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INELASTIC NEUTRON SCATTERING SPECTROMETER FOR THE IN-06 NEUTRON SOURCE AT THE MOSCOW MESON FACTORY

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ABSTRACT

In the spectrometers in which the so-called inverse geometry of scattering is used, the scattering neutron energy, E_2, is fixed and the initial neutron energy, E_1, is determined by source to sample time of flight. The inverse geometry method is a unique reliable means for determination of the absolute intensity of spectral lines. It is possible because this method allows experiments in a wide range transferred energies to be carried out without changing the experiment geometry. Such spectrometers possess a good definite dependence of the transfer energy on momentum transfer. This allows one to extract complementary to optical methods information from the experimental data.

The KDSOG-M spectrometer was created at the IBR-2 pulsed reactor of JINR for investigation of the lattice dynamics of solids and simultaneous analysis of the phase structure of samples. For analysis of the scattering neutron energy polycrystal filters and single crystals are used.

Creation of the IN-06 neutron source based on the proton accelerator of the Moscow meson factory leads to the necessary formation of a scientific research program for condensed matter physics. Re-equipment of the KDSOG-M spectrometer for use at the IN-06 neutron source includes preparation of an instrumental basis for carring out experiments in solid state physics and other fields (biophysics, applied science and so on).

This work is a project for transfer and updating the inverse geometry inelastic neutron scattering spectrometer KDSOG-M for use at the IN-06 neutron source of Moscow meson factory.

Keywords: Inelastic scattering, Inverse geometry

1. The IN-06 neutron source

The principle of operation of the IN-06 slow and fast (spallation) neutron source for neutron investigation in the branches of condensed matter physics and nuclear physics is based on use of the pulsed proton beam and accelerator-storage complex of the Meson factory of the State Scientific Centre Institute for Nuclear Research of the Russian Academy of Science and uranium targets [1].

The neutron source is planned to be put into operation in stages. In the first stage, the use of 4 experimental channels inside the experimental hall (neutron channel N1-N4) is planned. Flight paths in the first stage will be up to 30 m. In 1998 another three channels with flight paths up to 100 m, which terminate in experimental pavilions, will be in use.

The layout of the IN-06 experimental hall is shown in Fig. 1. Basic parameters of the IN-06 neutron source in the first stage is as follows: thermal neutron peak flux ~4×10^{14} n/cм^2/s, thermal neutron average flux ~0.8×10^{12} n/cм^2/s, thermal neutron pulse width ~50 μs at a frequency of 50 Hz.

In addition, changing the non-multiplying target to a multiplying target is supposed. It will increase the thermal neutron flux density by 1-2 orders of magnitude. Creation of a storage ring will decrease the thermal neutron pulse width.

Since the length of flight paths in the first stage are limited to 30 m (channel N1), creation of spectrometer with moderate resolution and high luminosity is the optimum version. A spectrometer like the KDSOG-M

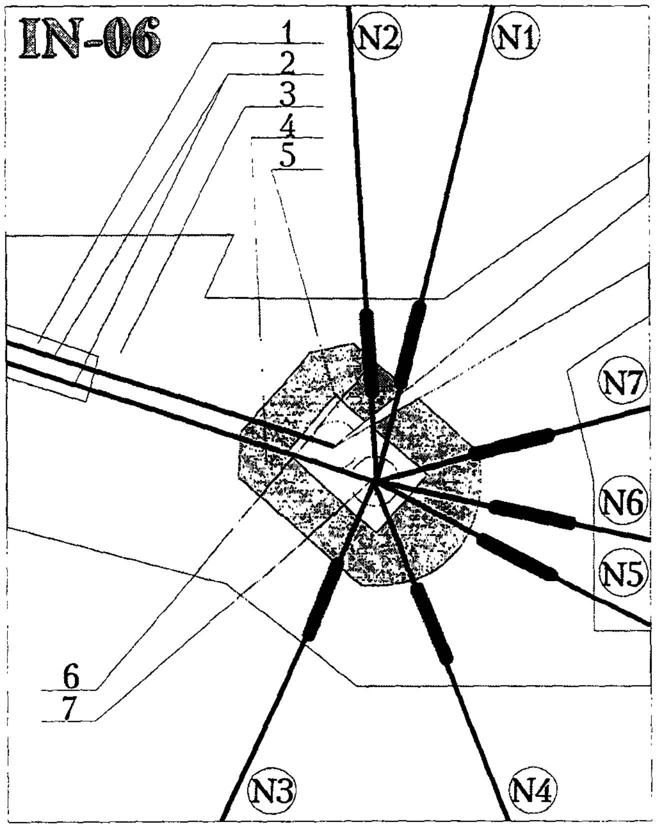


Fig. 1. The layout of the IN-06 neutron source experimental hall:

