01-Instrumentation and Experimental Techniques (X-rays, Neutrons, Electrons)

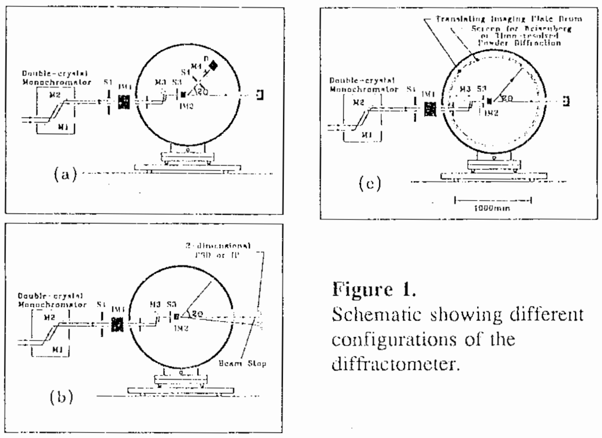

Figure 1. Schematic showing different configurations of the diffractometer.

PS–01.05.05 CATION DISTRIBUTION IN ZN-OXIDE SPINELS. By W. Schäfer[1], G. Will[2] and J. Gal[2], [1]Mineralogical Institute, University Bonn, Neutron Diffraction Group KFA Jülich, Bonn, Poppelsdorfer Schloß, 5300 Bonn, Germany; [2]Ben Gusion University, Beer Sheva, Israel.

The cation distribution in 4 compounds: $ZnAl_2O_4$, $ZnFe_2O_4$, $TiZn_2O_4$ and $SnZn_2O_4$ has been determined by neutron diffraction. Part of the investigations were done by conventional monochromatic powder diffraction at the FRJ-2 reactor in Jülich, part by TOF-measurements at the spallation sources ISIS. In both cases a position sensitive linear detector has been used.

The diffraction measurements were preceded by Mössbauer studies, which yielded contradicting results. The question arose whether the compounds crystallize as normal spinels or as inverse spinels. Only neutron diffraction with sufficient differences in the scattering lengths between Zn and the other cations will give the proper result.

The analysis was done by the Two-Step-Method with first a profile analysis and profile fitting yielding intensities for each reflection. The actual analysis and the cation distribution was then done with the POWLS least squares/program. Procedures and results will be shown.

01.06 – Open Commission Meeting on Neutron Diffraction – Complementarity of Neutron Sources

OCM–01.06.01 SCIENCE FROM PULSED SPALLATION NEUTRON SOURCES. By J L Finney, ISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot, Oxon, OX11 0QX, UK.

Conventional wisdom has it that pulsed neutron sources should be used when high energy and high momentum transfer is needed. This advantage over continuous reactor sources arises from the presence in the under-moderated spectrum of a significant high energy, low wavelength component, and facilitates high energy excitation studies and access to high scattering vectors. The time structure of the neutron pulse, however, allows a wide range of science to be performed that would be difficult, inefficient, or impossible on continuous sources. These advantages include very high resolution in both space and time, measurements over wide dynamic ranges of both energy and momentum transfer, the exploitation of fixed scattering geometries, and very low backgrounds.

These advantages have been exploited to great effect in areas of interest to crystallographers. Examples include the structure solution and refinement from powder data of systems for which single crystals were previously required, the detailed exploration of diffuse scattering, and the simultaneous measurement of both structure and dynamics in changing systems. Again contrary to conventional wisdom, pulsed sources are powerful sources of cold neutrons, and examples will be given of structural work exploiting long wavelength neutrons.

Although pulsed sources are relatively young, they have developed rapidly and are now established as powerful sources which have particular strong advantages. They are also capable of further development, as witnessed by proposals in both Europe and the USA for new sources up to 30 times the power of the ISIS source in the UK.

