Preface

RULES FOR POWDER-DIFFRACTION SOFTWARE

We remember all too well the days in the seventies we walked up and down the road from our laboratory to the University Computing Centre with punchcard trays. We were doing our Ph.D.work, were actively engaged in the use of powder-diffraction methods and were developing software for the application of deconvolution and α_2-component stripping methods. This recollection serves to illustrate that in those days commercial software for the evaluation of diffraction data did not exist and that computer power and facilities, in nowadays eyes, were of the primitive sort: we had to go physically to the "main frame" computer (IBM 360/65) and could only dream of powerful PC's, notebooks, floppy disks and the "internet". In fact even the software to steer the goniometers for data accumulation was partly laboratory made. Measured intensities were recorded on punched paper tape and formatting of the data occurred in the personally favoured, local style.

Contrasts of the past with current practice appear evident. One could think that the present-day provision of fully automated performance of measurements and on-the-spot evaluation of the measured data using commercial software packages has brought paradise on earth for the powder diffractionist. The truth is that on the one hand indeed we recognize the virtues of modern computer power but on the other hand suffer from the accidents and calamities that naturally accompany a development that exceeds the speed limit on the motorway to heaven.

Recently a number of "old" diffractometers in the laboratory in Delft had to be replaced. Not that the goniometers themselves were worn out or inappropriate for current research wishes. The principal reason for replacement was that the computer hardware used for control of the instruments was old (PDP-11 MINC; 32 kB(!); 8 (!) inch floppy disk), broke down frequently and the producer could not guarantee continued service, and, above all, replacement of the computer hardware plus rewriting of the software that was laboratory made was as expensive as acquisition of new, complete diffractometer systems. It hurts to have to abandon a good, in principle useful and accurate instrument (in particular because we did our Ph.D.work on it; but that is sentimentality), just because of such side-effects of a development that in principle is desired.

Undoubtedly, as can be learned from the above example, the future belongs to the commercially available software for data acquisition and evaluation. But then certain quality conditions have to be imposed and satisfied. This situation has not been attained at all.

An issue of great concern is the presence of blunt flaws in the programs sold. These can be straight bugs in the program, but here we mean in particular the methodological errors as for example inherited from the original program developer, and which may be detectable with only the greatest difficulty. Examples to illustrate the reality of what is meant can be given easily. A well known program package allows the fitting of line profiles according to certain profile-shape functions. One of these is the pseudo-Voigt function. This function is well defined in the field of powder diffraction. However, the program uses an analytical description of this function that is quite different from the accepted one. After "discovery" of this artefact, it has led us to indicate in papers, when appropriate, something like "fitting has been performed using the pseudo-Voigt profile-shape function as defined in the software package.....". Further, in an, again very well known, software package in a program for stress analysis ($\sin^2\psi$ method) the Eulerian (tilt) angle ψ was taken as $+\psi$ at places where it should have been $-\psi$, and vice versa, which has drastic consequences for the interpretation of the stress tensor. No doubt that the reader can add a long list of other examples.

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Some of the difficulties as indicated in the preceding paragraph could have been avoided if the program descriptions would have been more precise and accurate. It is also striking that normally the names of the original authors of the code for a certain data-evaluation method are not given in the description of the program and also the references to the specific literature (on which a method is based) are often absent or usually very incomplete. This is not only very unfair to the original developers of a method and also, as often, the program (the commercial supplier should not suggest unjustly an intellectual ownership), but also makes clear where the moral responsibility for errors of principle and shortcomings resides. Obviously any legal liability remains with the commercial supplier, who so to say owns the copyright but does not have the spiritual ownership.

A main problem of commercial software regards the data files. Not only their contents is deficient usually, but their structure can be problematic and, above all, the accessibility of the data (as measured and after evaluation) is never satisfactory. Until recently often producers even deliberately made access to the data files impossible; a morally objectionable act. Also, it happens normally that the software packages for data evaluation are composed of programmes of the most various origins (the majority of these programmed methods for data interpretation (as profile unravelling, Rietveld refinement, line-broadening analysis, stress determination, etc., etc.) have been provided by you and us) and accordingly their data files are structured differently, which has led to the situation that the end user often has to reformat the data files himself if more than one program for data evaluation has to be applied to the same set of experimental data, whereas this problem of course should have been solved by the commercial supplier of the whole package.

Accepting that for many applications of data acquisition and evaluation we as powder diffractionists will be end users of commercially available software, we should be active to develop and impose a general attitude with respect to demands that commercial software should satisfy. Treatment of data files, program descriptions and support continued through the years are a few of related important worries that concern us all.

It is not the first time in science that uneasiness with commercial software has been expressed. Thus about 10 years ago a format was proposed for X-Ray Powder Diffraction data files (deduced from a comparable format for spectroscopic data: Appl. Spectrosc. 42 (1988)151-161). In even more recent years the International Union of Crystallography (IUCr) has initiated the development of a special CIF (Crystallographic Information File: see http://www.iucr.ac.uk/iucr-top/cif/pd/index.html for more details) a presciption for the details which should be provided in any case regarding powder diffraction data as measured and as evaluated. These details as such should be accessible at least from results provided by commercial software. But clearly this is not enough. A more self-assured attitude of the powder diffractionists in this matter is in order to bring about a higher level of quality and reliability in commercial software. Then two routes appear possible. A more assertive behaviour of the individual powder diffractionist will gradually lead to the improvement sought for, or the powder-diffraction community acts as a whole by defining prescriptions and, for example, conferring an official quality mark, and thereby a more rapid betterment seems achievable. The last approach may perhaps best be realized through action of the Powder Diffraction Committee of the IUCr.

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Editorial Notes

Just as for all previous EPDIC conferences the proceedings are published in two books. The first book, i.e. Part 1, contains the papers devoted to developments in the methods and techniques of powder diffraction and the second book, i.e. Part 2, presents the papers with a focus on results obtained by application of powder- diffraction methods to specific classes of materials. Reviewing the proceedings of EPDIC-1, -2, -3, -4 and -5 the ratios of the numbers of papers in Part 1 and Part 2 are found to be 1, 0.7, 0.5, 1 and 0.9. The total number of papers published in the proceedings for each of the conferences ranges from about 120 to over 150.

The subdivision of the papers over the sections within Part 1 and Part 2 has been changed somewhat compared to the proceedings of EPDIC-4. The chapter "Characterization of thin layers" - that first appeared in the EPDIC-3 proceedings - has been transformed to a section of chapter I "Method Development", because more and more analyses become rather specific for thin layers. The chapter *"In-situ*, time dependent powder diffraction" (new for EPDIC-4) has been continued as a special field of applications. Although the emphasis in these papers is on the results obtained for certain materials, just as holds for the papers of Part 2, the *in-situ* technique often cannot be applied straightforwardly: it requires special accessories and data-evaluation techniques to be developed for the system investigated. This justifies that the chapter remains incorporated in Part 1. (Without this special chapter the ratio of the numbers of papers in Part 1 and Part 2 would have been 0.6, just as for EPDIC-4 !)

Each of the five proceedings of EPDIC has its own peculiarity. In the present case a strikingly low number of methodological papers on neutron powder diffraction occurs: only one ! Does this mean that it is right now in full bloom ? The answer is to the neutron powder diffractionists.

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