

MS40-2-5 How to do it? On-line single-crystal irradiation and spectroscopic measurements at in-house X-ray diffraction laboratory

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Abstract

With the development of hardware and ideas in crystallography field single-crystal studies becomes more and more demanding, thus more and more often a need of use complementary techniques in order to support X-ray diffraction data occurs.

Ideally, all complementary techniques should be used on the exactly same sample, in the exactly same conditions as for X-ray diffraction measurement. This however requires all the experimental set-ups mounted within the diffractometer, what creates difficulties due to limited space and goniometer movements during X-ray diffraction measurement. On the other hand, goniometer allows a crystal orientation in chosen direction, what is crucial for spectroscopic measurements.

In the literature most of on-line experimental set-ups are mounted at synchrotron facilities,^{1–14} where space requirements are not that demanding, and very often hardware capabilities are greater. In-house solutions are rarely described.^{15,16}

In this presentation we will focus on techniques requiring proper wavelength guiding from UV-IR range acting as external stimulus inducing structural changes within a crystal or to perform spectroscopic measurements on a single crystal. Our set-up is designed by crystallographers for crystallographers. We tried to find user friendly solutions, providing high efficiency and universal applications avoiding compromises.

We will discuss mostly the practical aspects when building on-line set-ups from sample preparation, through the selection of optics and data processing, to the analysis of the results. We will point out the biggest difficulties and most challenging topics with presentation of ready apparatus solutions with description of used components and applications, such as optical absorption and photoluminescence measurements on a single crystal.

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Fig. 1. The design of the experimental set-up

