matice [7], a výpočet analytických derivací intenzit s využitím algoritmů pro derivace vlastních vektorů a vlastních hodnot matice [8]. V oddělení strukturní analýzy je již po mnoho let vyvíjen krystalografický výpočetní systém Jana (současná verze Jana2006, [9]), a tento systém chceme využít jako základ pro implementaci nové metody.

Závěr

Nová laboratoř elektronové difrakce při Oddělení strukturní analýzy Fyzikálního Ústavu AV ČR, v.v.i. vznikla s cílem zavést, rozvinout a využívat metodu precesní elektronové difrakce pro kvantitativní strukturní analýzu krystalů už od velikosti několika desítek nanometrů. Laboratoř je vybavena transmisním elektronovým mikroskopem Philips CM120 a precesním zařízením SpinningStar. Cílem rozvoje experimentální i výpočetní metodiky je vývoj metody pro řešení a upřesňování krystalových struktur nanokrystalů, a její aplikace na současné problémy v oblasti materiálových věd.

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European Infrastructure for Study of Neutron Scattering

EVROPSKÉ INFRASTRUKTURY PRO STUDIUM NEUTRONOVÉHO ROPZTYLU

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The contribution will be published in next issue.

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NEUTRON DIFFRACTION EXPERIMENTS ON MEREDIT INSTRUMENT

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Introduction

Neutron powder diffractometer called MEREDIT is available for general and dedicated research use in the Nuclear Physics Institute in Řež from the beginning of the year 2009. Since that time we have made some very interesting measurement using this instrument together with application of all available sample environments which the diffractometer is equipped with. Unfortunately most of the demand for the beam time came from the foreign institutions. So the purpose of this presentation is to bring to Czech research community the information about the the neutron powder diffraction instrument what is accessible "at home" and demonstrate on several examples what the *neutrons* diffraction can do and what kind of problems can help with in point of view of the structure.

MEREDIT instrument

MEREDIT instrument is placed on the horizontal channel number 6 in the experimental hall of the light water reactor LVR15 in Řež. The layout of the instrument is shown on the Fig. 1. Three different wavelengths of the neutrons available for the diffraction experiments can be selected by two automatically exchangeable monochromators. The details about the secondary neutron beams is written in the Tab. 1. The multi-detector bank consists of 35 individual ^{3}He detectors in front of each is 10' Soller collimator. The diffraction pattern can be collected from 2° up to 148° in 2 with different step size

For dedicated measurement use the instrument is equipped with different sample environments. Vacuum furnace covers the temperature range from room tempera-

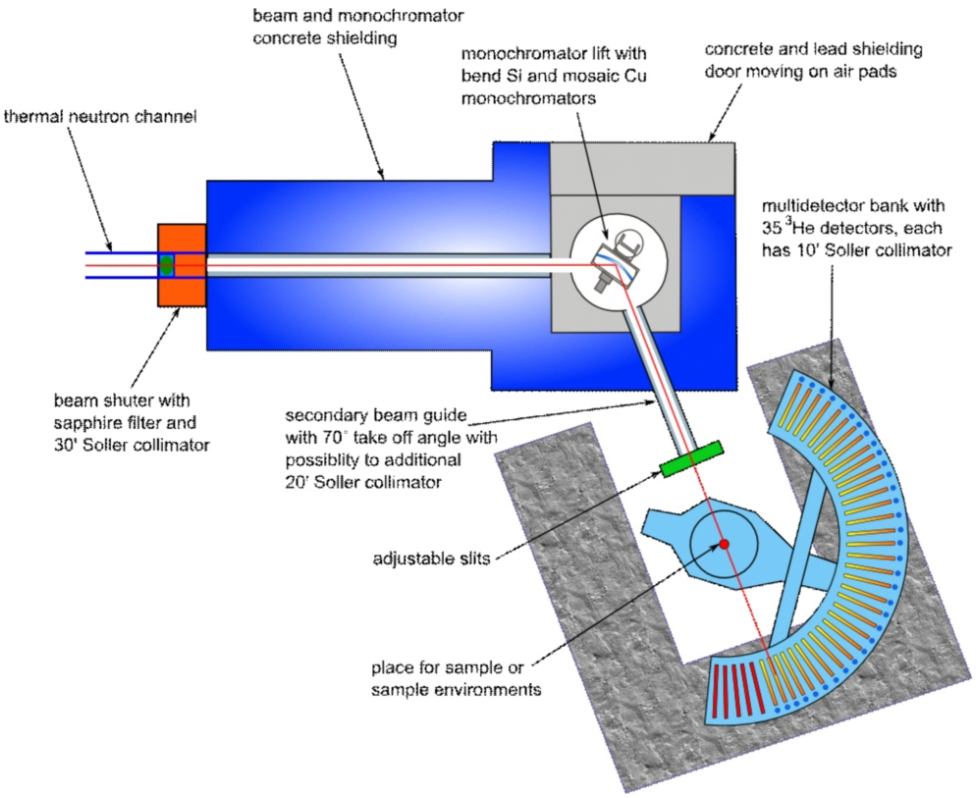

Figure 1. Layout of the MEREDIT instrument.

ture up to 1000 °C and close cycle cryostat goes from room temperature down to 10 K. Carousel for placing up to 6 powder samples and Euler goniometer are also available. A special deformation rig permits *in-situ* measurements under uniaxial stress/pressure or fatigue cycles. More information about the instrument, sample environments, resolution function etc. can be found on the web page of the instrument [1].

