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High-precision determination of residual stress of polycrystalline coatings using optimised XRD-sin 2ψ technique

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High-precision determination of residual stress of polycrystalline coatings using optimised XRD- $\sin^2\psi$ technique

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Abstract

The aim of the research is to optimize the XRD- $\sin^2\psi$ technique in order to perform high precision measurement of surface residual stress. Residual stresses existing in most hard coatings have significant influence on the adhesion, mechanical properties and tribological performance. In the XRD- $\sin^2\psi$ stress measurement, the residual stress value is determined through a linear regression between two parameters derived from experimentally measured diffraction angle (2θ). Thus, the precision coefficient (R^2) of the linear regression reflects the accuracy of the stress measurement, which depends strongly on how precise the 2θ values are measured out of a group of very broad diffraction peaks. In this research, XRD experiments were conducted on a number of samples, including an electron beam evaporated ZrO_2 based thermal barrier coating, several magnetron sputtered transition metal nitride coatings, and shot-peened superalloy components. In each case, the diffraction peak position was determined using different methods, namely, the maximum intensity (I_{max}) method, the middle point of half maximum (MPHM) intensity method, the gravity centre method, and the parabolic approaching method. The results reveal that the R^2 values varied between 0.25 and 0.99, depending on both the tested materials and the method of the 2θ value determination. The parabolic approaching method showed the best linear regression with $R^2 = 0.93 \pm 0.07$, leading to high precision of the determined residual stress value in all cases; both the MPHM ($R^2 = 0.86 \pm 0.16$) and gravity centre ($R^2 = 0.91 \pm 0.11$) methods also gave good results in

most cases; and the I_{\max} method ($R^2 = 0.71 \pm 0.27$) exhibited substantial uncertainty depending on the nature of individual XRD scans.

1 Introduction

Residual stresses have significant influence on the properties and performance of engineering materials such as wear resistant coatings [1], work hardened surfaces [2], welds and castings [3]. For hard coatings grown by physical vapour deposition, residual stresses are developed under intensive ion bombardment, which may lead to poor adhesion strength to the substrate surface and subsequently affect the wear resistance and corrosion resistance. For surface strengthening of metallic components, shot peening is a widely used technique to improve the fatigue resistance where the beneficial effect derives from the built-up of a compressive surface residual stress. The origin of residual stresses in metal welds is the inhomogeneous heating and subsequent cooling of the welds and the adjacent regions. Residual stresses have been recognised as one of the major causes of welding failures. In many circumstances, it is recommended to precisely measure and control the residual stresses.

Residual stresses can be measured by using various techniques including X-ray diffraction (XRD), neutron diffraction, wafer curvature, hole drilling, ultrasonic method, and electrical-magnetic methods [4]. Among these techniques, both the XRD and wafer curvature techniques are widely used for the determination of surface residual stresses whereas few literatures reported comparison between the two techniques. In literatures [5 - 6], the residual stresses of magnetron sputtered CrN and TiN coatings deposited on thin silicon wafers were measured using both the XRD and curvature techniques, which reported good consistence in the results obtained from the two techniques. In literature [7], substantially different values of residual stress on zirconia thermal barrier coatings were measured using the two techniques. The wafer curvature method was established following the famous Stoney's formula and is able to measure the macro average stress in a surface layer or a coating based on assumptions of homogeneous, isotropic and linear elastic coating and substrate [8]. To ensure sufficient precision in the curvature measurement, in many cases the coatings for stress measurement

were deposited on specially prepared thin and large size silicon wafers [5 – 7, 9] or steel sheets [10].

In contrast, the XRD- $\sin^2\psi$ technique was developed from the theories of crystallography and solid mechanics [11 – 13]. Given the limited penetration of X-rays in solid surfaces, what the XRD- $\sin^2\psi$ technique measures is the surface residual stress in a depth of up to a few micrometers. In experiments, the XRD- $\sin^2\psi$ stress measurement starts from XRD scans at a series of fixed incident angles and over a pre-defined diffraction angle. In each obtained scan, the chosen diffraction peak position has to be accurately determined, i.e. the 2θ value has to be measured from a very broad and sometimes irregularly shaped peak. The obtained 2θ values are then used to perform the linear regression in order to obtain the slope and intercept values to be used for the stress calculation.

