## Project information

| | |
|---|---|
| **Project full title** | European network for developing new horizons for RIs |
| **Project acronym** | EURIZON |
| **Grant agreement no.** | 871072 |
| **Instrument** | Research and Innovation Action (RIA) |
| **Duration** | 01/02/2020 – 31/01/2024 |
| **Website** | https://www.eurizon-project.eu/ |

## Deliverable information

| | |
|---|---|
| **Deliverable no.** | D3.12 |
| **Deliverable title** | **Python based data analysis software for advanced polarized neutron diffractometers** |
| **Deliverable responsible** | Dr. Arsen Goukassov |
| **Related Work-Package/Task** | WP 3 Task 3.5 |
| **Type (e.g. Report; other)** | Report |
| **Author(s)** | Dr. Arsen Goukassov |
| **Author(s) affiliation** | Leon Brillouin Laboratory CEA-CNRS |
| **Dissemination level** | |
| **Document Version** | |
| **Date** | 05/01/2024 |
| **Download page** | |

## Document information

| Version no. | Date | Author(s) | Comment |
|---|---|---|---|
| 2 | 13.05.2024 | Dr. Arsen Goukassov | |
| | | | |
| | | | |
| | | | |
| | | | |
| | | | |
| | | | |
| | | | |
| | | | |

### Table of Contents



This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 871072.

**Task 3.5: Prototype of advanced polarized neutron diffractometer [CEA-LLB; FZJ, ESS, ILL]**

Aim of the WP is prototyping of new elements improving the performance of polarized neutron diffraction experiments on advanced neutron sources. CEA-LLB is involved in the building of five instruments at ESS under construction, including the polarized neutron diffractometer MAGIC. LLB will conduct calculations and optimization and assure the design of spin handling devices, flippers, guide fields needed for polarized single crystal diffractometers as well as the software necessary for the data analysis adapted for area detectors. Developed software will be implemented at polarized neutron diffractometer POLI of the JCNS at the MLZ and will be accommodated for further using on diffraction instruments DREAM and MAGIC at the ESS.

**D3.12: Python based data analysis software for advanced polarized neutron diffractometers [48]**

**Report on D3.12**

The main goal of the LLB in the second stage of the CREMLIN+ project started in 2022 was a development of modern data analysis software for polarized neutron diffraction, which can be used in different neutron research center like ILL, FRMII and ESS under construction. This was necessary taking into account that currently available softwares in this domain, such as CCSL library and FULLPROF has been created several decades ago and was becoming out of date.

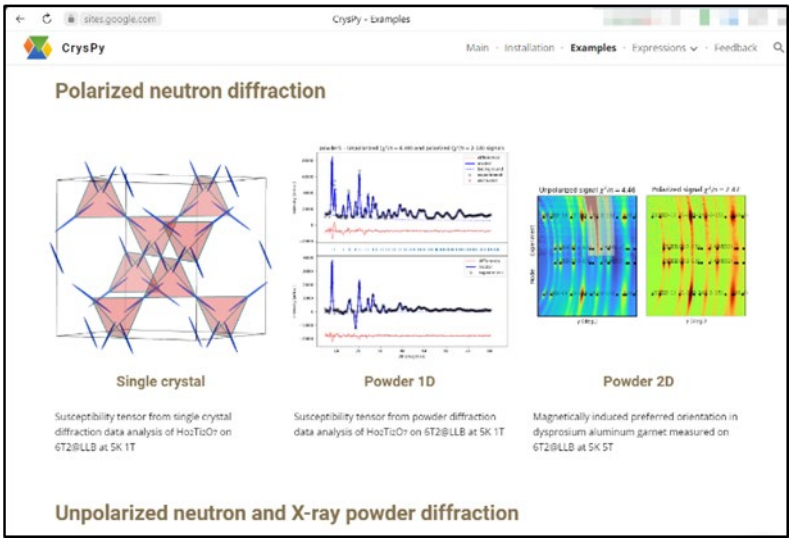
Such a software CrysPy has been created in the LLB using Python language. CrysPy is an open source program package that was developed for polarized neutron diffraction data analysis. The package allows the data treatment both for powders and single-crystal samples. Nuclear and (commensurate) magnetic structures refinement can be also perfomed based on the unpolarized neutron diffraction and X-ray diffraction data. CrysPy is currently the only one library in the world that allows analyzing polarized neutron diffraction experiments both on single crystals and powders. Developed by LLB the latest release of CrysPy includes the following features:

- **Two-dimensional Rietveld refinement procedure.** Two-dimensional area detectors increase the efficiency of the instrument by an order of magnitude. Moreover, in polarized neutron diffraction experiments the variation of intensity along the Debye cones can be used for the separation of nuclear and magnetic scattering contributions, as neutrons are sensitive only to the magnetic moment perpendicular to the scattering vector. For these reasons, the two-dimensional Rietveld refinement procedure implemented in the CrysPy library allows one to obtain a precision in the determination of the magnetic anisotropy close to that obtained in the single-crystal diffraction experiments. In the case of “magnetically textured” samples, the given procedure has significant perspectives as it does not require a high instrumental resolution due to the fact that different types of reflections with similar Bragg angles are spread over the Debye cones;

This project has received funding from the European Union’s Horizon 2020 research and innovation programme under grant agreement No. 871072.

- **Magnetization density reconstruction.** Currently used refinement procedure employs so-called dipole approximation for the magnetic form factor. It assumes that the spatial distribution of the magnetization density of an ion is isotropic, which is valid as long as it is larger than approximately the mean radius of the unpaired electrons. Newly developed maximum entropy reconstruction procedure in CrysPy taking into account the local anisotropy goes beyond the dipole approximation. This should stimulate the development of direct methods of non-collinear magnetization density reconstruction in anisotropic compounds based on the joint multipole- or wave-function refinements, thus shedding a light on the anisotropy of compounds with unquenched orbital moments, primarily of lanthanides and irridates. See (I.Kibalin, A.Gukasov, PRB, 2022) for more information;
- **Time-of-flight diffraction experiments with polarized neutrons**. The novel high-performing time-of-flight diffractometer MAGiC, which is under construction at the EES, will generate rather complex three-dimensional angular- and wavelength-dispersive data that cannot be routinely treated using the standard software packages. Thus, the development of appropriate software for the analysis of such complex experimental data is a desirable and inevitable step. The current release of the CrysPy library currently allows handling either one-dimensional angular or time-of-flight diffraction profiles measured with polarized neutrons;
- **Software dissemination.** The software dissemination efforts foster further innovation in CrysPy development and expand LLB collaboration with scientific centers. The source code of the CrysPy library has been published on the GitHub server: github.com/ikibalin/cryspy. The educational materials and 'training' experimental data are presented on the internet page: www/cryspy.fr.

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 871072.


CrysPy library has been presented at the conference ICDM9, 2022 (Aarhus, Denmark), the Robert-Stewart school (Nancy, France), 2022, the workshop in ILL (Grenoble, France), and the joint ESS ILL user meeting (Lund, Sweden), 2023, International Conference on Superconductivity and Magnetism ICSM2023, AOCNS2023 and others.

**Publications related to the Cryspy library**

**CrysPy developments:**

I.A. Kibalin, A. Gukasov, Local magnetic anisotropy by polarized neutron powder diffraction: Application of magnetically induced preferred crystallite orientation. Physical Review Research, 1 (2019) 033100

I.A. Kibalin, F. Damay, X. Fabreges, A. Goukassov, and S. Petit, Competing Interactions in Dysprosium Garnets and Generalized Magnetic Phase Diagram of S = 1 spins on a Hyperkagome Network, Physical Review Research, 2 (2020) 033509

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 871072.

