Residual stresses determination in textured substrates for plasma sprayed coatings

J Capek¹, Z Pala⁴,² and O Kovarik¹

¹ Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University in Prague, Trojanova 13, 12000 Prague, Czech Republic
² Institute of Plasma Physics, Za Slovankou 1782/3, 18200 Prague, Czech Republic
E-mail: capekjir@fjfi.cvut.cz

Abstract. In this contribution, we have striven to respond to the desire of obtaining the residual stress tensor in both cold-rolled and hot-rolled substrates designated for deposition of thermal coatings by plasma spraying. Residual stresses play an important role in the coating adhesion to the substrate and, as such, it is a good practice to analyse them. Prior to spraying, the substrate is often being grit blasted. Residual stresses and texture were quantitatively assessed in both virgin and grit blasted sample employing three attitudes. Firstly without taking preferred orientation into account, secondly from measurements of interplanar lattice spacings of planes with high Miller indices using MoKα radiation. And eventually, by calculating anisotropic elastic constants as a weighted average between single-crystal and X-ray elastic constants with weighting being done according to the amount of textured and isotropic material in the irradiated volume. In the ensuing verification analyses, it was established that the latter approach is suitable for materials with either very strong or very weak presence of texture.

1. Introduction

Joint occurrence of texture and residual stresses in metals is no rarity and it is well known that determination of the stress tensor by X-ray diffraction is not, in this case, a straightforward task and calls for both experimental procedures and data processing algorithms beyond the standard ones employed for isotropic and fine-grained polycrystalline materials. For now, a universal approach with the potential to correctly and properly evaluate the residual stresses in textured materials is, sadly, still lacking and this issue is tackled either, in the worst scenario, by neglecting the texture or by choosing one of the hitherto proposed methods.

The value and homogeneity of residual stresses and surface roughness of materials used as substrates for thermal coatings have also significant influence [1] on their adhesion. Grit blasting not only leads to rough surface and redistribution of residual stresses, but also considerably changes the preferred orientation in the affected surface layer. In this particular study, we analysed hot-rolled and cold-rolled steel substrates dedicated for ceramic coating deposition by WSP (water-stabilized plasma) spraying [2]. Particles of ceramic material are melted in the plasma jet and solidify upon impacting the substrate; hence, the overall properties of substrate-coating interface, including residual stresses, play in important role in the fatigue resistance [3] of the sprayed component.

2. Theory

Except for the so called sin²ψ method, the most widely used approach for macroscopic residual stresses determination, there also exists an algorithm proposed by Winholtz and Cohen [4] which is distinguished by lower calculation error. This method does not require any linear approximation but determines the unknown stress tensor components by least-squares minimization of the difference \( \chi^2 \), see equation (1), between calculated \( \varepsilon^{calc} \) and measured \( \varepsilon^{meas} \) lattice strain, where the unknown stress components \( \sigma^\epsilon \) are refined.

\[
\chi^2 = \sum_i \left[ \varepsilon_i^{calc} (\sigma^\epsilon) - \varepsilon_i^{meas} \right]^2 .
\]  (1)

For stress determination in textured materials, Hauk and Nikolin [5] suggested analysing diffraction planes \( \{hkl\} \) with high values of Miller indices. In this case, the diffraction profiles of this work must maintain attribution to the author(s) and the title of the work, journal citation and DOI.

Published under licence by IOP Publishing Ltd
contribute to X-rays diffracted by higher number of differently oriented grains and the deviation from the linearity in the sin²ψ plot is practically non-existent even with presence of strong texture. For iron-based materials, it is suitable to use MoKα radiation and measure \{732+651\} diffraction profile. The main advantage of this method is suppression of texture influence on residual stress analysis, but overlapping and relatively low diffracted intensity count among its disadvantages.

More appropriate methods are those which do not use X-ray elastic constants (XEC), but the so-called X-ray stress factors (XSF). These parameters are functions of (i) Miller indices, (ii) angles φ, ψ, representing rotation of specimen, and (iii) texture. Viewing textured material as a state of grains’ ordering somewhere between ideal polycrystal and single-crystal, it should be possible to propose an algorithm for residual stress determination by combining textured and non-textured state. On the basis of a work by Dölle [6], the program was developed for calculation of the residual stress state in specimens with preferred orientation. Equation (2) represents determination of XSF \(R_{ij}\):

\[
R_{ij} (hkl, \varphi, \psi) = \frac{\lambda^i r_{ij} (hkl) + \lambda^a S_{ij}}{\lambda + \lambda^a}, \tag{2}
\]

