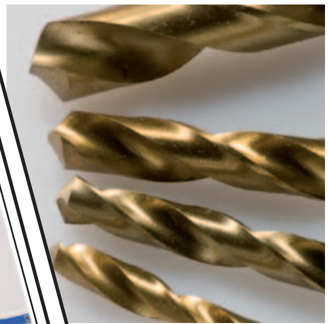
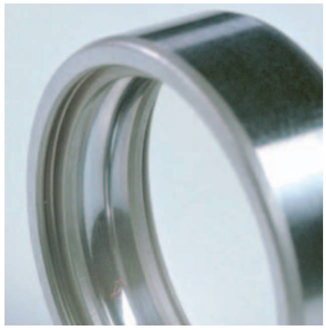
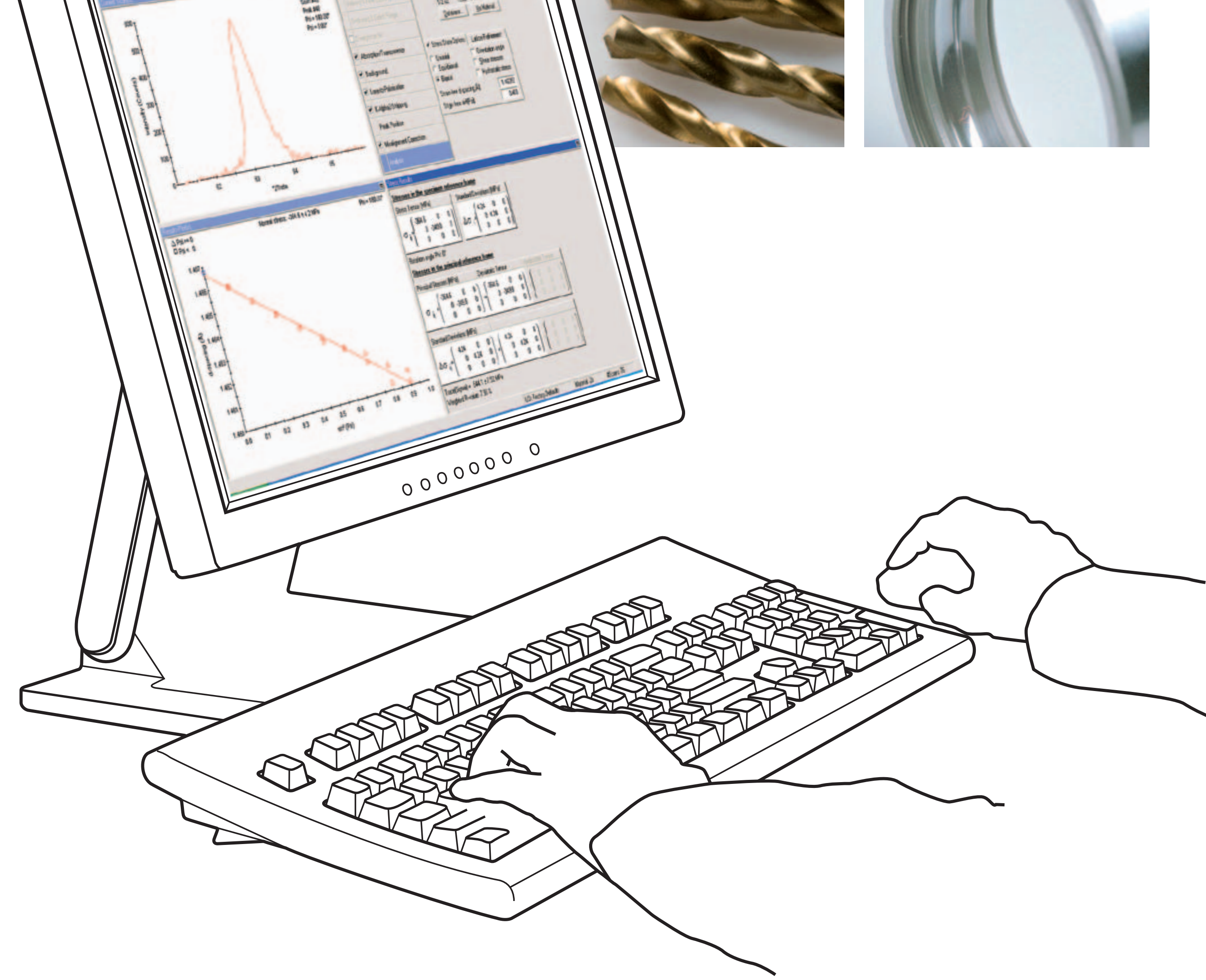
PANalytical

