Ultima IV
X-RAY DIFFRACTOMETER

1. Introduction

Ultima IV is an advanced and versatile X-ray diffraction system equipped with a precision-engineering horizontal-sample X-ray diffractometer together with a conventional X-ray generator and a sealed-off X-ray tube. Ultima IV is specially designed to allow for simple and reproducible changeovers form one selected configuration to another and vice versa.

A variety of configurations from a conventional model for an analysis of powder samples to an advanced model for the characterization of thin film samples can easily be selected by selecting and combining a goniometer, an optical system, a slit, a detector and various special- purpose attachments.

2. Instrumentation

2.1. System expandability

Ultima IV with a basic configuration is shown on the left-hand side of Fig. 1. The diffractometer uses conventional para-focus X-ray optics for routine X-ray analysis including crystalline phase identification.

This basic configuration can be upgraded by adding cross beam optics (CBO) unit to the incident beam. The CBO converts the original focusing optics to the parallel-beam optics. Ultima IV with the parallel-beam optics (see the middle figure in Fig. 1) can be used for the characterization of thin films, small-angle scattering study, micro-spot X-ray diffraction analysis, *in-situ* dynamical measurements, powder crystal structure determination and refinement, precision lattice parameter determination.

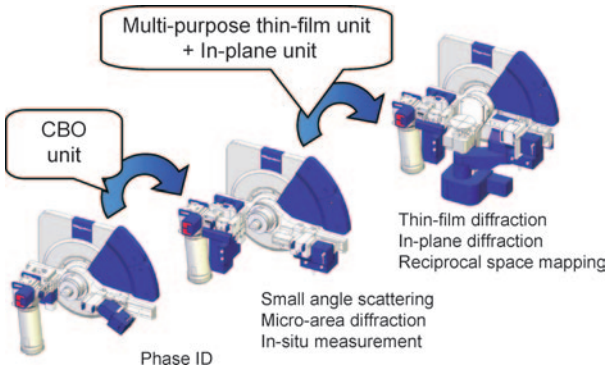

Fig. 1. Examples of the combination of units.

The Ultima IV system can further be expanded by the addition of an in-plane unit as shown on the right-hand side of Fig. 1. The addition of an in-plane unit makes it possible for the Ultima IV diffractometer to measure crystal planes that are perpendicular to the sample surface. This upgraded system can be especially useful to the characterization of the surface of a thin film, the recording of a reciprocal lattice map.

In addition, there is a wealth of various specially designed attachments that can easily be used with an Ultima IV system. With advanced engineering designs all units and attachments can simply and reproducibly changeovers from one to another.

2.2. Automatic instrument alignment

A computer program can be used to automatically align the entire diffractometer system by adjusting all

Fig. 2. Easy-to-use design based on ergonomics.

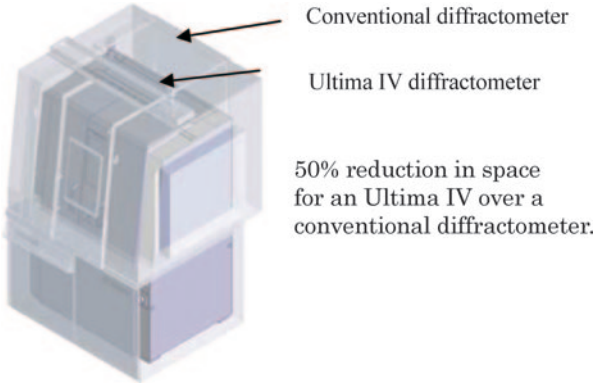

Fig. 3. Comparison of the size of an Ultima IV with that of a conventional diffractometer.

the movable optical axes when the system is first installed and when any unit or attachment is added or removed. This allows the Ultima IV system to be automatically and properly aligned at all times.

2.3. Enhancements of usability

The Ultima IV system is specially designed based on ergonomic considerations so that a user does not have to take an improper posture when mounting or dismounting a sample, a CBO unit, an in-plane unit, an attachment, or an X-ray tube.

As shown in Fig. 2, the height of the sample holder in Ultima IV is as low as 1000 mm from the floor and the opening width of the safety front door is as wide as 600 mm.

Attachments each equips with a hot plug, which enables a user to connect it to the instrument main unit without the need to turn off the power of the instrument. This makes it easy for a user to add or remove a unit or an attachment. Therefore, a series of measurements, such as an *In-situ* measurement using a high-temperature unit, a residual stress measurement using a distortion attachment, a qualitative analysis using a rotating sample holder, and/or a small-angle scattering measurement using a transmission sample holder, can be accomplished in one day.

The use of a horizontal sample holder makes it possible to study a variety of samples including powders, thin films, viscous samples and liquid samples.

2.4. Compact size and light weight

The size and weight of the main unit of a conventional diffractometer system are 1200 mm wide, 1300 mm deep, and 750 kg in weight. A Ultima IV diffractometer system is specially designed to have a compact size of 800 wide, 1100 mm deep and only 610 kg in weight. Therefore, an Ultima IV system requires significantly less installation space and loading on the floor. The height of the instrument is also reduced from 1920 mm for a conventional diffractometer system to 1630 mm for an Ultima IV system (Fig. 3). These features make it possible to install an Ultima IV system in a small laboratory.

3. Safety features

Ultima IV is designed under the newest and most assured safety regulations in complying with the latest international safety standards.

The X-ray generation unit can be controlled only from the host computer, and is equipped with an interlocking mechanism to prevent a danger of exposure to X-rays when X-rays are generated and the shutter is opened.

In emergency, the entire system can be shut off by turning a breaker-power switch located at the lower right on the front panel of the instrument.

4. D/teX Ultra, an advanced and high-performance X-ray detector

A D/teX Ultra detector can be used on an Ultima IV diffractometer for high-intensity, high-precision and high-sensitivity X-ray measurements.

D/teX Ultra gives up to 100-time intensity gains over those of a conventional scintillation counter. Therefore, the measurement time can be greatly reduced, and the measurement speed can be dramatically increased. D/teX Ultra also has high-energy resolution, and this can used to reduce the secondary fluorescence X-rays from a sample. Therefore, the use of a D/teX Ultra detector can greatly increase the performances of an Ultima IV diffractometer.

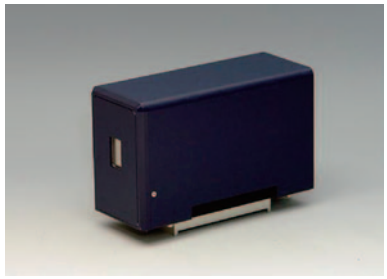

Fig. 4. D/teX Ultra detector.