I.A. Kibalin and A. Gukasov, Asphericity of magnetisation density and anisotropy in rare-earth pyrochlores via polarized neutron diffraction and iterative entropy maximization, submitted Phys. Rev. B, 105 (2022) 104411

**CrysPy using**

I. V. Golosovsky; I. A. Kibalin; A. Gukasov; A. G. Roca; A. López-Ortega; M. Estrader; M. Vasilakaki; K. N. Trohidou; T. C. Hansen; I. Puente-Orench et al. Elucidating Individual Magnetic Contributions in Bi-Magnetic Fe3O4/Mn3O4 Core/Shell Nanoparticles by Polarized Powder Neutron Diffraction. Small Methods, 2023-10 DOI: 10.1002/smtd.202201725

Sandeep K. Gupta, Hannah H. Nielsen, Andreas M. Thiel, Emil A. Klahn, Erxi Feng, Huibo B. Cao, Thomas C. Hansen, Eddy Lelièvre-Berna, Arsen Gukasov, Iurii Kibalin, Sebastian Dechert, Serhiy Demeshko, Jacob Overgaard*, and Franc Meyer. Multi-Technique Experimental Benchmarking of the Local Magnetic Anisotropy of a Cobalt(II) Single-Ion Magnet. JACS Au 2023, 3, 2, 429–440

W.J.A. Blackmore, S.P.M. Curley, R.C. Williams, S. Vaidya, J. Singleton, S. Birnbaum, A. Ozarowski, J.A. Schlueter, Y.-S. Chen, B. Gillon, A. Goukassov, I. Kibalin, D.Y. Villa, J.A. Villa, J.L. Manson, P.A. Goddard, Magneto-structural Correlations in Ni2+-Halide···Halide-Ni2+ Chains, Inorganic Chemistry, 61 (2022) 141

I. Kibalin, A. Gukasov, Quantifying Magnetic Anisotropy Using Polarized Neutron Powder Diffraction, Neutron News, (2021) 1

E.A. Klahn, A.M. Thiel, R.B. Degn, I. Kibalin, A. Gukassov, C. Wilson, A.B. Canaj, M. Murrie and J. Overgaard, Magnetic anisotropies of Ho( III ) and Dy( III ) single-molecule magnets experimentally determined via polarized neutron diffraction, Dalton Transactions, 50 (2021) 14207

E.A. Klahn, E. Damgaard-Møller, L. Krause, I. Kibalin, A. Gukasov, S. Tripathi, A. Swain, M. Shanmugam, J. Overgaard, Quantifying magnetic anisotropy using X-ray and neutron diffraction, IUCrJ, 8 (2021) 833

M. Souhassou, I. Kibalin, M. Deutsch, A.B. Voufack, C. Lecomte and N. Claiser, Spin-resolved charge density and wavefunction refinements using MOLLYNX: a review, Acta Cryst., B77 (2021) 706

E.K. Nigmatullina, I.A. Kibalin, V.P. Sedov, A.A. Borisenkova, A.A. Bykov, I.V. Golosovsky, 'Phantom' atoms and thermal motion in fullerene C60 revealed by x-ray and neutron diffraction, Journal of Physics: Condensed Matter, 33 (2021) 455401

L. Ding, C. Hu, E. Feng, C. Jiang, I.A. Kibalin, A. Gukasov, MF. Chi, N. Ni and H. Cao, Neutron diffraction study of magnetism in van der Waals layered MnBi2nTe3n+1, Journal of Physics D: Applied Physics, 54 (2021) 174003

I. Kibalin, A.B. Voufack, M. Souhassou, B. Gillon, J.-M. Gillet, N. Claiser, A. Gukasov, F. Porcher and C. Lecomte, Spin-resolved atomic orbital model refinement for combined charge and spin density analysis: application to the YTiO3 perovskite, Acta Crystallographica Section A, 77 (2021) 96

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 871072.

Currently, various approaches to the description of magnetic anisotropy, beyond the local susceptibility model, are being developed, which will be included in the future CrysPy library releases. The new approaches will enable to describe local magnetic anisotropy and bulk magnetization within the framework of the same model. The complementarity of polarized neutron diffraction experiments with magnetometry measurements should attract interest to the polarized neutron diffraction in chemical laboratories involved in the studies of magnetic anisotropy of various modern materials, such as molecule magnets, nanoparticles, and frustrated systems.

The software CrysPy is now used in LLB, ILL, ORNL, FRMII and ESS.

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 871072.