_{x_{i-1}}^{x_i} \sigma_i(x) dx, \quad (A5)$$

and

$$M = \frac{1}{h} \sum_{i=1}^n \int_{x_{i-1}}^{x_i} \left(x - \frac{h}{2} \right) \sigma_i(x) dx, \quad (A6)$$

where σ is the effective axial applied stress. On substituting (A4) into (A5) and (A6) the following expressions are obtained on changing the variable of integration:

$$F = h\sigma = \sum_{i=1}^n \int_{\varepsilon_{i-1}}^{\varepsilon_i} \Phi_i(e) \frac{de}{\hat{\varepsilon}}, \quad (A7)$$

and

$$M = \frac{1}{h} \sum_{i=1}^n \int_{\varepsilon_{i-1}}^{\varepsilon_i} \left(\frac{e - \varepsilon}{\hat{\varepsilon}} - \frac{h}{2} \right) \Phi_i(e) \frac{de}{\hat{\varepsilon}}, \quad (A8)$$

where $\varepsilon_i = \varepsilon + \hat{\varepsilon} x_i$ denotes the axial strain on the interface $x = x_i$.

It is now observed that for a laminate, with a specified uniform temperature distribution defined by the value of ΔT , subject to a given bending moment per unit area M , and to an effective applied axial stress σ , the relations (A7) and (A8) enable the parameters ε and $\hat{\varepsilon}$ to be calculated and substituted into (A4) enabling the axial stress distribution $\sigma_i(x)$ in each layer to be found. On using (A7) the relation (A8) may be written in the form

$$M + \frac{1}{2} h\sigma = \frac{1}{h} \sum_{i=1}^n \int_{\varepsilon_{i-1}}^{\varepsilon_i} \frac{e - \varepsilon}{\hat{\varepsilon}^2} \Phi_i(e) de. \quad (A9)$$

A4 Comments on the cracking of a thin elastic layer on a thick substrate

The analysis described above, to account in an approximate way for the effects of plasticity during the combined tensile and bending loading of a multi-layered system, is now applied to a simple system comprising a very thin elastic coating, having thickness in the range 0.1-10 μm , that is perfectly bonded to an elastic-plastic substrate having a thickness that has a thickness in the range 0.1-1 mm. The applied bending load is assumed to be such that, in the absence of tensile loading, the coating deforms in a state of tension rather than compression. The phenomenon of interest is the prediction of cracking in the elastic coating in the presence of elastic-plastic deformation in the substrate, and of thermal residual stresses.

It is clear from experiments that the substrate can exhibit significant elastic-plastic deformation before the first through-thickness coating crack forms. The above analysis enables this deformation to be predicted in an approximate way. The coating crack is assumed to form under conditions of fixed loading, and as the coating is very thin compared to the thickness of the substrate, the additional deformation arising from crack formation will be very small when compared to the deformation that has occurred prior to crack formation. Any plastic flow that occurs during crack formation will either be associated with the macroscopic deformation of the system, or with localised plastic flow in the substrate associated with the stress concentration at the crack tip. Both these types of plastic deformation are assumed to be negligible when compared to the deformation present just before the first crack forms.

When adopting an energy balance approach to crack formation it is necessary to be able to calculate the energy of unit length of the layered system both with and without a crack. The deformation change arising from the formation of the first crack is assumed to be elastic so that existing methods of estimating the energy change can be used. It should be noted that the effective fracture energy resulting will, however, be affected by the localised plastic

deformation associated with the crack tip. In particular the fracture energy will be greater than that which would result if no plastic had deformation occurred, as there is a localised energy dissipation resulting from the localised plastic flow near the crack tip. This is exactly the situation for the analysis of fracture in homogeneous systems when small-scale yielding conditions prevail. For this case the cracks are analysed using the energy release rate G defined for linear elastic materials, and the effect of plasticity is absorbed in the critical value G_c of the energy release rate such that fracture occurs when $G > G_c$. The approach to be adopted for the prediction of fracture in an elastic coating is fully consistent with this approach.