RESIDUAL STRESS ANALYSIS

Stress
and
Stress Plus







The Analytical X-ray Company

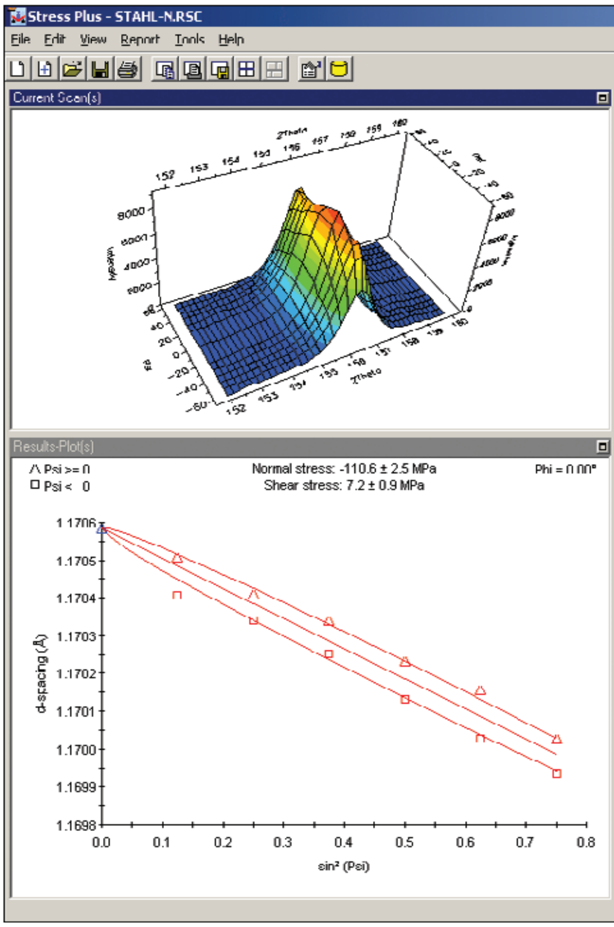
Overview

The PANalytical software package Stress combines classical single-{hkl} uni-directional and multi-directional (full tensor) residual stress analysis with both an X-ray elastic constants (XEC) database and all the established methods for determining peak position. In addition, there is an improved routine for correcting minor misalignments of either the specimen or the diffractometer. A free choice of user-configurable defaults and instant recalculation of all results upon even the smallest change of input parameters, make Stress suitable for both routine analysis and research applications.

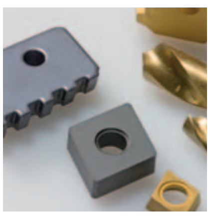
PANalytical Stress Plus offers the benefits of the intuitive Stress package together with the advanced functionality of the proprietary and unique Stress Plus module. It supports analysis of all data generated by modern techniques used to analyze residual stress in polycrystalline coatings. These include grazing incidence, multiple {hkl} peaks, combined tilts and/or specific sample tilts.

The software is part of a complete solution that includes PANalytical's Empyrean hardware platform and the stress measurement capabilities of Data Collector. Stress and Stress Plus can be used interactively on screen or may be run automatically via the command line interface. Running under Windows® 7 Professional (64-bit) or Windows XP® Professional (32-bit), this application features a split screen user interface, ensuring a complete overview of scans, parameters, $\sin^2\psi$-plots and numerical stress results in a single application window. The complete on-line help system explains every function specific to the program. Novice users are introduced to the basic features through the use of worked examples explained in the Quick Start Guide.

Stress and Stress Plus are part of PANalytical's XRD Software range which uses the XRDML data format. Also existing stress data in the .rsc format can be processed.

