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

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New Japanese Spallation Neutron Source (JSNS), Material 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) and Total Diffraction (NOVA)) have al and Special Environment (SPICA)) have already put out the first data and made good scientific results. Furthermore, two other diffractometers (Earth science (PLANET) and Special Environment SPICA) are constructing now.

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 (Z-Code is development code-name). Fig.1 shows the overview of Z-Code. It is the integrated environment for finding out crystal structure using various analysis methods from powder diffraction data. For example, It has the general functions of Indexing, Peak Searching, Structure Matching from the 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 have released the new Rietveld analysis software called "Z-Rietveld" with the users 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 structure refinement. Z-Rietveld has demonstrated nice refinements of 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.

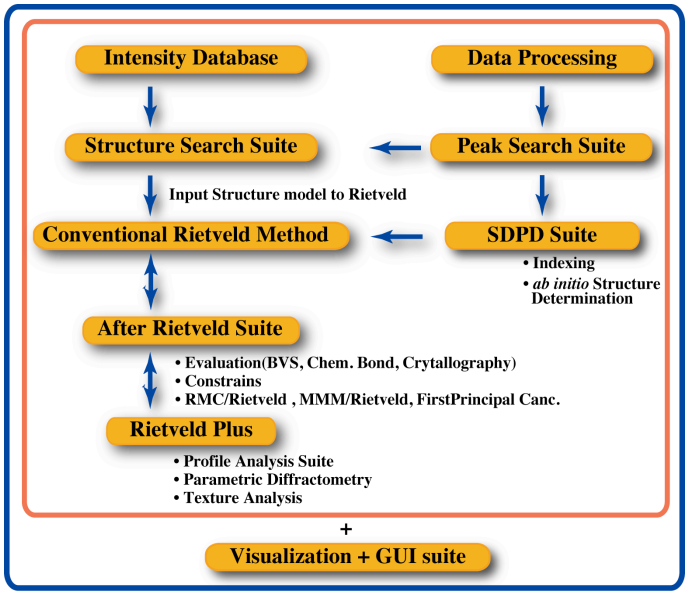

Fig. 1 The overview of Z-Code. Z-Code is still under development for both professional and beginners.