Constants \(\lambda^i\) and \(\lambda^a\) denote the volume ratio of untextured and textured parts in the specimen, respectively, dependent on the individual inclination during measurement and corresponding to relative intensities of PF (pole figure). Parameters \(r_{ij}\) represent the combination of XEC calculated on the basis of the selected linear elastic model and \(S_{ij}\) represent single-crystal elastic constants in the laboratory reference frame. Residual stresses are calculated following Winholtz and Cohen method using XSF. For this particular approach, it is necessary to comply with specific conditions; otherwise the calculation error grows rapidly. In particular, this method is applicable in the case of very weak, or virtually non-existent, texture, and also when strong and sharp texture is present.

3. Experiment
The analysed samples were made of ISO 630:1980 steel. One sample was hot-rolled (RH) and the other cold-rolled (RC). After this procedure, each sample was grit blasted by coarse corundum particles with an incidence angle of 75° on one side of both samples (RH-blasted and RC-blasted). Strains were measured in three directions on the rolling plane. Stresses determined in the directions parallel with the rolling direction (RD) are termed stresses \(\sigma_{RD}\), perpendicular (transversal direction) stresses \(\sigma_{TP}\). Stresses termed \(\sigma_{ij}\) halve RD and TD and measurements in this direction are carried out in order to compute \(\sigma_{ij}\) stress tensor component. The shape of primary beam had a rectangular shape with dimensions 10×1 mm². Generally with tilt increasing, the irradiated surface area enlarges and the penetration depth decreases. We assumed biaxial state of stress and used the Winholtz and Cohen method to compute residual stresses. Diffraction profiles of \{211\} and \{732+651\} of bcc iron were analysed by CrKa and MoKa radiation, respectively. Profiles corresponding to Kα radiation were fitted by Pearson VII function. In the generalised Hooke’s law, we used XEC obtained in accordance with Eshelby-Krömer model [7] using single crystal elastic constants for iron \(S_{ij} = 7.6\) TPa⁻¹, \(S_{12} = -2.8\) TPa⁻¹, \(S_{44} = 8.6\) TPa⁻¹. Very important parameter to calculate residual stresses correctly, especially the component \(\sigma_{G3}\), is stress-free lattice plane distance \(d_0\). This parameter was determined on the basis of finding the so-called stress-free direction \(\psi^*\) of the RH sample according to the algorithm that can be found [8] in chapter 2.112c, which yielded the value of 0.117024 nm for \{211\} planes.

The texture was qualitatively determined using Schultz reflection geometry and radiation from X-ray tube with cobalt anode. The CoKa radiation was used, because 1D detector for CrKa was not at our disposal; the effective penetration depth \(T^0\) of CoKa for \{110\}, \{200\} and \{211\} profile is 5 μm, 7 μm and 9 μm, respectively which is approximately 1.5 higher values
than 3 μm, 5 μm and 6 μm for CrKa. The shape of primary beam was rectangular with dimensions 0.25×1 mm². Pole figures were re-calculated from the orientation distribution function which was calculated on the basis of WIMV method [9] from measured PF.

4. Results

Components of macroscopic residual stress tensors relevant for surface layers can be seen in Tab. 1, where CrKa (XSF) means that the method using XSF was employed. Next, the values listed for CrKa and MoKa are based on the XEC for random texture. Pole figures of {211} planes are seen for cold-rolled sheet in Fig. 1.

**Table 1.** Surface distributions of macroscopic residual stresses.

| Stress, MPa | Radiation | RC     | RH     | RC-blasted | RH-blasted |
|-------------|-----------|--------|--------|------------|------------|
| $\sigma_{RD}$ | CrKa      | -70 ± 5 | -6 ± 8 | -141 ± 3   | -201 ± 3   |
|             | CrKa (XSF)| -147 ± 6| -187 ± 10 |
|             | MoKa      | -61 ± 7 | -24 ± 6 | -205 ± 14  | -260 ± 13  |
| $\sigma_{45}$| CrKa      | -85 ± 5 | -14 ± 6 | -132 ± 5   | -200 ± 5   |
|             | CrKa (XSF)| -130 ± 7| -170 ± 12 |
|             | MoKa      | -37 ± 4 | -11 ± 4 | -200 ± 15  | -252 ± 9   |
| $\sigma_{TD}$ | CrKa      | -125 ± 3| 2 ± 10 | -142 ± 3   | -194 ± 6   |
|             | CrKa (XSF)| -130 ± 4| -174 ± 13 |
|             | MoKa      | -33 ± 8 | -16 ± 3 | -188 ± 16  | -212 ± 16  |
| $\sigma_{33}$ | CrKa      | -15 ± 8 | 10 ± 10 | -19 ± 2    | -29 ± 3    |
|             | CrKa (XSF)| -19 ± 2 | -14 ± 4 |
|             | MoKa      | 33 ± 4 | 73 ± 2 | 165 ± 7    | 149 ± 6    |