A consequence of the methodology described is that the fracture energy that will be measured in a fracture experiment will be a characteristic of both the coating and the substrate. The value measured can, however, be applied to predict cracking in coatings and substrates having different thicknesses, or including additional coating layers having different properties.

A5 Modelling the effects of plastic deformation in steel layers

A multi-layered system containing elastic layers and elastic-plastic steel layers is now considered. For the steel layers, a plasticity model is used when the uniaxial yield stress was taken to be $\epsilon_y = 200$ MPa. The incremental plasticity model used is the standard Mises yield surface with associated flow and isotropic hardening. The properties for steel are used where $E = 210$ GPa and $\nu = 0.29$ for the elastic region, and for the plasticity model the elastic-plastic stress-strain curve assumed is specified by the data given in Table A1.

Table A1 Stress-strain values used for plastic substrate modelling.

Stress (MPa)	Elastic strain (%)	Plastic strain (%)	Total strain (%)
0	0	0	0
200 (Yield stress)	0.0952	0	0.0952
246	0.1171	2.35	2.47
294	0.1400	4.74	4.88
374	0.1781	9.35	9.53
437	0.2081	13.77	13.98
480	0.2286	18.0	18.23

A6 A comparison of the analytic model with finite element analysis (FEA)

A finite element model was constructed and used to compare layer stress profile predictions with those determined by the analytical model for a coated system under uniaxial loading. Results were generated for an uncracked coated model with an elastic coating and an elastic-plastic substrate and also just the elastic-plastic substrate only. A combined axial strain and axial bending strain were applied to the coated system which consisted of a 3 μm thick titanium nitride (TiN) coating applied to a 900 μm thick steel substrate, as shown in Figure A2. The moduli, Poisson's ratios and thermal expansion coefficients for TiN and steel are shown in Table A2.

Table A2 Coating (TiN) and substrate (steel) property data.

	E (GPa)	ν	α ($^{\circ}\text{C}^{-1}$)
TiN	425	0.2	1.0×10^{-5}
Steel	210	0.29	1.2×10^{-5}