Advantages and disadvantages of using the neutron diffraction

The neutron diffraction if very useful probe technique because of these main advantages:

- deep sample penetration
- "see" the light elements
- distinguishing of elements lying beside in periodic table
- direct interaction with magnetic structure

There also exist disadvantages. The main disadvantages are that for the neutron diffraction experiment you need a large quantity of the sample and the neutron flux is not so high – long counting time.

Let demonstrate on the real examples measured on MEREDIT instrument the above mentioned advantages and try to compare the results with X-ray diffraction experiments.

Deep sample penetration

This advantage allows you to use vast kind of closed sample environments (furnace, cryostat, magnet, etc.). In other hand you will collect the information from the whole volume of your sample – useful when studying internal changes in the sample (residual material stress/strain) or want to use non-destructive internal probe for ex. cultural heritage investigation.

"See" light elements

In some cases important properties of material is bind with the light elements such as O, N, C or H(D). Such kind of elements is hardly possible to "see" by X-ray diffraction but neutrons provide very powerful tool to describe them. In the Fig. 2 are electron and nuclear density calculated from the X-ray and neutron powder diffraction data of lanthanum silicate, respectively. It is clearly visible that the "visibility" of the oxygen atoms which is crucial for this oxygen-ion conductive material is limited in the case of the X-ray diffraction. The hydrogen storage materials are also very important kind of materials what can be studied by the neutron diffraction. Especially in the point of view of content of the hydrogen that is enter to the structure. Example of such investigation is made on the intermetallic compound $ScAl_{0.8}Mg_{0.2}$ [2].

Distinguishing of elements lying beside in periodic table

Scattering amplitude for X-ray increases with the atomic number but in the case of neutrons it is not dependent on position in the periodic table. In some case as for ex. Mn or Ti the scattering amplitude is even negative. It means that we are able distinguish two atoms beside in periodic table (Fe/Mn) and say if these atoms are in the structure ordered or not. The example is given in the ferromagnetic material $FeMn(Si_{0.5}P_{0.5})$ studied by X-ray and neutron diffraction.

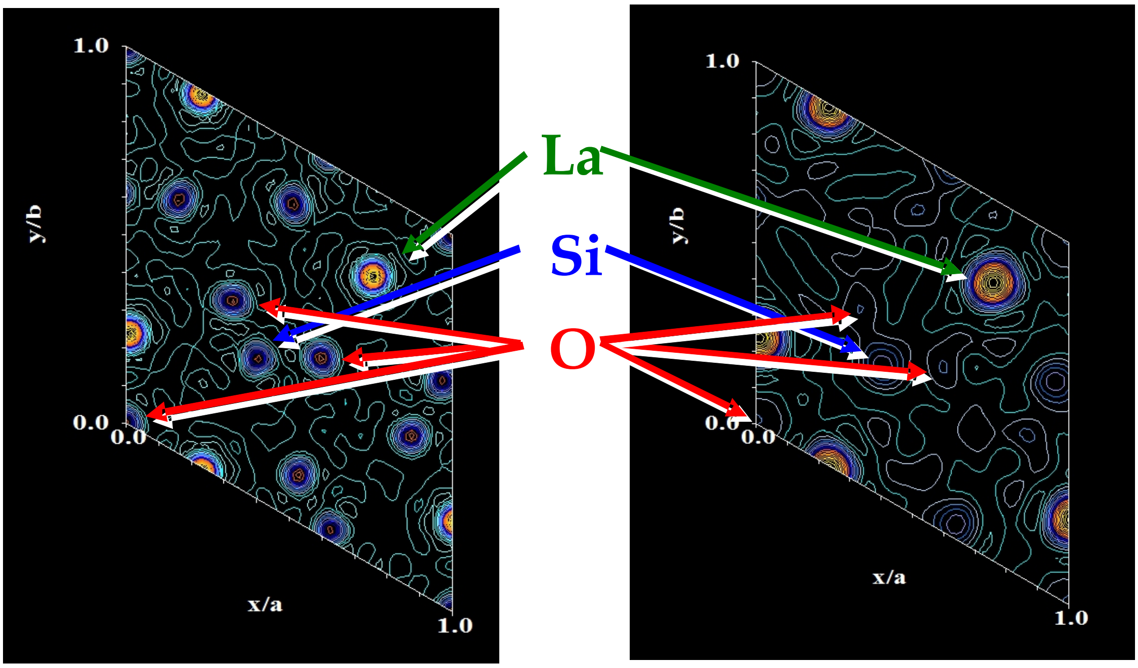

Figure 2. Nuclear (left) and electron (right) density map of the plane (001) at z = Ľ of the lanthanum silicate.

Direct interaction with magnetic structure

Due to the fact that neutron posses the spin what can interact with the spins in the sample we can get by using neutron diffraction the information about the magnetic structure. Even the neutron diffraction can solve the complex magnetic structures the example of how the spin arrangement is "visible" by neutrons is made on simple structure of FeS. FeS shows the antiferromagnetic structure with propagation vector *k*=(0, 0, 0).

Conclusion

Contribution to solve some kind of problems by using the neutron powder diffraction can be very significant. So don't think of neutron powder diffraction as a competitive method to the X-ray or electron diffraction but as a complementary tool which can push you further in your investigation. Moreover notice that we have such tool now in the Czech republic and it is open for collaboration.

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