A NEW HIGH PERFORMANCE HIGH-RESOLUTION POWDER DIFFRACTION SYSTEM AND ITS APPLICATIONS TO CRYSTAL STRUCTURE ANALYSIS

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Structural information of crystalline materials is very important in conducting research and development of industrial materials. Single crystal technique can straightforwardly provide us the information. Experimental products obtained are, however, often polycrystalline materials. Three-dimensional reciprocal space data are required for solving and refining crystal structures, while a problem of peak overlaps is inevitable in powder diffraction. Sophisticated techniques such as the Rietveld method, direct-space methods, have been developed for solving the problem, whereas a high-angular resolution powder diffraction data are always an essential requisite.

A single-crystal analyzer (SCA) is one of the best choices as an X-ray optical device for obtaining high-angular resolution and low background intensities. Its best performance can be obtained by combining it with high brilliance parallel beam from synchrotron radiation (SR) sources. Intensity gains in high resolution and high-speed experiments in several SR facilities have been further multiplied by using multiple-detector systems (MDS). With a laboratory X-ray source, diffracted intensities from the SCA are lower than those from a SR source. A popular way of increasing diffraction intensities is to use a rotating anode X-ray generator and/or a graded multi-layer mirror. To introduce the MDS similar to those used in several SR facilities, however, makes the laboratory diffractometer system more complex and very expensive.

In the present paper, a high-performance high-resolution powder diffraction system will be presented. The angular resolution is the same as that obtained with the SCA, while the intensity gain is greater by one order of magnitude. High performance of the present system could be obtained with a newly designed multi-crystal analyzer. Some examples of application to structure determination and refinement will be presented.