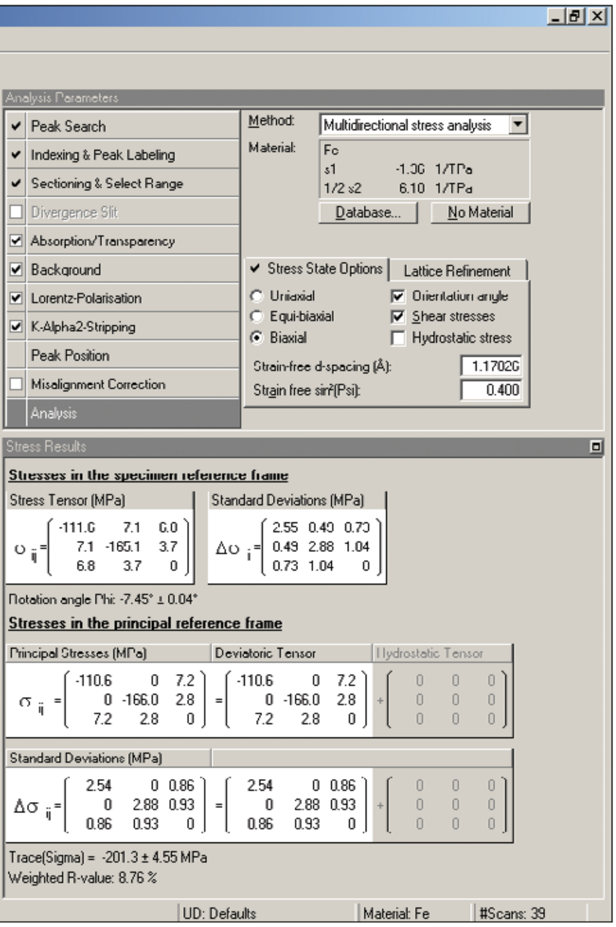


Main application window



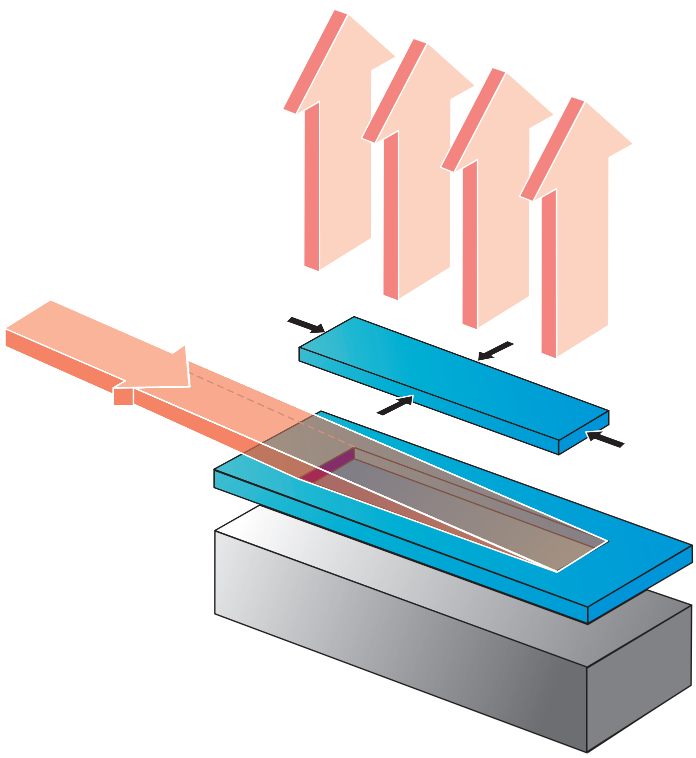
Stress features

- Designed for classical single-{hkl} $\sin^2\psi$ stress analysis
- Interactive calculations and complete, automatic analysis
- Wide choice of pattern treatment and peak position methods
- Elastic constants database and a built-in XEC calculator
- Reliable results with simple routine to correct for minor misalignments
- Analysis on combined data sets from multiple measurement files



Stress Plus additional features

- Software for analysis of residual stress in polycrystalline coatings
- Support for grazing incidence XRD data
- Multiple-{hkl} $\sin^2\psi$ stress analysis
- Support of combined tilts measurements
- Comprehensive routine to evaluate and correct for all minor misalignments
- Enables qualitative evaluation of stress gradients in coatings or bulk samples



