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Product Information

THE WORLD OF THE INTEGRATED RIETVELD ANALYSIS SYSTEM FAT-RIETAN
A MESSAGE TO USERS OF THE RIGAKU VERSION

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A Rietveld analysis program RIETAN is the one and only software that can be applied to the refinement of intensity data measured by any of angle-dispersive X-ray diffraction (including SR), angle-dispersive neutron diffraction and TOF neutron diffraction in virtually the same procedu re.[1],[2] This program has lots of features for crystallographic calculation and is so user-friendly that even the novice at computer or crystal analysis can easily run it. It is designed to have the computer make up for user's want of ability and experience. Thus, in Jappn, RIETAN has already established its position as a *de facto* standard of Rietveld analysis programs. Most educational and research institutions and private businesses now employ RIETAN.

One of the salient features of RIETAN is the provision of manuals that contain exceedingly minute explanations. For instance, a manual for angle-dispersive diffraction contains pages as many as 130. RIETAN may be said to be a rare program for crystallographic computation in Japan because it has such thoroughgoing documentation. These manuals not only scrupulously cover information required for a wide range of users, both beginners and experts of crystal analysis alike, but also contain detailed descriptions not found in conventional manuals. Notable in particular are explanations in a simple style about that minimum knowledge of crystallography by citing examples which is indispensable for running RIETAN, such as how to read "International Tables", the meanings of symmetry operations, complex lattices, equivalent positions, temperature factors, and so on. Such descriptions are very favorably received because they have hitherto been entirely omitted from conventional software packages associated with crystallography. Besides, a detailed report on the newest version of this program[3] is also available.

The weakest point of a previous version of RIETAN was that it was "isolated" software. Because it was not connected to other programs for crystallographic calculation, users had to reenter basic input data on symmetry operations, atomic names, etc. along with results of refinement (structure parameters, lattice constants and their standard deviations) at the time of running the related programs. Parameters refined by Rietveld analysis are no more than expressionless numbers. Needless to say, the whole aspect of crystal structure analysis can be understood only after the validity of a structure model is checked by Fourier (D) synthesis, interatomic distances and bond angles are calculated, and crystal models are plotted. However, because reentry of the above data was a terribly troublesome "dirty work", RIETAN users including me always tended to neglect utilization of the related programs, which leads to dilution of the significance of Rietveld analysis despite collection of intensity data over long hours.

It was toward the end of 1987 that Rigaku Corporation set on the work of modifying RIETAN to a menu-operation system. I checked menus as they came out bit by bit from Rigaku and indicated improvements to be made. What I noticed soon was that unless a variety of related programs should be connected to RIETAN in such a way as to enable execution of them without the need of reentries, RIETAN would lose much of its raison d'&tre as commercial software. Without the provision of such related programs from the maker side, it would be difficult for users to connect these programs to RIETAN by themselves unless they have accumulated expert knowledge about crystal analysis.

[1] F. Izumi: Nippon Kessho Gakkai Shi (J. Crystallogr. Soc. Jpn., in Japanese), **27**, 23 (1985).

[2] F. lzumi, H. Asano, H. Murata and N. Watanabe: J. Appl. Crystallogr., **20**, 411 (1987).

[3] F. Izumi: RIGAKU J., **6**, No. 1, 10 (1989).

Even if they succeeded in obtaining the related programs, it would be almost impossible for them to transport it to a computer which is connected to a powder diffractometer in use or to redesign it to a menu-operation system or to connect it to RIETAN. Such software, if available, must be also useful to those who run RIETAN on mainframe computers.

With the above idea in mind, I started integration of the Rietveld analysis system in June or so of the following year. The new system to be born was given a development code, FAT-RIETAN (stout-size RIETAN). Efforts were devoted at the same time to polish up the substance of RIETAN, especially the output feature of crystallographic data. The progress of programming work was slow, however, partly because I was busily engaged in research and others at that time in the aftermath of "superconductivity fever". Finally, in February 1989, the connection to ORTEP-II, the last phase of the work, was completed, and thereby RIETAN was reborn from a naive stand-alone software to a full-fledged integrated system.

In the Rigaku version of the FAT-RIETAN system, the following programs (① - ⑥) and data bases (⑦ - ⑨) are organically combined with each other to produce a harmonious, integrated environment. The environment thus prepared not only allows Rietveld analysis and simulation of powder diffraction patterns but also makes other crystallographic calculations easily challengeable.

① RIETAN

The Rietveld analysis of X-ray powder diffraction data. It is also possible to simulate X-ray powder diffraction patterns of compounds whose structures have already been analyzed.

② GENREF

Calculation of the diffraction indices and peak positions of a compound whose space group is known. It can also compare the obtained peak positions with an observed pattern so as to examine the diffraction indices and presence of impurities.

③ FRS

Fourier and D syntheses based on F_o estimated from the results of Rietveld analysis so as to plot contour maps.