The accuracy of the XRD- $\sin^2\psi$ residual stress measurement depends on the minimization of various measurement errors derive from several sources, e.g. the material to be measured, the instrument setup and the data processing [4, 11 – 13]. In terms of the tested materials, it is often the case that the surfaces to be measured are not ideally flat, may contain coarse crystalline grains, strong texture, high density of lattice defects and an in-depth stress gradient. Consequently, the diffraction peaks obtained in such materials have different scales of broadening, roughening and asymmetry. Provided that other errors have been minimized, such as those caused by the instrumental setup and the Lorenz-Polarization-Absorption factors, then it is the precise positioning of the diffraction peak, i.e. the 2θ angle, which eventually determines the precision of the residual stress calculation. In the literatures [11 – 12] several peak positioning methods have been recommended for quantitative XRD work. For example, the diffraction peak position 2θ can be defined as the angle referring to the maximum X-ray intensity (i.e. the I_{\max} method), the middle position of the width at half maximum intensity (the MPH method) or the geometric centre of the whole diffraction peak (the gravity centre

method). Alternatively, the 2θ value can also be determined by the line approach method, which applies a known mathematical expression to approach the experimentally obtained XRD curve and then works out the peak position of the mathematical expression as the 2θ value. The best known approaching process has been the parabolic approaching. Obviously, determination of the 2θ values by using the different methods mentioned above is expected to have substantial uncertainty. This is true especially when real materials to be tested have coarse and or extremely fine grain sizes, high density of lattice defects, texture, or in-depth stress gradient. In these circumstances, how the diffraction peaks are measured becomes a decisive factor to the precision of residual stress determination.

Although XRD- $\sin^2\psi$ technique has been widely used in stress measurement [1, 5 – 7, 11 – 14], however, little published work is available which provides a systematic evaluation of the influence of the different 2θ value determinations on the precision of the residual stress calculation. Obviously this lack of knowledge brings about remarkable uncertainty in stress determination. This paper aims to evaluate the effect of different diffraction peak positioning methods on the precision of the linear regression data processing employed in the XRD- $\sin^2\psi$ residual stress measurements. A number of typical materials have been selected in these experiments, including PVD hard coatings, thermal barrier coating and shot peened superalloy components. For each diffraction peak curve obtained, the above mentioned peak positioning methods were applied to determine the Bragg diffraction angles. The residual stress values were then derived from the measurements and were compared with each other.

2 The XRD- $\sin^2\psi$ technique

The XRD- $\sin^2\psi$ technique calculates the residual stresses existing in the surface layer of polycrystalline materials by assuming a plane-stress state. The theory of the technique can be

found in numerous literatures, e.g. in [1, 7, 12 - 14]. Figure 1 illustrates schematically the in-plane stress σ_ϕ with respect to the two principal stress components σ_1 and σ_2 . When a X-ray beam hits the sample surface at an incident angle Ω , those grains, with their (hkl) lattice planes meeting the Bragg diffraction condition and having an off-axis angle ψ with respect to the sample surface normal, emit a diffraction X-ray beam at a diffraction angle 2θ . Then the d-spacing $d_{\phi\psi}$ of the (hkl) lattice plane is measured. The principal formula for the XRD- $\sin^2\psi$ stress measurement can be written as:

$$\frac{d_{\phi\psi} - d_0}{d_0} = \left(\frac{1 + \nu}{E}\right) \cdot \sigma_\phi \cdot \sin^2(\psi) - \left(\frac{\nu}{E}\right) \cdot (\sigma_1 + \sigma_2) \quad (1)$$

where E and ν stand for the Young's modulus and the Poisson's ratio normal to the (hkl) orientation of the material respectively, and d_0 the lattice spacing at stress-free condition. It should be pointed out that, the surface of a polycrystalline material contain large quantity of grains having different orientations and, more importantly, these grains exhibit an elastic anisotropy. In order to describe the deformation of the individual crystallites and hence the lattice spacing due to an in-plane stress state, a grain interaction model is needed [15 – 16]. It was reported that only in the rare case of a (001) or (111) textured film of cubic material the film is in plane elastic isotropic and no grain interaction model is needed [6]. In the present paper we assume elastic isotropy in the individual crystallites and hence forgo the use of a grain interaction model.

