SIMULTANEOUS FITTING OF DIFFERENT SPECTROSCOPIC DATA: FEATURES AND RECENT APPLICATIONS OF THE EFFI CODE

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As scientists examine more and more complex phenomena and systems, are taking into account more details, they are more frequently faced with the necessity of *simultaneous* evaluation of raw data of measurements performed on the same sample with different methods and/or with the same method at different temperature, pressure, magnetic field, etc. This need is justified by the fact that such experimental data partly depend on the same set of parameters, viz. the physical parameters of the sample, i.e., the parameters the experimentalist is typically interested in. Lacking suitable programs for the simultaneous evaluation of all these data, the experimentalist is often forced to evaluate some of the parameters from only one kind of measurements and to keep these parameters constant when evaluating other experiments, an obviously incorrect approach. Besides, for different theories different programs are used, which makes very difficult tuning parameters of such theories to each other and to extend or modify the theories used for describing different experimental data.

Over the past years, we have developed the general and versatile data fitting environment EFFI (Environment For FItting) [1], which has been very efficiently applied for the evaluation of many sets of 'conventional' transmission and 'synchrotron' Mössbauer spectra the latter including grazing-incidence, i.e., synchrotron Mössbauer reflectometry (SMR) [2] measurements, both time-differential and time-integral. Presently, EFFI is capable of simultaneously fitting several data sets of the following kinds of experiments:

- Conventional Mössbauer absorption and emission spectroscopy
- X-ray reflectometry
- Nuclear resonant forward scattering of synchrotron radiation: time differential mode
- Nuclear resonant forward scattering of synchrotron radiation: stroboscopic mode
- Synchrotron Mössbauer reflectometry: time integral, time differential and stroboscopic modes
- Specular polarized neutron reflectometry
- Off-specular polarized neutron reflectometry

Beside the enumerated spectroscopies, a programmer interface is provided to include new theories. The versatility of EFFI is ensured by handling constraints in terms of general and editable correlation matrices linking parameters of different theories and thereby defining the real physical parameters.

The main and yet essential disadvantage of the old versions of EFFI was the fact that its user interface was written using development tools available in the eighties and, therefore, in spite of its scientific merits, its user-friendliness was considerably limited.

We are presenting the test version of a new generation of EFFI. This environment, based on a user interface written in C++, is a widely available, free, thoroughly documented program. Extended capabilities of EFFI include an up-to-date and user-friendly graphical user interface, which may be developed further as an international project of several groups active in the field and to complement its present capabilities by theories of new experimental methods, including off-specular neutron reflectometry, off-specular synchrotron Mössbauer reflectometry, i.e., methods, which are being increasingly used in the field of magnetic thin film research.

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[1] H. Spiering, L. Deák, L. Bottyán, Hyperfine Interact. 125 (2000) 197.
[2] D.L. Nagy, L. Bottyán, L. Deák, E. Szilágyi, H. Spiering, J. Dekoster, G. Langouche, Hyperfine Interact. 126 (2000) 353.
[3] http://www.dynasync.kfki.hu/