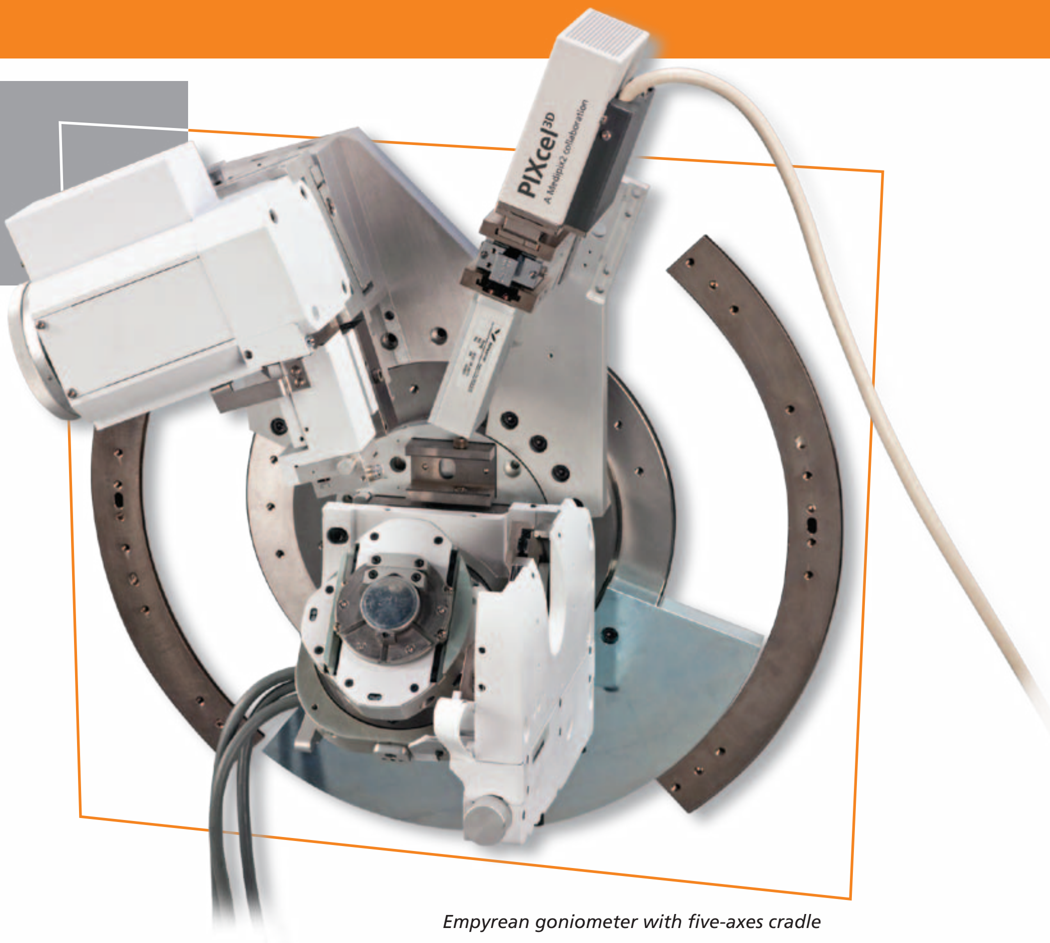
Grazing incidence stress measurement

Residual stress analysis

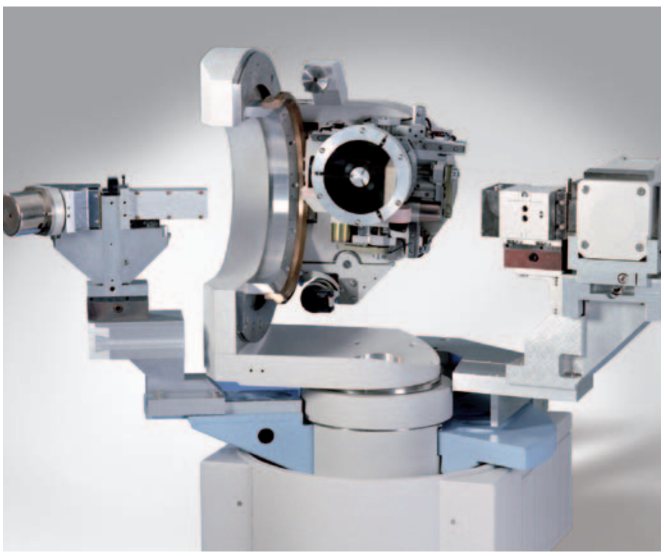
Classical stress measurements

PANalytical Stress is dedicated to the analysis of XRD residual stress measurements according to the classical single-{hkl} sin²ψ method. Both measurement types, known as the chi-stress (formerly known as psi-stress) and omega-stress variant are covered.

Chi-stress measurements are typically performed on a diffraction system with a point focus configuration that is also suitable for texture analysis. In this configuration a poly-capillary X-ray lens can be applied to minimize the effects of defocusing. For very small samples, the mono-capillary optics module is the correct choice. Sample tilting is always performed by a special cradle, an Empyrean five-axes cradle or an MRD cradle, with a motorized chi (psi) axis. For extra large samples, PANalytical offers a large MRD XL cradle or the Empyrean three-axes cradle.



Empyrean goniometer with five-axes cradle



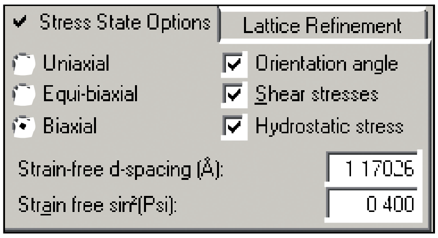
X'Pert PRO MRD

Omega-stress measurements are performed on a line focus diffractometer as used for phase analysis. Sample tilting is carried out by the independent omega axis of the goniometer. For extra heavy samples, virtual tilting with the theta-theta goniometer is a suitable option. Such a configuration may also include an X-ray mirror, beneficial when measuring curved samples.

PANalytical

Stress state options

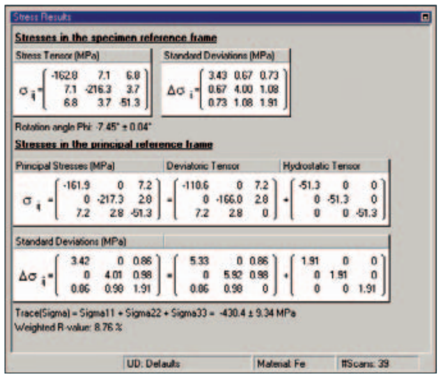
PANalytical Stress offers the analysis of various stress states. Optionally these can be combined with determining the rotation angle, shear stresses or the hydrostatic stress component. The latter includes triaxial stress analysis on the basis of the deviatoric-hydrostatic stress tensor approach.



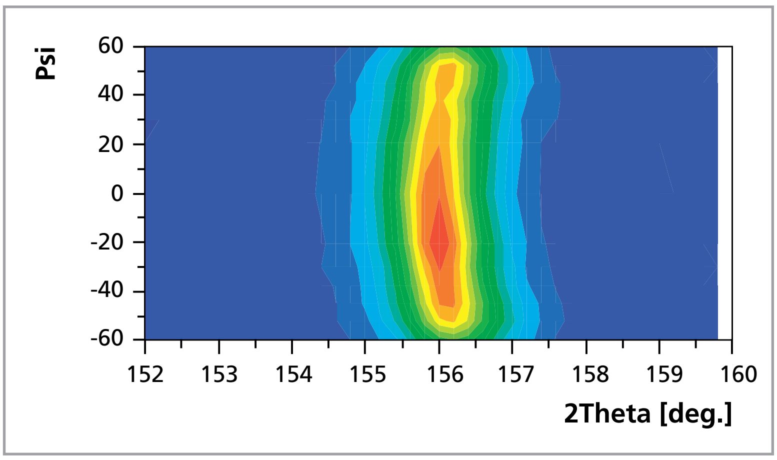
Stress state options

Deviatoric-hydrostatic approach

Triaxial stress analysis requires the use of all available information, including those data which in principle are less reliable. This leads to confusing results for the total stress tensor. Stress (Plus) takes the deviatoric-hydrostatic approach, separating reliable and less reliable information effectively. The deviatoric stress tensor is based on reliable, relative peak shift data while the hydrostatic stress tensor uses less reliable, absolute peak position data.