Assuming $\sigma_\phi = \sigma_1 = \sigma_2$ when the in-plane stress σ_ϕ is independent of the orientation,

Equation (1) can be re-written as:

$$\mathbf{d}_{\phi\psi} = \left[\left(\frac{1 + \nu}{E}\right) \cdot \sin^2(\psi) - \left(\frac{2\nu}{E}\right) \right] \cdot \sigma \cdot d_0 + d_0 \quad (2)$$

Then Equation (2) can be treated as a linear function $\mathbf{Y} = \mathbf{a} \cdot \mathbf{X} + \mathbf{b}$ by letting:

$$Y = d_{\phi\psi} = \frac{\lambda}{2 \cdot \sin(\theta)}; X = \left[\left(\frac{1+\nu}{E} \right) \cdot \sin^2(\psi) - \left(\frac{2\nu}{E} \right) \right] \quad (3)$$

Therefore after making a series of XRD scans covering a known Bragg 2θ at fixed glancing angles Ω_i (for $i = 1, 2, 3$, etc.), the Bragg diffraction half angle θ_i can be measured in each diffraction peak and the associated off-axis angle ψ_i is calculated according to the relation $\psi_i = \theta_i - \Omega_i$. The obtained θ_i and ψ_i are subsequently used to calculate the data group $\{X_i, Y_i\}$ according to Equation (3), from which a linear regression processing of Equation (2) is used to obtain the value of the constants **a** and **b**. Finally the in-plane stress σ , as well as the strain-free lattice d-spacing d_0 , can be obtained from the relations $d_0 = b$ and $\sigma = a/d_0$ respectively.

3 Experimental

Table 1 shows the sample materials used in the residual stress measurement. Samples 1 – 8 are magnetron sputtered transition metal nitride coatings grown in three different laboratories using various magnetron sputtering processes. The TiAlN/VN is a nano-structured TiAlN and VN multilayer coating grown by unbalanced magnetron sputtering deposition [17]. The TiAlCrYN is another unbalance magnetron sputtered coating having chemical composition of $Ti_{0.43}Al_{0.52}Cr_{0.03}Y_{0.02}N$ [17]. The TiCN and TiSiCN coatings were grown by plasma enhanced magnetron sputtering deposition [18]. The TiN and CrTiAlN coatings were grown by close field unbalanced magnetron sputtering deposition [19]. Details of the deposition, structure characterization, and properties of the coatings have been published in previous publications [17 - 19]. Sample 9 is a tetragonal ZrO_2 based thermal barrier coating (TBC) grown by an electron beam PVD process. Samples 10 - 12 are Ni-Cr superalloy components subjected to a shot peening surface strengthening at different conditions. The TBC and superalloy samples were provided by a UK based aerospace company.

A computer programmed Philips X-Pert X-ray diffractometer was employed for the X-ray diffraction work, using a Cu K_{α} radiation source ($\lambda = 0.154056$ nm for $K_{\alpha 1}$) working at 40 KV and 40 mA. The incident X-ray beam was introduced through a 15 mm width window, a 0.5° divergence slit and a 0.25° anti-scattering slit, to hit the sample surface at a fixed incident angle Ω . A computer controlled Omega-goniometer was used for the ψ tilt. For each sample the lattice plane used for the stress measurement was experimentally selected following a Bragg-Brentano ($\theta - 2\theta$) XRD scan. As a criterion for the selection, the selected diffraction peak should be a well-shaped high-intensity single diffraction peak, i.e. not significantly overlapping with diffractions of the substrate material. The Ω values and the diffraction peak chosen for each sample are listed in Table 1. At each incident angle Ω , a slow $\Omega - 2\theta$ scan was undertaken for the selected diffraction peak range at a small step size of 0.0167° and a step period time between 200 and 400 seconds depending on the sample material. Because the aim of the research was in the comparative study between different peak positioning methods, a simplification was made by assuming the elastic constants of the nitride coatings to be $E = 300$ GPa and $\nu = 0.23$. The E and ν values of the TBC and superalloy materials were taken from the literature [14].

