DIFFRACTION ELASTIC CONSTANTS FOR ARBITRARY SPECIMEN AND CRYSTAL SYMMETRIES

Accurate determination of residual stresses by means of diffraction relies on the knowledge of the elastic constants that translate lattice strain into macro-stress. Because of the difference between the elastic behavior of the aggregate and that of a single crystallite, the straightforward relationship between strain and stress as mediated by single crystal or polycrystal elastic constants no longer holds. Instead, the relationship between lattice strain and macro-stress is mediated by diffraction elastic constants (DEC).

Very recently, we proposed a theory that allows a transparent calculation of DEC. This theory applies for almost the entire range of polycrystalline elasticity, including that for aggregates of arbitrary phase composition and arbitrary symmetry, both of the aggregate and of the constituents [1]. Results show that for a particular crystallographic plane (*hkl*) and an arbitrary anisotropic material there are usually six independent DEC. These DEC depend on the orientation of the scattering vector, on the grain shape, and on the elastic constants both of the crystallites and of the aggregate. Figure 1 shows Young's modulus vs. the orientation parameter for different crystallographic planes (*hkl*) of two plasma-sprayed coatings with different types of anisotropy. Calculated DEC for comparison to measurement were not previously available.

Figure 1 also illustrates the difference between the anisotropy of the aggregate and that of the crystallites that comprise the aggregate. The slope of E_{hkl} vs. Γ depends mostly on the ratio

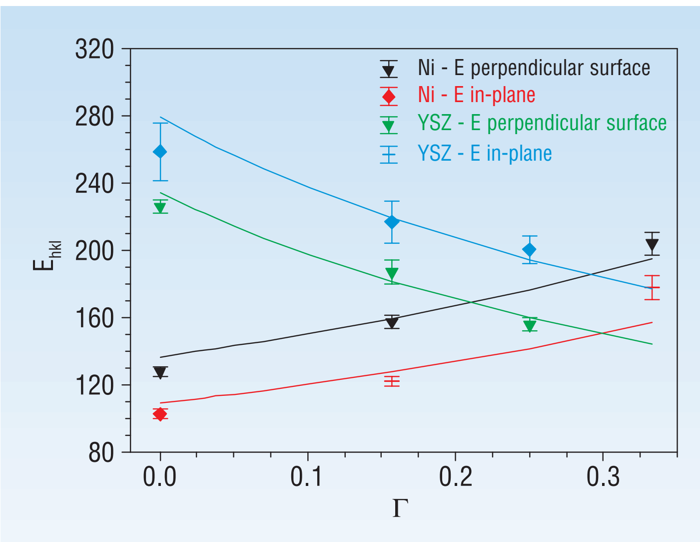

FIGURE 1. Young's modulus vs. orientation parameter for a metallic nickel coating and a ceramic YSZ (ZrO_2+8%Y_2O_3) coating deposited by plasma spraying. Solid lines indicate calculated values, points are measured values.

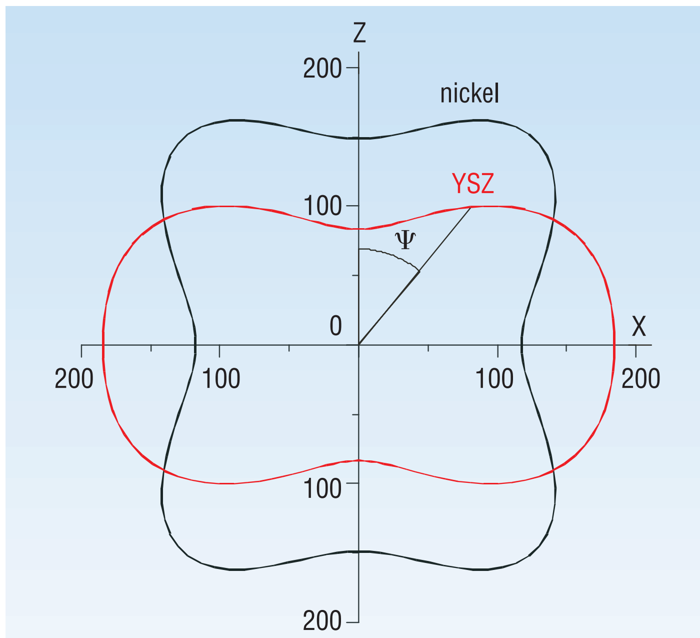

FIGURE 2 . Central section of the representation surface for Young's modulus in a nickel coating and a yttria stabilized zirconia coating. The length of the radius vector for a certain tilt angle Ψ is equal to Young's modulus in units of GPa. These values were calculated from hkl-dependent elastic constants measured by neutron diffraction. The z-direction is perpendicular to the surface of the coating. All in-plane directions are equivalent due to the transversal-isotropic elastic symmetry of sprayed coatings.