Stress results window



Isolines plot

Residual stress analysis

Uni-directional and multi-directional stress analysis

PANalytical Stress offers both uni-directional and multi-directional (full tensor) stress determination. Uni-directional stress analysis calculates the stress in the direction of the diffraction plane only. Multi-directional analysis fits the ellipsoid stress function to the results of all measurement directions and calculates directly the full stress tensor.

Results of stress measurements can be expressed in two unit systems:
- International SI units (MPa)
- Imperial units (psi)

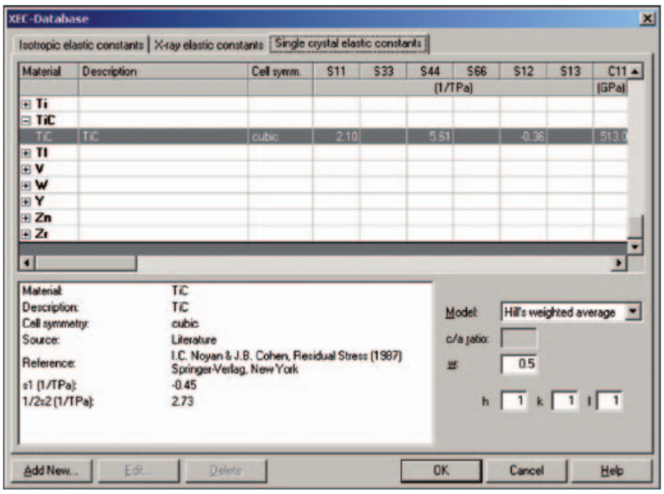
XEC calculator

The built-in X-ray elastic constants (XEC) calculator offers 5 different methods to calculate the XECs S_1 and ½ S_2 as needed for residual stress analysis:
- Isotropic case
- Reuss
- Voigt
- Hill's weighted average
- Quasi-isotropic model

Elastic constants database

An elastic constants database with over 400 verified literature entries is included. Data retrieval is possible for:
- Isotropic elastic constants
- X-ray elastic constants
- Single crystal elastic constants

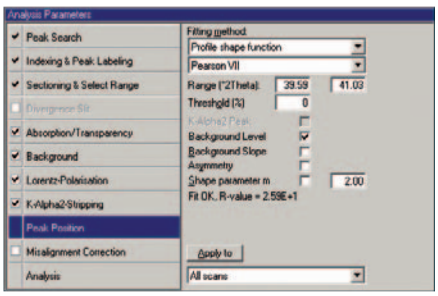
Addition of more elastic constants defined by the user is possible too.



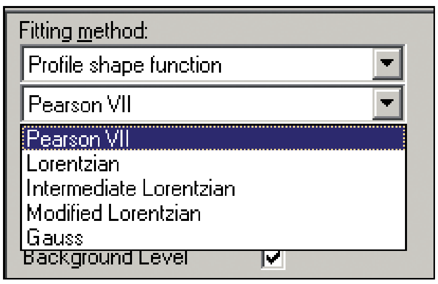
Elastic constants database with built-in XEC calculator

Peak position determination

Uniquely for a residual stress program, Stress offers all the widely accepted methods for determining a peak position:
- Center of gravity
- Centered center of gravity
- Parabola fit
- Profile shape function fit
- Middle of width at % height
- Manual position
- Cross-correlation function