Prior to the diffraction peak measurement, the obtained XRD curves were treated by 9-point averaging, the Lorentz-polarization-absorption corrections [12], and background removing. Each treated curve was then analysed to determine the diffraction peak angle 2θ using four peak positioning methods shown in Table 2. For each series of XRD scans the obtained data group $\{\Omega_i, 2\theta_i\}$ was used for the residual stress calculation by the linear regression as described in Equations 2 – 3. In addition to the slope \mathbf{a} and the intercept \mathbf{b} which were used to calculate the residual stress value, the precision factor (\mathbf{R}^2) and the standard deviation of the slope ($\Delta\mathbf{a}$) were also determined. Then the error of the stress arising from the regression

treatment was determined as $\Delta\sigma = \Delta a/d_0$. Finally, the calculated residual stress was expressed as $\sigma \pm \Delta\sigma$.

4 Results and discussion

4.1 Diffraction angles determined by different peak positioning methods

As an example of the residual stress measurements, Figure 2a shows a group of XRD scans obtained on the magnetron sputtered TiN coating. These Ω - 2θ scans were acquired in the 2θ period $35.5^\circ - 37.5^\circ$ and at a range of Ω angles from 8.5° to 31° , referring to the off-axis angles $\psi = 10^\circ \sim -13.5^\circ$. The diffraction peak angles (2θ) measured by using the four different methods are plotted against the off-axis angle ψ in Figure 2b. The four peak positioning methods led to different 2θ values for each XRD scan. The 2θ values determined by the I_{\max} method show large irregular variation, whereas those measured by the other methods show a smooth variation with the off-axis angle ψ . Figure 2c shows the linear regressions referring to the data groups measured by the I_{\max} and parabolic approaching methods. Note that the two peak positioning methods give rise to different precision factors with $R^2 = 0.96$ for the parabolic approaching and $R^2 = 0.47$ for the I_{\max} respectively.

4.2 Effect of diffraction peak positioning methods on the measured residual stress values

Table 3 summarizes the residual stress values of the sample materials determined by using the four peak positioning methods. The un-peened NiCr superalloy sample exhibits low residual stress, which was expected as a result of the manufacturing (machining) process, compared to the residual stresses in the shot-peened samples. The shot peening treatment resulted in significant level of residual compressive stresses. The TBC sample, a thick oxide

coating grown by electron beam evaporation, shows typically low residual stress. The TiCN and TiSiCN coatings, being grown by plasma assisted magnetron sputter deposition [18], all exhibit low compressive stresses, which favours good adhesion property and erosion resistance especially for the large thickness (i.e. over 30 μm). It was noted that the silicon-containing nanocomposite coatings show higher residual stress than the ternary TiCN. However, further discussion of the effect of chemical composition on the residual stress is not a topic of this paper. The TiAlCrYN coating shows residual compressive stress, but with lower values than in our previous measurements [17, 20]. The TiN and CrTiAlN coatings, being grown by close field unbalanced magnetron sputter deposition, show high compressive stresses. The high residual stress is related to the high hardness, dense deposited structure, and the (111) texture resulted under the deposition conditions [19]. The relationship between the coating density, texture and residual stress can be found in our previous publication [21]. The TiAlN/VN coating shows high levels of compressive stress which is in consistent with our previous reports [17, 21].

The magnitude of the difference in the measured compressive stress when measured by I_{max} and parabolic methods was dependent upon the material system and varied from +163% to -29%. The most common difference was of the order of $\pm 20\%$.

