

Open Source Software for Quantitative X-ray Microanalysis: openMicroanalysis

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It goes without saying that the microanalysis community heavily depends on software. Quantification software, simulation programs, and physical quantities databases are essential tools for today's microanalysts. Many software are available either as commercial, personal/research group internal or not openly distributed, free to download and use, and open source. Without a doubt all types of software play an important role in the community, but we believe that open source software is the best approach to foster innovation and exchange ideas while offering the same level of validation and transparency as peer-reviewed scientific work. The ability to read the code gives users access to all mathematical algorithms, alternate implementations, further optimizations or special cases. Most importantly, open source software enables innovation as the scientists can improve or develop new algorithms, without starting from scratch, but using building blocks already available.

We therefore propose to start a community-driven open source project to centralize physical quantity databases and algorithms used for x-ray quantification. The principal objective is to encourage collaborative work in microanalysis by providing the necessary building blocks for new projects. We chose two directions to accomplish this objective: (1) to accept source code donations from scientists in order to collect different implementations of current algorithms, models and databases used in x-ray quantification, and (2) to review, validate and implement them into a coherent, verified, interchangeable sets of building blocks. Although the development of new algorithms or end-user software is not explicitly envisaged at this stage, we strongly believe that this fundamental work will facilitate the creation of new projects for the microanalysis community.

Recently, the CalcZAF software, which was previously free to download, was made open sources by the authors and is now hosted as part of the openMicroanalysis project. Its implementation of different models can now be studied and openly discussed while any modification can be tracked and suggested. Through this first donation, the following ones and the core development, programming best-practices in the open source ecosystem (version control, code proposal, issue tracker, documentation, testing, and release system) are advocated to facilitate and encourage collaborative work.

The roadmap of the second and main direction of the project, the development of building blocks needed in microanalysis, is shown in Figure 1. It consists of three phases. The first phase is the development of fundamental libraries covering all physical quantities required for x-ray quantification like x-ray transitions data, mass absorption coefficients, cross sections, etc. The second phase is related to x-ray intensities. It is separated in two concurrent phases which involves the implantation of algorithms for (a) modelling x-ray generation and calculating x-ray intensities, and (b) extracting x-ray intensities from experimental data. The third and last phase combines the results from the previous phases with the aim to validate the implemented correction models with experimental data. In sum, the outcomes of each phase can serve as building blocks for new projects in microanalysis, for example, to improve or develop new quantification algorithms.

We chose the Apache License Version 2.0 [1] for the main project because it is a permissive license which allows the code to be included in commercial and open source software while requiring any code modification in derivative software to be clearly stated. This license allows the openMicroanalysis project to reach a larger community than other open source licenses.

As aforementioned, one of the strongest project goal is to be community-driven. We encourage everybody from the microanalysis community to participate as the project does not only need programmers, maintainers and contributors, but also experts to review current and new models, and users to give feedback and request features useful for their research and experiments. Furthermore, the contribution of quality experimental data will be essential for the validation of the models.

References:

[1] Apache License: <http://www.apache.org/licenses/LICENSE-2.0>
 [2] openMicroanalysis Website: <http://www.openmicroanalysis.org/>
 [3] openMicroanalysis Discussion forum: <https://groups.google.com/forum/#!forum/openmicroanalysis>

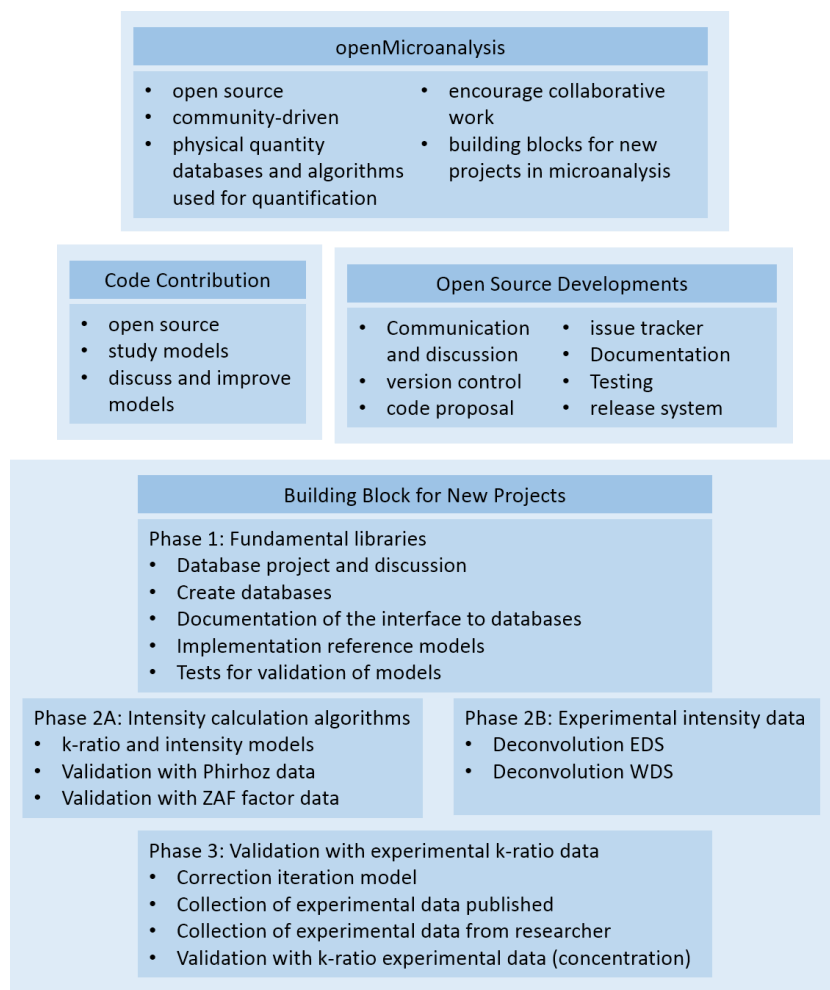


Figure 1. The roadmap of the main direction of the openMicroanalysis project.