Peak position determination parameters



Drop-down list box containing the profile shape functions

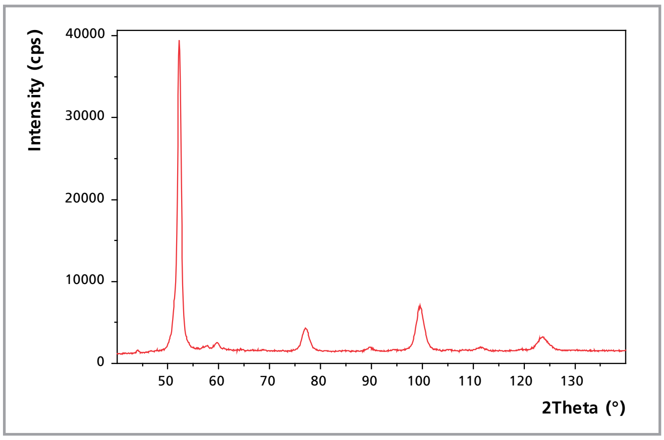
Solutions for steel components

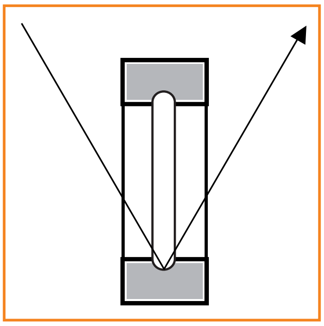
Example: Ball bearing outer ring

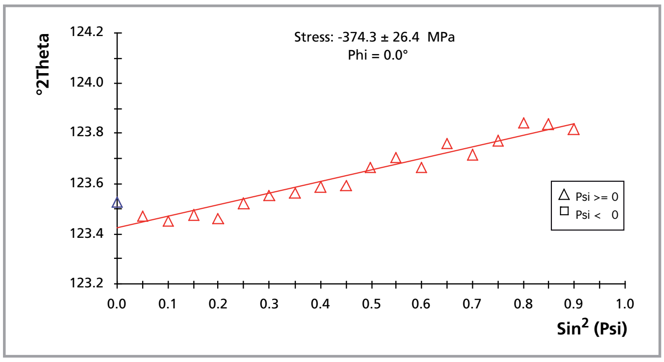
Classical single-{hkl} chi-stress measurement on the inner raceway of a ball bearing outer ring.

Measured on an X'Pert Powder system with open Eulerian cradle using an X-ray lens in the incident beam, a 0.27° parallel plate collimator and a proportional detector in the diffracted beam.

Equivalent measurement data can be obtained on Empyrean systems equipped with a five-axes or three-axes cradle.
A moderate compressive stress of -374 MPa is found.







STRESS PLUS ONLY

Residual stress analysis

Residual stress in polycrystalline coatings

PANalytical Stress Plus is designed for analysis of residual stress in polycrystalline coatings. Such measurements could be of grazing incidence beam, on multiple {hkl} peaks, using combined tilts of chi and omega, or a combination of these advanced options.

The measurement strategy used depends on the nature of the coating and substrate. Polycrystalline coatings can range from nanocrystalline, randomly oriented to highly textured: substrates can be of any nature, from amorphous, polycrystalline to single crystal.

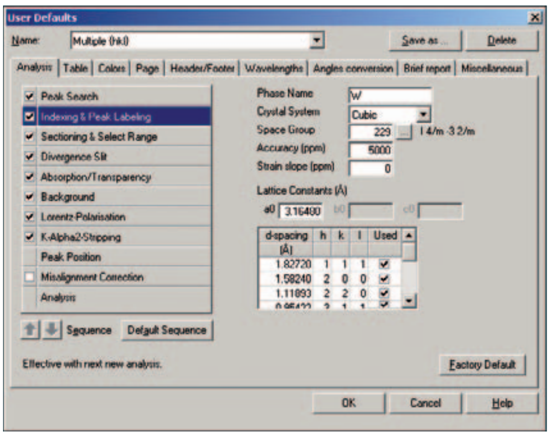
The optimum diffraction optics for measuring residual stresses in coatings may range from traditional Bragg-Brentano focusing beam geometry to modern parallel beam geometry with either point or line focus.

Overview of attainable (+) and unattainable (–) combinations of coatings and substrates

Substrate	Coating				
	Amorphous	Polycrystalline			Single crystal/ Epitaxial
		Nano-crystalline	Randomly orientated	Highly textured	
Amorphous	-	+	+	+	-
Polycrystalline	-	+	+	+	-
Single crystal	-	+	+	+	-

Indexing of multiple-{hkl} stress measurements

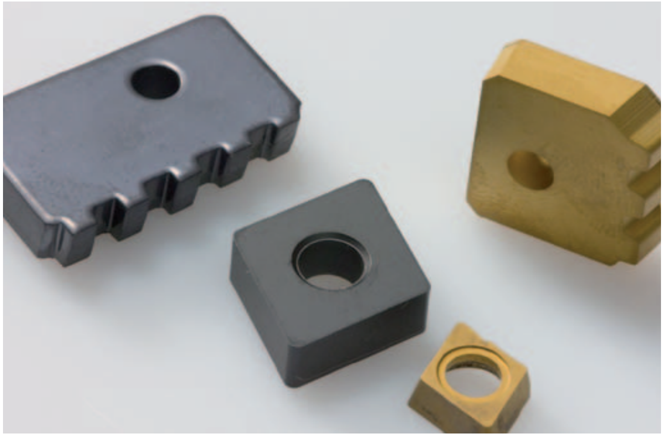
A unique, smart algorithm assigns the {hkl} indices to the analysis peaks, recognizing the correct peaks despite the position shifts that occur because of stresses in the sample. Two parameters are accessible for fine-tuning to individual situations.