4.3 Effect of diffraction peak positioning methods on the precision of the measured stresses

In Table 3, the precision \mathbf{R}^2 values are shown to vary between 0.25 and 0.99 depending on the sample materials and on the peak positioning methods. It shows that low \mathbf{R}^2 values result in high values of the standard deviation of stress measurements. For some samples, such as the TiCN, TiAlCrYN and CrTiAlN-1, all the measurements show \mathbf{R}^2 values higher than 0.9 regardless of the peak positioning methods applied. This may be attributed to good quality of

the original diffraction data, including high intensity and or well-shaped diffraction peaks with good symmetry. On other samples, such as TiAlN/VN, TiN, un-peened Ni and CrTiAlN-3, the obtained R^2 values vary with the peak positioning methods.

In general, the parabolic approaching method gave rise to high R^2 values in all cases with one exception of low value $R^2 = 0.76$ for the NiCr-1 supper alloy sample. The overall average for the R^2 value obtained using the parabolic approaching method is $R^2 = 0.93 \pm 0.07$, suggesting that the parabolic approaching measurement gives consistently high precision.

The I_{\max} method, however, shows poor precision with the R^2 value as low as 0.25, which therefore led to large scattering of the determined residual stress values. The overall performance of the I_{\max} method is $R^2 = 0.71 \pm 0.27$. The performance of the other peak positioning methods lie between the parabolic approaching and the I_{\max} , with $R^2 = 0.86 \pm 0.16$ for the MPHMM and $R^2 = 0.91 \pm 0.11$ for the gravity centre methods respectively.

A survey of the R^2 distribution as a function of the peak positioning methods is shown in Figure 3. The parabolic approaching measurement assumes a symmetric profile in the top part ($I > 0.7I_{\max}$) of the diffraction peak in order to determine the top of peak position. Therefore, the lower parts of the diffraction peak, have much less effect on the measurement. The I_{\max} method, on the other hand, took account only a single point of a diffraction peak which has the maximum intensity. Uncertainty following this method could easily be caused by factors such as asymmetry, broadening and scattering fluctuation in the top period. Consequently this method is the most unreliable. In extremely cases, the obtained R^2 was as low as 0.25. For the other two methods applied, the MPHMM method uses the two half-maximum points in the diffraction curve to determine the peak position, whereas the gravity centre method takes the whole diffraction peak area into account. The R^2 values obtained following these two methods are significantly higher than the I_{\max} method and slightly lower than the parabolic approaching method.

4.4 Errors arising in the XRD- $\sin^2\psi$ residual stress measurement

According to literatures [22], the errors in the XRD- $\sin^2\psi$ residual stress measurement may arise from the following aspects:

- Errors in the diffraction peak measurement and in the XRD instrument setup;
- Nonlinear $d \sim \sin^2\psi$ relations due to the grain interactions and in-depth stress profile;
- Anisotropic elastic property of crystalline materials.

In the first, any error arising in the measured 2θ values will bring about errors in the two linear regression variables and thus lower the precision of the linear regression. This is because, as described in Equation (3), both variables in the linear regression formula are determined from the diffraction angle 2θ . However, large errors may be resulted in the diffraction peak positioning, which is especially true when most of the stressed surfaces give rise to large linear broadening in the diffraction peaks due to their nano- or sub-micron-scale grain sizes (e.g. in PVD coatings) or due to the high density lattice defects (e.g. in plastically deformed surfaces). It is unfortunate that there were only very limited number of literatures which provided the methods of diffraction peak positioning, e.g. the middle-width method in [23] and the 50% parabolic approach in [6], where in most other literatures the applied methods were not mentioned at all [7, 14, 24 – 27]. In the current research, it has been the first time that large number of experiments are conducted to show the substantial influence of the diffraction peak positioning methods on the precision of residual stress measurement. The parabolic approaching has been approved to be the most reliable method to conduct residual stress measurement at high precise.

Secondly, non-linear relationship may exist between the two regression variables in Equation (3) either due to grain interactions or due the existence of a depth profile of residual stress.

