

XRD COMBINATORIAL SCREENING SYSTEM WITH AUTOMATED REFLECTION-TRANSMISSION CONVERSION

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A system designed for X-ray diffraction combinatorial screening can be converted automatically between transmission mode and reflection mode (patent pending). The choice between reflection and transmission modes depends mostly on the design of the sample plate and the way sample was prepared. In many XRD combinatorial screening applications, such as polymorphism studies in pharmaceutical chemistry, a typical 2θ measuring range is from 2 to 60°. One option is to run the combinatorial XRD screening in transmission mode in order to avoid the defocusing effect associated with reflection mode diffraction. In the transmission mode X-ray diffraction measurement, the incident beam is typically perpendicular to the sample so the irradiated area on the specimen is limited to a size comparable to the X-ray beam size. In some cases, however, the XRD screening has to be done in reflection mode due to the restriction of the sample plate. Most existing X-ray diffractometers for combinatorial screening are dedicated for either reflection mode or transmission mode. Some systems may be able to do both modes, but the configuration is typically optimized for one mode and the other mode can be done with only limited types of samples or sample plates. A sample plate for combinatorial screening is preferably aligned in horizontal direction. During the screening process the sample plate moves only in the horizontal direction with translation. The sample library will not rotate away from the horizontal direction. This is necessary for holding powder samples or liquid samples in the sample plate. If a reflection mode diffraction data were collected on a system with transmission configuration, the sample plate would have to be rotated away from the horizontal position. The powder samples on a plate may fall off or cross contaminate in a non-horizontal position. The same is true if a transmission mode system is used for reflection mode diffraction. This new design makes the conversion between transmission mode and reflection mode easy and automatic. The system can run at optimum configuration for both reflection and transmission modes because the sample library is always in the horizontal position.