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$2C_{44}/(C_{11}\text{-}C_{12})$ which is > 1 for nickel and < 1 for YSZ. The aggregates exhibit generally transversal isotropic elastic symmetry but again with a different anisotropy in the metallic coating ($C_{11}/C_{33} < 1$) and in the ceramic coating ($C_{11}/C_{33} > 1$). This anisotropy causes a substantial difference between E_{hkl} normal and perpendicular to the coating surface.

While the data in Fig. 1 still depend on the crystallographic plane (*hkl*) they can also be used to estimate the overall elastic constants of the aggregates that, in turn, yield the directional dependence of the mechanical value of Young's modulus. This distribution forms a surface with rotational symmetry around the coating surface normal vector as illustrated by a central section shown in Fig. 2.

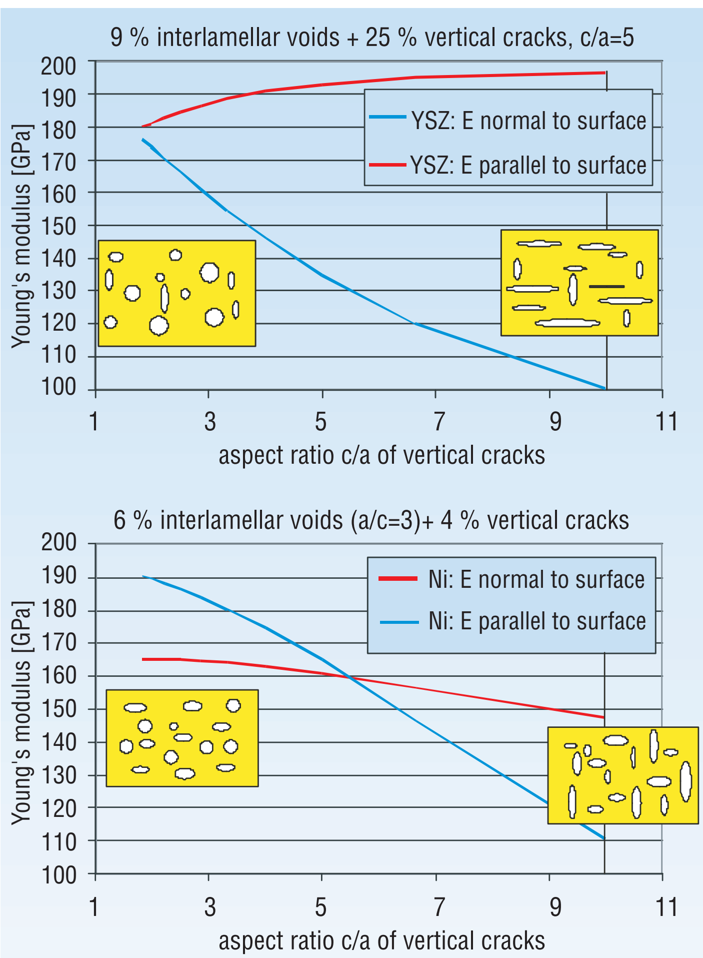

FIGURE 3. Young's modulus for the YSZ coating (a) and for the nickel coating (b) vs. the pore aspect ratio. The vertical lines at aspect ratio of 10 indicate where the best agreement is found with experimental results.

The elastic anisotropy of sprayed coatings has its roots in their microstructure. In the complete absence of preferred crystallite orientation, the responsible factor is the porosity and alignment of elongated voids and cracks resulting from the spray process. These voids can be treated as another phase with very low elastic moduli. This way it is possible estimate the overall elastic constants if the distribution of pore shapes and volume fractions are known.

In the case that the aggregate constants are already known, the reverse approach of estimating a pore distribution can offer some insight into the properties of different coatings. Figs. 3a and b show where the best agreement was found for plasma sprayed metallic and ceramic coatings. The main difference is that the pore structure of the ceramic coating is dominated by interlamellar (horizontal) voids, while the concentrations of horizontal voids and vertical cracks are more balanced in the metallic coating.

REFERENCES

[1]. T. Gnäupel-Herold, J. Matejicek, and H.J. Prask, "Mechanical Properties of Plasma Sprayed Coatings - Measured by Diffraction," to be published in *Proc. of the 9th Int. Metallurgical Conf. Metal 2000, Ostrava, Czech Republic*, May 16-18, 2000; T. Gnäupel-Herold, and H.J. Prask, "Diffraction Elastic Constants for Arbitrary Specimen and Crystal Symmetries: Theory and Practical Consequences," in *Proc. of the 6th Int. Conf. on Residual Stresses (ICRS-6)*, (IOM Communications Ltd., UK, 2000), pp. 243-250.