For the former, because the XRD- $\sin^2\psi$ stress calculation was originally developed to calculate macro residual stress in the surface of isotropic polycrystalline materials, the anisotropy of individual crystallites was not taken into account. In the past, several grain interaction models were proposed to address this issue, including the Voigt and the Reuss models which assume equal strain tensor and equal stress tensor respectively, the Neerfeld-Hill model suggesting the arithmetic average of X-ray and macroscopic elastic constants calculated from the Voigt and the Reuss models. More details of grain interaction models can be found in literatures [5, 16, 28]. For the latter, a depth profile of residual stress in coatings and thin films can be formed due the structural evolution during their growth [29 – 30]. For plastically deformed surfaces, e.g. after shot-peening or machining, the depth profile of residual stress is attributed to the varying plastic strain at different depth. These result in a nonlinear and splitting $d \sim \sin^2\psi$ curve [12 – 13].

Moreover, the error may also derive from improper adoption of the elastic modulus E and Poisson's ratio ν values in the calculation because of the remarkable anisotropic elastic property of crystalline materials. In case of TiN coatings, for example, the E_{macro} , $E_{(111)}$ and $E_{(200)}$ are different from each other whereas the anisotropy ratio was reported in a range of 1.26 ~ 3.8 [31].

Despite of these errors, the XRD- $\sin^2\psi$ technique is still considered as a reliable method for residual stress measurement in many applications, where the main concern is focused on the relative change of residual stress, instead of its absolute values, as a function of material processing parameters, such as the variation of substrate bias voltage in magnetron sputtering deposition, or different particle energies in shot-peening surface hardening. Nevertheless, accurate determination of diffraction angle is essential for precise measurement of residual stress whenever the XRD- $\sin^2\psi$ technique is applied. It is hoped that the results obtained from the current research will help for this purpose.

5 Conclusions

The precision of residual stress measurement using the XRD- $\sin^2\psi$ technique depends strongly on the accurate determination of diffraction peak positions. In this research, four widely used methods of peak positioning have been evaluated in term of the precision of the residual stress measurement and measurements have been carried out on a number of different sample types. The following conclusions can be drawn:

- (1) The parabolic approaching method obtained the best linear regression with $R^2 = 0.93 \pm 0.07$, leading to high precision determination of the residual stress value for all materials. This method is therefore recommended for the diffraction peak positioning of high precision residual stress measurement.
- (2) Both the gravity centre and MPHMM methods rank below the parabolic approaching but also show good results in most cases. These methods are also recommended for residual stress measurement.
- (3) The I_{\max} method is not recommended for residual stress measurement as it exhibited substantial uncertainty depending on the nature of individual XRD scans.

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Table 1 Sample materials and XRD parameters

No.	Material	E [GPa]	ν	(hkl)	2θ	Ω
1	TiAlN/VN	300	0.23	(220)	$60^{\circ} - 68^{\circ}$	$5^{\circ} - 55^{\circ}$
2	TiAlCrYN	300	0.23	(422)	$130^{\circ} - 135^{\circ}$	$5^{\circ} - 30^{\circ}$
3	TiCN	300	0.23	(422)	$121^{\circ} - 129^{\circ}$	$5^{\circ} - 55^{\circ}$
4	TiSiCN-1	300	0.23	(422)	$121^{\circ} - 129^{\circ}$	$5^{\circ} - 55^{\circ}$
5	TiSiCN-2	300	0.23	(422)	$121^{\circ} - 129^{\circ}$	$5^{\circ} - 55^{\circ}$
6	TiN	300	0.23	(111)	$35^{\circ} - 38^{\circ}$	$8.5^{\circ} - 31^{\circ}$
7	CrTiAlN-1	300	0.23	(422)	$131^{\circ} - 138^{\circ}$	$5^{\circ} - 25^{\circ}$
8	CrTiAlN-2	300	0.23	(422)	$131^{\circ} - 138^{\circ}$	$5^{\circ} - 25^{\circ}$
9	TBC	70	0.23	(321)	$102^{\circ} - 104^{\circ}$	$5^{\circ} - 40^{\circ}$
10	NiCr-0	214	0.31	(311)	$89^{\circ} - 93^{\circ}$	$12^{\circ} - 45^{\circ}$
11	NiCr-1	214	0.31	(311)	$89^{\circ} - 93^{\circ}$	$12^{\circ} - 45^{\circ}$
12	NiCr-2	214	0.31	(311)	$89^{\circ} - 93^{\circ}$	$12^{\circ} - 45^{\circ}$