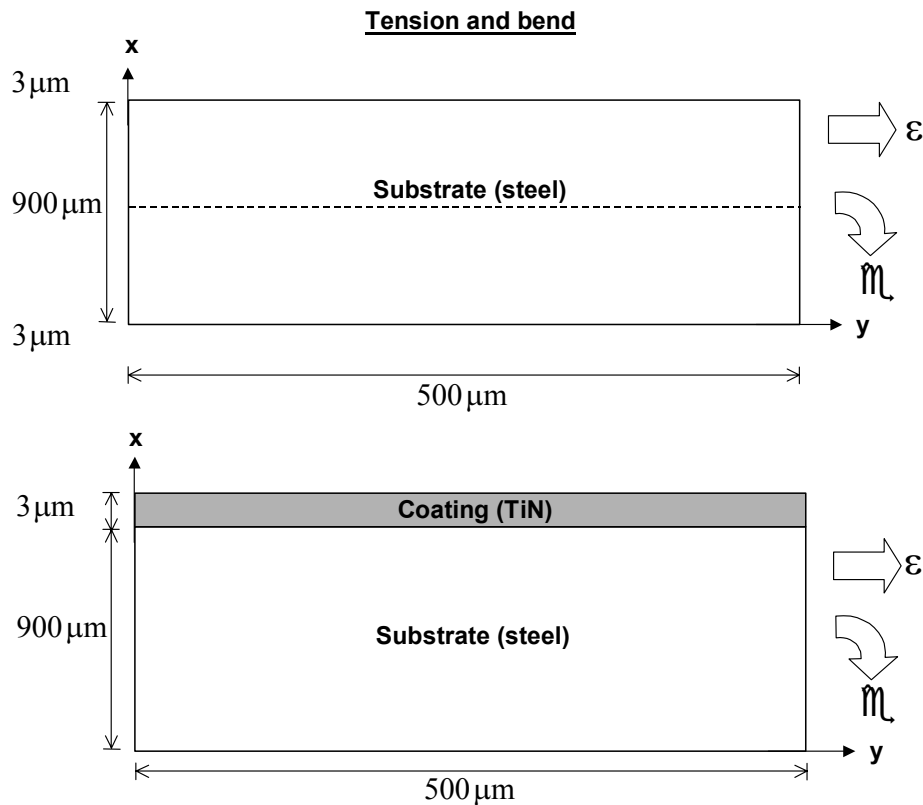
The length of the sample is set at 1000 μm with a plane of symmetry at $y = 500 \mu\text{m}$ on which the shear stress is $\sigma_{xy} = 0$. Both the FEA and analysis in this report effectively model a two-dimensional system where unit width is assumed. Boundary conditions imposed on the two-layer system were horizontal displacements between 9.53 μm (at $x = 903\mu\text{m}$) and 0.5 μm (at $x = 0$), increasing linearly with increasing height. For the combined bending and tension case, the axial displacement at was set at $v = (0.001 + 0.00002x)L$ where $L = 500 \mu\text{m}$ resulting in an application of an axial strain $\epsilon = 0.001$ and curvature of $\hat{\epsilon} = 0.00002 \mu\text{m}^{-1}$. For the substrate only, the horizontal displacements applied were between 9.53 μm (at $x = 0$) and 0.5 μm (at $900\mu\text{m}$), increasing linearly with increasing height, resulting in an axial strain of $\epsilon = 0.01906$ and curvature of $\hat{\epsilon} = -2.00667 \times 10^{-5} \mu\text{m}^{-1}$.

It should be noted that to compare with the analytical model the coated system is subjected to a uniaxial strain only and the stress is fixed at zero in the transverse direction. The FEA calculations were run using the ABAQUS finite element software. The mesh was made up of type CPE8 elements, which are 8-noded bilinear plane strain elements. These elements have been used successfully for other models of cracked coatings.

Table A3 shows a comparison of the values at the free surface and interface of the coating and substrate for the analytical model and FEA. The loading conditions chosen produce stresses where the substrate behaviour is plastic. Figures A4, A5 and A6 show the axial through-thickness stress profiles calculated by the analytical model and FEA for the coated system (coating and substrate) and substrate only. As can be seen the analytical model accurately predicts the stress behaviour calculated by FEA in all cases.

Table A3 A comparison of axial stresses calculated by the analytical model and FEA.

	Axial Stress Coating (MPa)	Axial Stress Substrate (MPa)
Analytical Model	8100.50 (free surface) 8075.00 (interface)	200.09 (free surface) 234.96 (interface)
FEA	8101.00 (free surface) 8076.00 (interface)	210.10 (free surface) 235.00 (interface)

*Figure A2 Schematic diagrams of the combined axial tension and bend loading modelled by FEA for the substrate only and two-layer coated systems.*

The values for the axial global stress and axial bending moment, calculated by averaging the axial stress for each layer, are shown for the steel only system and TiN/steel coated system in Table A4.

Table A4 Global axial stresses and bending moment calculated by the analytical model

	Axial Global Stress (MPa)	Axial Bending Moment (MNm^{-1})
Steel only	217.58	2.624×10^{-3}
Coated System	263.24	2.632×10^{-3}