OCM–01.06.02 PULSED NEUTRON SOURCES AND STEADY REACTOR SOURCES By Y, Endoh, Department of Physics, Tohoku University Aramaki Aza Aoba, Aoba ku, Sendai, 980, Japan

We have argued for a long time the necessity of the complimentary usage of both steady and pulsed neutrons for condensed matter science in particular. In early days, we have developed pulsed neutron scattering techniques by carrying out experiments at the electron lineac facility of Tohoku University. Pulsed neutrons has been delivered since the late 60′ s. In 1981, the first pulsed spallation neutron beam was delivered at the National Laboratory for High Energy Physics (KEK) in Japan after three year′ s construction of this neutron facility, KENS. It was once the most intense and also the first full scaled pulsed neutron facility in the world. Since then KENS has been improved by the renewal of the spallation target as well as intensifying the proton accelerator, but it is a far small scaled facility compared with the world biggest neutron facility of ISIS at the Rutherford Appleton Laboratory.

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On the other hand, the JRR3M which is the medium flux reactor was started recently operation, which eases our frustrations due to the shortage of steady neutrons for a long period. Now Japanese neutron users can access to either facilities under the well organized user programs. Furthermore many are familiar to both pulsed and steady sources and enjoy the complementarity. Therefore soon or later the program will be arranged in such a way that we can access to both facilities more easily.

I will discuss in the presentation the complementarity of both neutron sources stressing both the scientific and technical merits by showing some real examples. Then I will present the future pulsed neutron project in Japan which is now proposed to the Japanese government.

OCM-01.06.03 CHEMICAL PHYSICS WITH ADVANCED NEUTRON SOURCES by J.W.White*, Research School of Chemistry, Canberra, ACT, 0200, Australia

This lecture will illustrate the variety of problems that can now be solved with modern neutron scattering methods and the feasibility of doing valuable but different types of experiment at neutron sources of different power and spectral characteristics. Examples from our recent work on Nucleation of Zeolites in silicate gels, Microphase separation in paraffin mixtures, Combined High resolution diffraction and inelastic scattering for Intercalates, will be used to illustrate methodological aspects of the complementarity that can be developed by astute optimisation of sources and instruments and some detail will be given on The superconductivity and Lattice Dynamics of Rb3C60 as an example of how a unique an insight into the mechanism of the superconductivity was recently obtained by neutron inelastic scattering.

As concerns Rb3C60 superconductivity, the phonon density of states of Rb3C60 has been measured above and below the superconducting phase transition temperature of 29K and in the energy transfer range 1<DE/meV<300 at an energy resolution DE/E=2%. Marked changes in the molecular vibrational spectrum of C60 are observed upon intercalation with rubidium. In particular the Hg modes at 54meV and Tlu mode at 66meV are strongly quenched and other modes are broadened and shifted. Distinct changes in the Hg, Tlu modes near 180meV and the Hg modes near 135meV are observed on passing through the superconducting transition temperature region. These changes strongly suggest the involvement of molecular motions in the superconductivity of these materials.

PS-01.06.04 SXD: SINGLE CRYSTAL STRUCTURAL AND DIFFUSE SCATTERING STUDIES BY TIME-OF-FLIGHT NEUTRON LAUE DIFFRACTION. by C.C.Wilson*, ISIS, Rutherford Appleton Laboratory, Chilton, Didcot, Oxon OX11 0QX, UK

SXD, the single crystal diffractometer at the UK Spallation Neutron Source ISIS, uses the Laue time-of-flight diffraction technique for structural studies. This method exploits the ability of an instrument equipped with a 2D position-sensitive detector (PSD) on a pulsed neutron source to access large volumes of reciprocal space in a single measurement and has significant advantages in many areas of structural work.

Among the areas in which SXD is routinely operating are the following:

- Structural studies: location of unknown atoms, especially hydrogen, water and other light units; the detailed study of hydrogen bonding in organic materials, especially in very strong hydrogen bonds; the study of long range (static) structural disorder, for example in minerals and cases where species are close in atomic number ; the exploitation of the high sin q/y measurements possible on a spallation source (greater than 3A-1) to measure high resolution effects;
- Diffuse scattering studies: the study of short range order and disorder; quantitative atomic level cluster modeling: quantitative Reverse Monte Carlo type modeling.
- Incommensurate structures and phase transitions: the study of magnetic structures, especially where the incommensurate peaks are in obscure or unknown regions; the monitoring of structural changes, where the technique is of especial use when the phase transition can be monitored and characterized through a small subset of reflections, as these can often be obtained in a single data histogram using time-of-light Laue diffraction.

This paper will present examples of the use of SXD in these areas.