Table 2 The diffraction peak positioning methods

Short name	Procedures
I_{\max}	The 2θ value is defined as the angle at the maximum intensity I_{\max} .
MPHM	<ol style="list-style-type: none"> 1. find out the I_{\max} value; 2. determine the values $2\theta_1$ and $2\theta_2$ from the curve referring to the half maximum intensity ($0.5 I_{\max}$); 3. $2\theta = 0.5 \times (2\theta_1 + 2\theta_2)$.
Gravity Centre	<ol style="list-style-type: none"> 1. make area integration from both sides of the diffraction curve; 2. find out the 2θ position which divides the diffraction peak area into two equal parts.
Parabolic approach	<ol style="list-style-type: none"> 1. Take the top part ($I > 0.7 \cdot I_{\max}$) of the curve to make a parabolic approach: $I = a \cdot (2)^2 + b \cdot (2) + c$; 2. $2\theta = \frac{-2a}{b}$.

Table 3 The mean value and standard deviation of residual stresses and the associated line regression precision R^2 determined by using different diffraction peak positioning methods

Coating	I_{\max}		MPHM		Gravity Centre		Parabolic	
	Stress [GPa]	R^2	Stress [GPa]	R^2	Stress [GPa]	R^2	Stress [GPa]	R^2
TiAlN/VN	-6.67 ± 3.14	0.43	-4.56 ± 1.89	0.49	-3.38 ± 0.99	0.66	-5.74 ± 0.88	0.89
TiAlCrYN	-0.56 ± 0.04	0.99	-0.84 ± 0.08	0.97	-0.79 ± 0.06	0.98	-0.74 ± 0.05	0.99
TiCN	-0.44 ± 0.03	0.98	-0.48 ± 0.03	0.98	-0.59 ± 0.03	0.99	-0.44 ± 0.04	0.97
TiSiCN-1	-2.94 ± 1.27	0.64	-0.76 ± 0.27	0.72	-0.81 ± 0.06	0.98	-1.12 ± 0.09	0.98
TiSiCN-2	-0.74 ± 0.05	0.98	-0.55 ± 0.05	0.98	-0.64 ± 0.02	0.99	-0.69 ± 0.04	0.98
TiN	-8.98 ± 4.74	0.47	-4.51 ± 0.45	0.96	-5.23 ± 0.82	0.91	-5.98 ± 0.60	0.96
CrTiAlN-1	-3.83 ± 0.29	0.98	-3.55 ± 0.31	0.98	-3.29 ± 0.30	0.98	-4.76 ± 0.67	0.94
CrTiAlN-3	-2.65 ± 1.15	0.64	-1.64 ± 0.33	0.89	-1.69 ± 0.23	0.95	-3.57 ± 0.76	0.88
TBC	-0.08 ± 0.02	0.76	-0.09 ± 0.01	0.98	-0.09 ± 0.01	0.91	-0.10 ± 0.01	0.93
NiCr-0	-0.40 ± 0.31	0.25	-0.35 ± 0.09	0.74	-0.22 ± 0.05	0.81	-0.31 ± 0.05	0.88
NiCr-1	-1.35 ± 0.23	0.77	-1.60 ± 0.27	0.78	-1.41 ± 0.23	0.78	-1.56 ± 0.28	0.76
NiCr- 2	-0.83 ± 0.54	0.37	-1.16 ± 0.12	0.96	-0.98 ± 0.06	0.98	-1.04 ± 0.08	0.98

Figure captions

Figure 1 A schematic diagram showing the set-up of the XRD- $\sin^2\psi$ in-plane stress measurement.

Figure 2 An example of data processing for the stress measurement, obtained from the TiN coating. (a) A group of XRD θ - 2θ scans at $\psi = -12.8^\circ \sim 13.3^\circ$; (b) Variation of the diffraction peak position (2θ) versus the off-axis angle (ψ); (c) Comparison of linear regressions between the I_{\max} and parabolic approaching methods.

Figure 3 Comparison of the values of the linear regression precision factor following the four diffraction peak positioning methods.