**Figure 1.** PF of {211} planes for RC (left) and RC-blasted (right) samples.

5. Discussion

Firstly, in the used experimental lay-out it was impossible to calculate stresses in virgin samples employing the method with XSF, because of a too coarse-grained material in the irradiated volume. Sadly we were not able to increase the irradiated surface area without significant defocusation errors. Hence, in virgin samples only calculation with texture omission and with MoKa can be compared which leads us to observation of fairly large discrepancies in stress values. The responsible factor for this is most likely twofold. Firstly different gauge volumes correspond to these values (with penetration depth for MoKa being approximately triple of $T_{ef}$ for CrKa) and since the presence of stress gradients in virgin
samples cannot be ruled out, it is not surprising that the presented values are not the same. Secondly, the first method uses algorithm for stress calculation in isotropic material while the investigated material was textured. As for the large discrepancy in $\sigma_{33}$ values in grit-blasted samples, the effect of stress depth gradient and difference in $T_{ef}$ should be considered.

The pole figures in Fig. 1 clearly show that grit-blasting leads to much lower degree of preferred orientation in surface layer. The main reason is most likely an increasing orientation spread in the grains due to plastic deformation. The stress tensor was evaluated in three manners for the grit blasted samples. Thus on the basis of the above mentioned model, XSF were calculated and afterwards residual stresses were determined. Because the level of preferred orientation in the blasted samples is very low, relative intensities are nearly one and resulting XSF almost equal XEC. Differences between values of stress components calculated according the first two approaches are very small as seen in Tab. 1. The reason for this observed difference stems from difference in relative intensities, i.e. even the very low level of texture has some influence on stress values. Hence, the applied method according to equation (2) leads only to small alterations in stress values for weak texture, which is in accordance with expectations. On the other hand, this algorithm remains to be verified on strongly textured samples.

6. Conclusion

Even though the values of residual stresses calculated with neglecting the texture in non-blasted samples show sound experimental error, they should not be trusted because the applied algorithm does not correspond to assumptions of the method. On the other hand, it was not possible to use the algorithm with XSF for determination of residual stresses because of coarse grained nature of the irradiated volume. Thus, to us it seems the most appropriate to use MoKα radiation for residual stress determination is such case. From pole figures, it is obvious that grit blasting of both cold and hot rolled steel surface leads to quantitative change in texture with very low level of preferred orientation in grit blasted surfaces. When we compare the two approaches without and with XSF, they lead to very similar values of stress. However, employing MoKα radiation correspond to different values of stress and one has to bear in mind a big difference in penetration depth which is almost threefold in comparison with CrKα. It should also be noted that grit-blasted hot-rolled sheet has larger values of compressive residual stresses when compared to cold-rolled.

Acknowledgements

J. C. acknowledges support of the Grant Agency of the Czech Technical University in Prague, grant No. SGS13/219/OHK4/3T/14. Z. P. was supported by GAP108/12/1872, a Czech Science Foundation grant.

References

[1] Harris A F and Beevers A 1999 *Int. J. Adhes. Adhes.* **19** 445–452
[2] Chraska P and Hrabovsky M 1992 *Therm. Spray: Int. Adv. Coat. Technol.* **1** 81–85
[3] Kovarík O et al. 2014 *Surf. Coat. Technol.* **251** 143–150
[4] Winholtz R A and Cohen J B 1988 *J. Phys.* **41** 189–199
[5] Hauk V and Nikolín H -J 1988 *Texture Microstruct.* **8/9** 693–716
[6] Dolle H 1979 *J. Appl. Cryst.* **12** 489–501
[7] Eshelby J D 1957 *Proc. Roy. Soc. A* **241** 376–396
[8] Hauk V, ed. 1997 *Structural and Residual Stress Analysis by Nondestructive Methods: Evaluation-Application-Assessment* (Elsevier) 640
[9] Kocks U F et al. 2005 *Texture and Anisotropy: Preferred Orientation in Polycrystals and their Effect on Materials Properties* (London, Cambridge University Press) 115–118