Indexing parameter window

Solutions for hard coatings

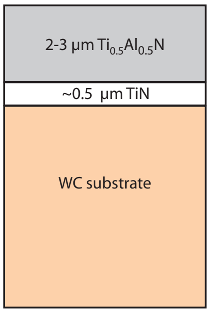
Example: TiAlN on WC

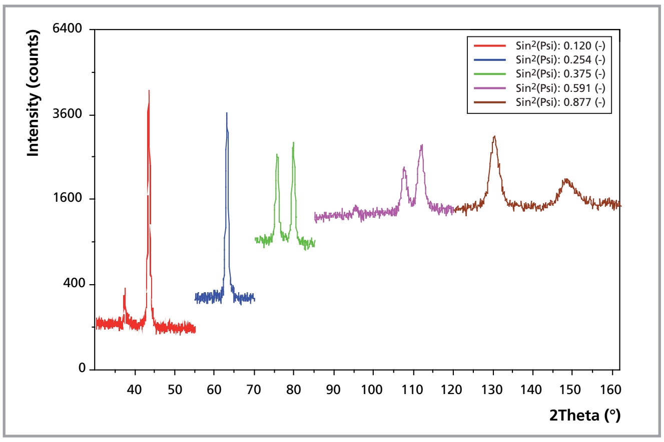


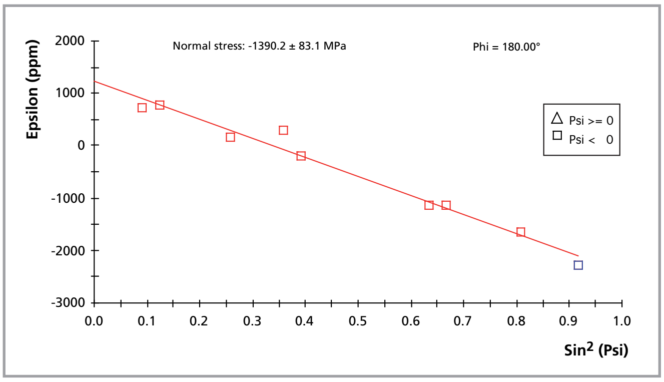
Grazing incidence multiple-{hkl} stress measurement on a coated tool insert.

Measured on an X'Pert PRO MRD system with 1° grazing incidence angle using an X-ray mirror in the incident beam, a 0.27° parallel plate collimator and a proportional detector in the diffracted beam. Equivalent measurement data can be obtained on Empyrean systems.

A very large compressive stress of -1390 MPa is found.

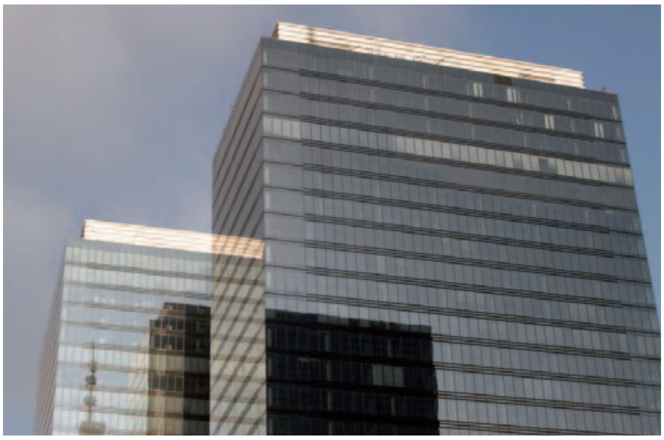




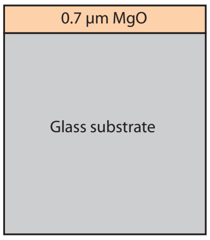


Residual stress analysis

Solutions for coatings on glass



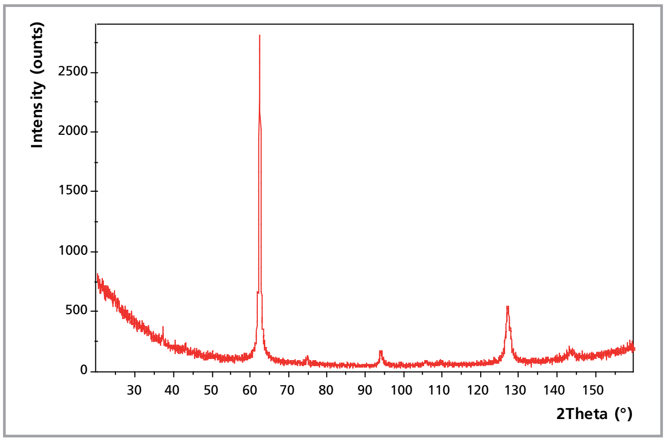
Example: MgO on glass

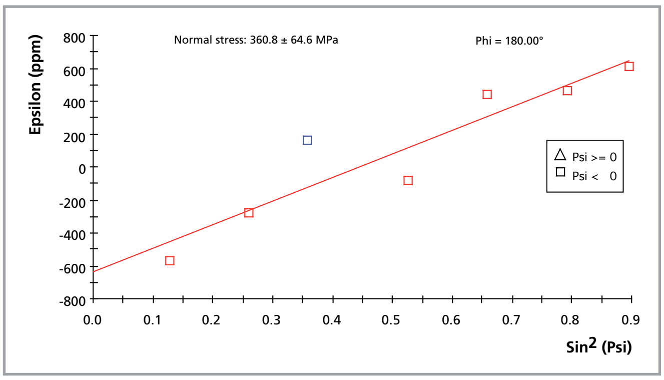


Grazing incidence multiple-{hkl} stress measurement on a coating on glass.