④ ORFFE

Calculation of interatomic distances and bond angles. This program is characterized by procedures for calculation of precise standard deviations.

⑤ ORTEP-II

Drawing of crystal structure models. This program has surprisingly abundant functions and is excellent in representing anisotropic thermal vibrations. In FAT-RIETAN, macro instructions for crystal model plotting are translated into instructions for ORTEP-II with a preprocessor called PRETEP.

⑥ LATTEN

Calculation of Madelung potentials by Ewald's method.

⑦ SPGRI

A data base containing information on 230 space groups described in "International Tables", Vol. 1.

⑧ SPGRA

A data base containing information on 230 space groups described in "International Tables", Vol. A.

⑨ ASFDC

A data base containing coefficients for calcula-tion of atomic scattering factors as well as correction terms for anomalous dispersion and atomic weights.

Provided in addition is a file manager to efficiently carry out copying, deletion, conversion, etc. of various files. All of these programs are capable of menu operation so that users can devote themselves to analysis without being aware of the presence of the operating system which is running behind FAT-RIETAN.

A drawback of menu operation is troublesome menu selection with a mouse. This is felt more and more as an operator gets familiar with the way of running programs. Another such drawback is that there are frequent occasions where users cannot make full use of program features. This tendency is stronger in particular with RIETAN, ORTEP-II or other programs which have many features and need a large amount of input data. The FAT-RIETAN system (Rigaku version) is designed to allow a jump to any optional entry section at the time of reediting input data, but even so it does not mean a solution to the latter problem. To cope with this, consideration is given in RIETAN and ORTEP-II so that the user can also directly edit input files with a full screen editor (vi or an optional Hitachi Editor).

What should be emphasized here is the educational significance of the FAT-RIETAN system. RIETAN and its related programs include most of crystallographic calculations required for single

crystal X-ray analysis except for an important analytical process for solving the phase problem[4].

Accordingly, this software group must be not only useful for development and identification of materials but also effective for the novice to learn the fundamentals of crystallography. Since for a long period, it has been my earnest wish that not only a handful of people who possess expensive four-circle single-crystal X-ray diffractometers but those who are routinely using powder diffractometers be familiarized with crystallography through RIETAN which is offered to help their studies. RIETAN is a massive program containing nearly 9000 lines. It lavishly uses arrays, moreover, in order to enhance the computation speed. As a result, it can hardly be run on conventional 16-bit personal computers. Intensity data had to be transferred to a large computer for analysis. No matter how excellent anysoftware may be, it is difficuitto expect its wide spread if it needs access to a large computer where file handling is troublesome, functions of editors are very poor, JCL is necessary, and an exorbitant charge for using has to be paid. I was therefore under the impression that for some time ahead it would be impracticable to run RIETAN on a computer connected to powder diffractometers.

When the development of a new diffractometer system, D/max-1000, was started, Rigaku made studies on the selection of a suitable computer but failed to reach an internal consensus. The matter was left as a pending issue. I happened to visit Rigaku in June 1987 and was asked for an advice on a computer for the D/max-1000 system. I recommended without hesitation the use of a 32-bit workstation with UNIX as an operating system. Since UNIX is a "seasoned" OS, it can be operated reliably without being troubled by bugs. Moreover, its multitask and multiwindow capabilities are fitted for simultaneous execution of measurement and data processing on separate windows. I must admit here that in recommending so, there was somewhat an underlying motive in me to transport RIETAN to the Rigaku system. Surprisingly enough, anyway, Rigaku instantly decided on the same day to employ a 32-bit UNIX machine for D/max-1000. Thus, my long cherished wish to carry out Rietveld analysis while simultaneously measuring diffraction data with a multitask and multiwindow system was at last fulfilled, although I made due efforts myself, too, to attain it. The significance of on-the-spot run of various crystallographic calculations (drawing) realized by the completion of the FAT-RIETAN system must be said immeasurable.

The RIGAKU version of the FAT-RIETAN system is the very product that has come out upon joint development by me and Rigaku Corporation. Its performance and ease of use have been thoroughly checked by us. As such, it is the only commercial software at present that can be safely recommended by me who created the original version. It has now left its developer's hand and is being routinely operated by users. During the process of such use, many more points to be improved will surface. I am eager to grow this software further to a more friendly and more refined one by positively incorporating users' requirements and new analytical procedures. It is my wish to mature it to a point where it can render full service as a bridge between powder diffractionists and crystallography. To this end, I welcome comments and information from users who may find problems or bugs upon actual run. I intend to cope with such matters as best as possible.

Lastly, I would like to express my sincere thanks to Mr. Masahiko Saito, Engineering Department of Rigaku Corporation. He took charge of actual modifications toward menu operation. He met my minutest requests and wrote programs, in the C language, containing lines as many as 7000 in total.

[4] For the solution of the phase problem, what most users of four-circle diffractometers carry out is merely the utilization of the direct method as a "black box". No particular high-level crystallographic knowledge is used for this purpose.