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Complementary studies of the structural properties of highly disordered materials by x-ray absorption and diffraction

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Nowadays technology very often takes advantage of the diversity of useful properties observed in highly disordered materials. The reliable characterization of such materials requires application of several methods providing complementary information. The complementary application of x-ray diffraction and absorption studies will be discussed basing on a few examples. One of them will be the group of non-stoichiometric composite transition metal complex salts, known as double metal cyanides (DMC). These materials are used as the industrial catalysts and form an interesting family of porous molecular materials with large fraction of the amorphous phase. This fraction may be obtained by introduction to the crystalline zinc hexacyanocobaltate (III) ($Zn_3[Co(CN)_6]_2 \cdot nH_2O$) organic ligands of different size. Depending on the type of ligands the catalysts exhibit different levels of activity. The crystalline zinc hexacyanocobaltate exhibits only very weak catalytic properties. Although they are frequently used in chemical industry the mechanism of catalytic activity is not known.

The other examples will concern magnetic semiconductors with intentionally introduced inclusions of secondary phases [1]. The structural and magnetic properties of such composites will be overviewed and advantage of applying for the same pieces of material several nondestructive techniques will be emphasized. In many cases the absence of diffraction peaks cannot guarantee the absence of other phases particularly when they result from the disordered nano-inclusions. The advantage of synchrotron based diffraction will be demonstrated in such a case.

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High-pressure diffraction studies at synchrotrons and in laboratories

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Since the late 1950's high pressure crystallography has become an efficient technique for crystal structure determinations and for monitoring phase transitions. The diamond-anvil cell was then designed and can be routinely applied in laboratories and dedicated beamlines of synchrotron and neutron facilities.

Synchrotrons provided new quality in X-ray diffraction and particularly in these experiments where very high intensity of the radiation is needed. It can be especially advantageous at high pressure crystallography, where the size of the sample is reverse to the attainable pressure. Moreover, because of the very high background, the time of data acquisition is often very long before sufficient signal-to-background ratio is obtained. In our research we study organic and organometallic compounds and the scattering of light atoms is relatively weak. Examples of single-crystal data measured in the lab with sealed X-ray tube and of the data collection repeated at the synchrotron will be compared. It can be shown that synchrotron is advantageous not only because of the beam intensity but also because of a tunable X-ray wavelength, low-beam diversion and small beam diameters. The disadvantages of high polarization and fluctuations in intensity in the synchrotrons can be easy corrected.

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