Development of a New Rietveld Code as Powder Diffraction Analysis Suite, Z-Code

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New Japanese Spallation Neutron Source (JSNS), Materials and Life Science Facility (MLF) in Japan Proton Accelerator Research Complex (J-PARC) has been inaugurated. Four different powder diffractometers (Super High Resolution (S-HRPD), High Throughput (iMATERIA), Engineering (TAKUMI), Total Diffraction (NOVA)) have already put out the first great data. Furthermore, two more diffractometers have been proposed. In this situation, new powerful and useful analysis software for powder diffraction data is desired. Since 2004, the powder diffraction group in J-PARC has started to develop a new powder diffraction analysis suite, Z-Code (code-name for the development). Fig.1 shows the overview of Z-Code. It is the integrated environment for finding out crystal structures using various analysis methods from powder diffraction data. For example, It has the general functions of Indexing, Peak Searching, Structure Matching from a Data Base, and Conventional Rietveld analysis. Z-Code also supports Texture analysis, Profile analysis, Fourier synthesis, and Maximum Entropy Method as the advanced analysis components.

We just released and began to test the new Rietveld analysis software called “Z-Rierveld” with the first users of the powder diffractometers in J-PARC. Z-Rietveld is the one component of Z-Code. It has a Graphical User Interface (GUI) and many powerful features for the refinement of crystal structures. Z-Rietveld has demonstrated nice refinements of a complicated structure models using multiple data sets, such as x-ray and neutron ones. In this presentation, more features and details of Z-Rietveld will be discussed.

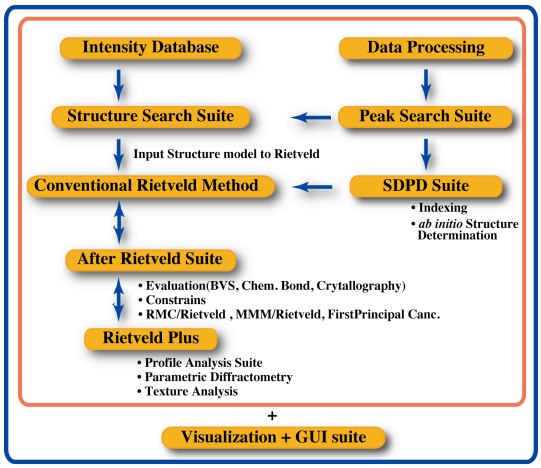

Fig. 1 The overview of Z-Code. Z-Code is still under development for both professional and beginners.