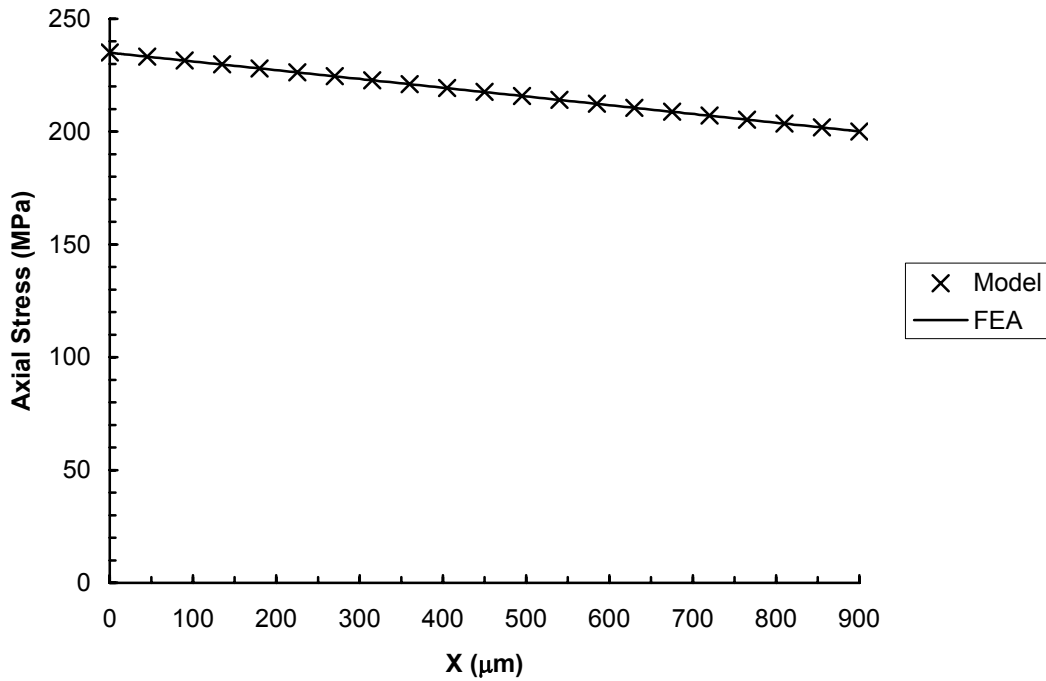


Figure A3 *A comparison of the through-thickness axial stress profile predictions from the analytical plasticity model and FEA for steel substrate only subjected to axial tension and bending.*