Measured on an X'Pert PRO MRD system with 0.5° grazing incidence angle using an X-ray mirror in the incident beam, a 0.27° parallel plate collimator and a proportional detector in the diffracted beam. Equivalent measurement data can be obtained on Empyrean systems.

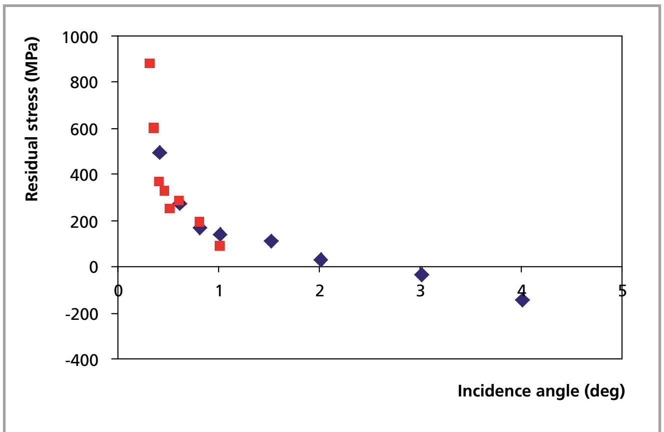
A large tensile stress of + 361 MPa is found. A stress gradient is present in the coating.

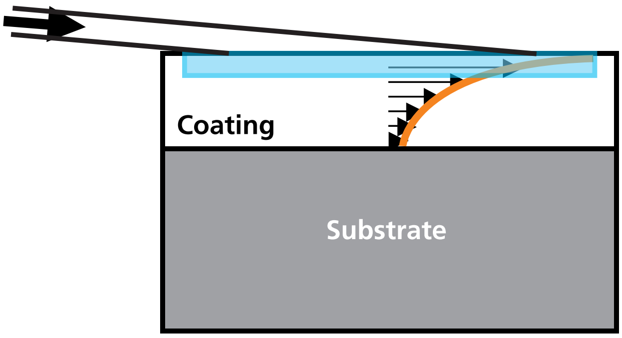




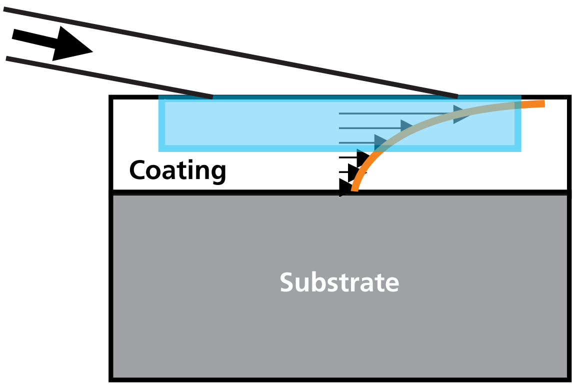
Qualitative stress gradient

Repeated stress measurements with grazing incidence angles ranging from 0.2° to 4° give qualitative information on the stress gradient.
A very large tensile stress of + 900 MPa is found near the surface.

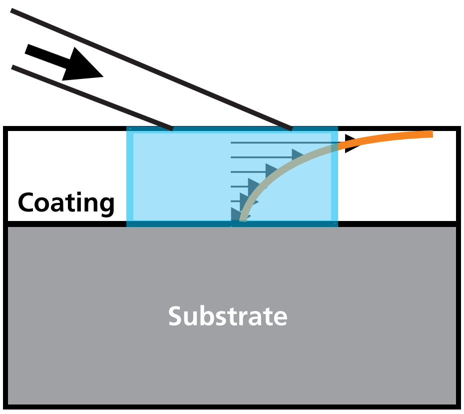




Small angle of incidence: analyzing stress near surface



Medium angle of incidence: analyzing stress near surface and deeper



Large angle of incidence: analyzing average stress of whole coating

PANalytical

Global and near

PANalytical
PANalytical is the world's leading supplier of analytical instrumentation and software for X-ray diffraction (XRD) and X-ray fluorescence spectrometry (XRF), with more than half a century of experience. The materials characterization equipment is used for scientific research and development, for industrial process control applications and for semiconductor metrology.
PANalytical, founded in 1948 as part of Philips, employs around 1000 people worldwide. Its headquarters are in Almelo, the Netherlands. Fully equipped application laboratories are established in Japan, China, the USA, and the Netherlands. PANalytical's research activities are based in Almelo (NL) and on the campus of the University of Sussex in Brighton (UK). Supply and competence centers are located on two sites in the Netherlands: Almelo (development and production of X-ray instruments) and Eindhoven (development and production of X-ray tubes). A sales and service network in more than 60 countries ensures unrivalled levels of customer support.
The company is certified in accordance with ISO9001-2008 and ISO 14001.

The product portfolio includes a broad range of XRD and XRF systems and software widely used for the analysis and materials characterization of products such as cement, metals and steel, nanomaterials, plastics, polymers and petrochemicals, industrial minerals, glass, catalysts, semiconductors, thin films and advanced materials, pharmaceutical solids, recycled materials and environmental samples.

Visit our website at www.panalytical.com for more information about our activities.

PANalytical is part of Spectris plc, the productivity-enhancing instrumentation and controls company

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