Invited Lecture

Revealing the local magnetic anisotropy by polarized neutron powder diffraction

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Magnetic anisotropy is an essential property of primary importance in areas ranging from molecular magnetism and magneto-optics to magnetoelectric transport. It is an inherent characteristic of magnetic materials that describes the response of magnetization to a magnetic field. Several techniques are currently used to extract information about bulk magnetic anisotropy; the most well-known are single crystal and torque magnetometry and ESR. However, all these techniques provide information about the bulk anisotropy of material [1].

A powerful alternative method for characterizing magnetic anisotropy is single-crystal polarized neutron diffraction (PND). In this approach, measured flipping ratios are used to fit the atomic magnetic susceptibility tensors for each of the magnetic atoms in the asymmetric unit, which allows one to quantify the magnetic anisotropy at the local level in paramagnetic compounds [2]. It is becoming a reference for mapping the magnetic anisotropy at the atomic scale in molecular magnets. However, it is still hardly applicable to a number of highly interesting powder materials, such as molecular magnets or nanoscale systems, because of the low luminosity of existing instruments and the absence of appropriate data analysis software. A library of dedicated computer code is now available at www.cryspy.fr, and, having established an initial proof-of-concept, the technique can be considered ready for application to novel systems [3]. Application of this technique to a range of polarized neutron powder diffraction (PNPD) measurements will be presented in the report (Fig.1) [4-6].

Furthermore, the PNPD technique has been recently applied to study the magnetic anisotropy of magnetically ordered compounds. In particular, PNPD data of Mn3O4 magnetic nanoparticles, analysed in the frame of the local anisotropy approach [7], is used to gain unprecedented detail on the contribution of the different magnetic sublattices on the magnetization process. The main results of this work will also be highlighted in the report.



Figure 1. (a) Magnetization components versus temperature for DyGaG. Insets show magnetization ellipsoids. (b) The measured and calculated flipping sum (top) and difference (bottom) diffraction patterns collected on $Co([(CH_3)_2N]_2CS)_2Cl_2$ at 2K, 5T.

- [1] Perfetti, M. (2017) Coordination Chemistry Reviews 348, 171-86.
- [2] Gukasov, A., Brown, P.J. (2002) Journal of Physics: Condensed Matter 14, 8831-39.
- [3] Kibalin, I. A., Gukasov, A. (2019) Physical Review Research 1, 033100.
- [4] Kibalin, I.A., Damay, F., Fabrèges, X., Gukasov, A., Petit, S. (2020) Physical Review Research 2, 033509.
- [5] Klahn, E.A., Damgaard-Møller, E., Krause, L. Kibalin, I., Gukasov, A., Tripathi, S., Swain, A., Shanmugam, M., Overgaard, J. (2021) IUCrJ 8, 833 41.
- [6] Golosovsky, I.V., Kibalin, I.A., Gukasov, A., Roca, A. G., López-Ortega, A., Estrader, M., Vasilakaki, M., Trohidou, K. N., Hansen, T. C., Puente-Orench, I., Lelièvre-Berna, E., Nogués, J. (2023) Small Methods 7(10), 2201725.
- [7] In process of submission to publication: Kibalin, I. A., Gukasov, A., Golosovsky, I. V., Roca, A. G., López-Ortega, A., Estrader, M., Hansen, T. C., Puente-Orench, I., Lelièvre-Berna, E., Nogués, J. Revealing the spin structure and local anisotropy in nanoparticles by polarized neutron powder diffraction: Mn₃O₄ and Fe₃O₄ as case studies.