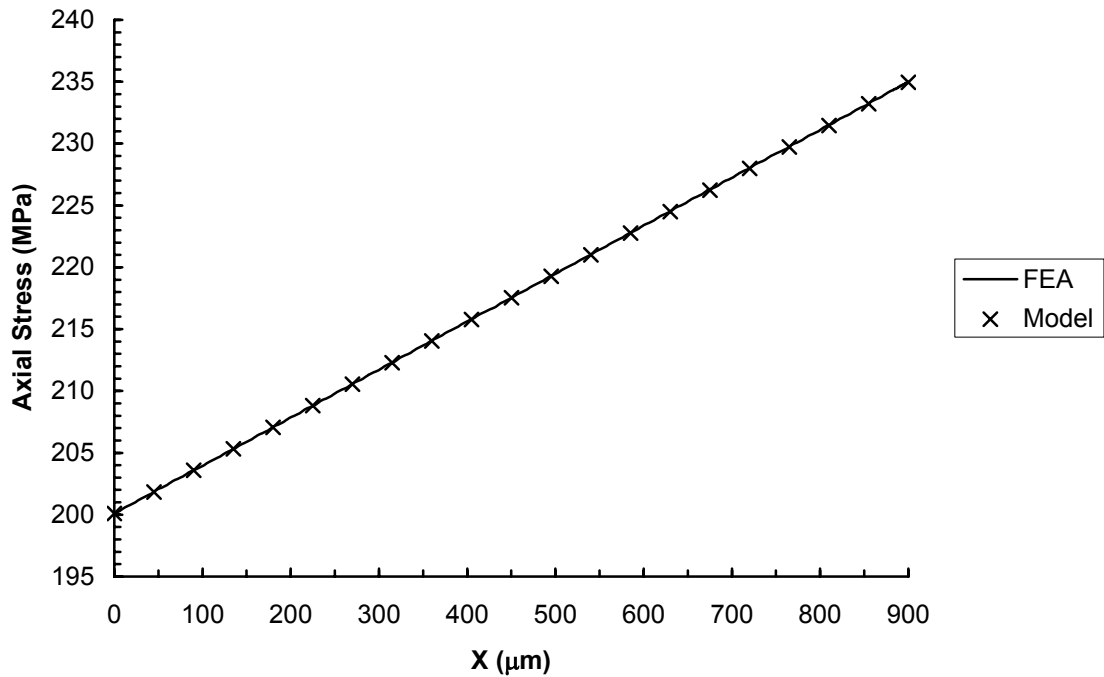


Figure A4 *A comparison of the through-thickness axial stress profile predictions from the analytical plasticity model and FEA for the steel substrate of a coated system subjected to axial tension and bending.*

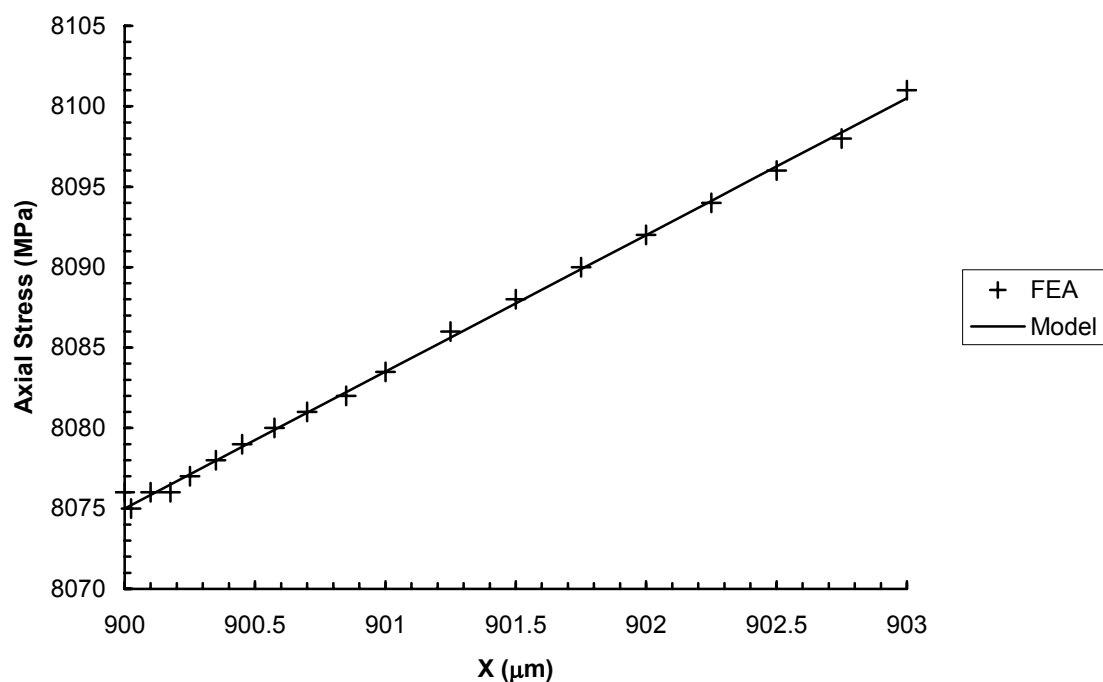


Figure A5 A comparison of the through-thickness axial stress profile predictions from the analytical plasticity model and FEA for the TiN coating of a coated system subjected to axial tension and bending.

A7 Conclusion

The approximate model for analysing the stress and strain distributions in a coated system subject to combined uniaxial loading and bending, that leads to yielding of the substrate, has been shown to give predictions that are in very good agreement with corresponding FEA solutions.