

RAPID COMBINATORIAL SCREENING BY TWO-DIMENSIONAL XRD

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The combinatorial chemistry requires rapid screening techniques to test and evaluate the variation of composition, structure and property across the material library. X-ray diffraction, especially two-dimensional X-ray diffraction is one of the most suitable rapid screening techniques because of the penetrating power, nondestructive to samples, fast data collection, and the abundant information contained in the two-dimensional diffraction pattern.

A two-dimensional diffraction pattern contains the information on structure, quantitative phase contents, crystal orientation and size distribution. All the information can be used as screening criteria. In combinatorial screening applications, sample cells are located close to each other. Therefore, the XRD screening process should also avoid cross contamination between adjacent cells in the material library. In many combinatorial screening applications, such as polymorphism studies in pharmaceutical chemistry and catalysis development in the oil industry, 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. The desired resolution and free from cross contamination in the same 2θ range can also be achieved in reflection mode diffraction by using a motorized retractable knife-edge. The motorized retractable knife-edge makes it possible to scan over the whole combinatorial library with automatic sample alignment.