1. *Accelerator*
2. *Proton beams*
3. *Shield*
4. *Concrete*
5. *Thermal shield*
6. *Channel gate*
7. *Neutron target*

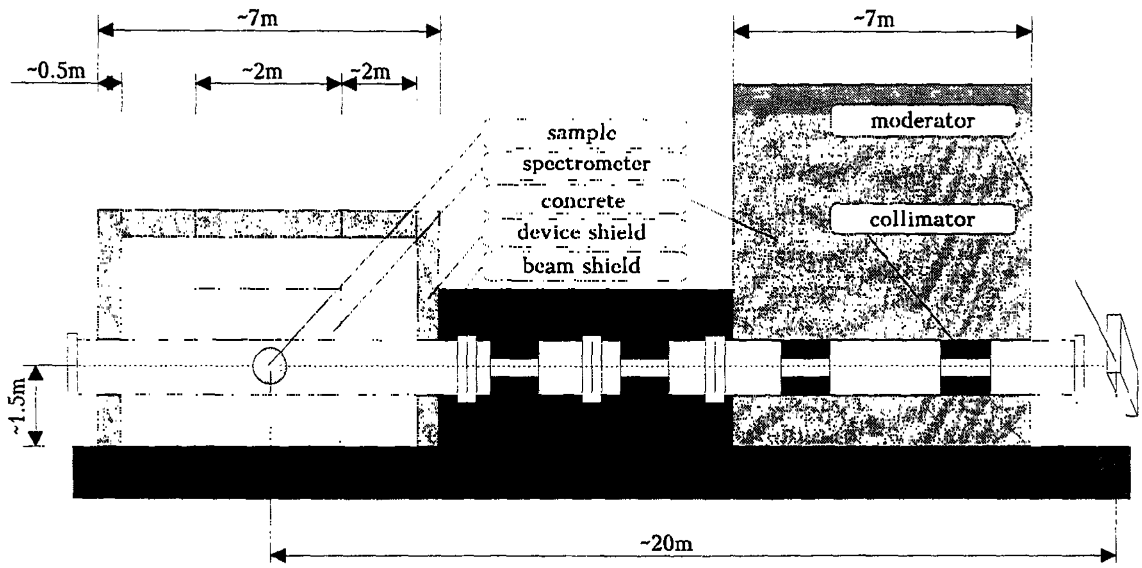


Fig. 2. Scheme of equipment and arrangement of shields.

spectrometer satisfies these requirements. Moreover, the smaller (compared to IBR-2) thermal neutron pulse width will allow an increase in spectrometer resolution. The scheme of spectrometer modernisation described below allows the use of time focusing and gives possibilities for step-by-step equipping of the spectrometer by supplementary section for investigation of inelastic neutron scattering.

Equipment and shielding for normal operation of the spectrometer, which must be placed in the IN-06 experimental hall, are shown in Fig. 2.

2. The KDSOG-M spectrometer

In 1984 the inelastic neutron scattering spectrometer using inverse geometry (see Fig. 3), KDSOG-M, was put into operation at the IBR-2 pulsed reactor [2]. The KDSOG-M spectrometer was designed for investigations of crystal lattice dynamics by inelastic scattering and for neutron diffraction studies simultaneously. That gave the possibility to investigate the phase composition of the sample which sufficiently increased the volume of information obtained from experimental data.

The most convenient conditions for carring out the experiments in condensed matter physics using the KDSOG-M spectrometer are available in the region of energy transfer below 50 meV (see Fig. 4). The composition of the low background level in this region of energy transfer, medium resolution and high luminosity allows the study of crystal lattice dynamics, its changes at phase transitions, vibration spectra of amorphous substances and low frequency intramolecular vibrations in molecular crystals. The values of the transition energies between the levels of paramagnetic ions in the crystal fields also lie in the same range.

At higher values of energy transfers (up to 500 meV) despite the background increases and the resolution becomes worse, it is still possible to

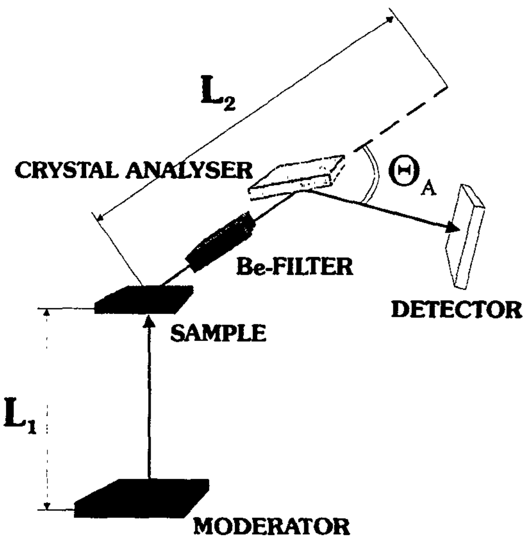


Fig. 3. The inverse geometry method.

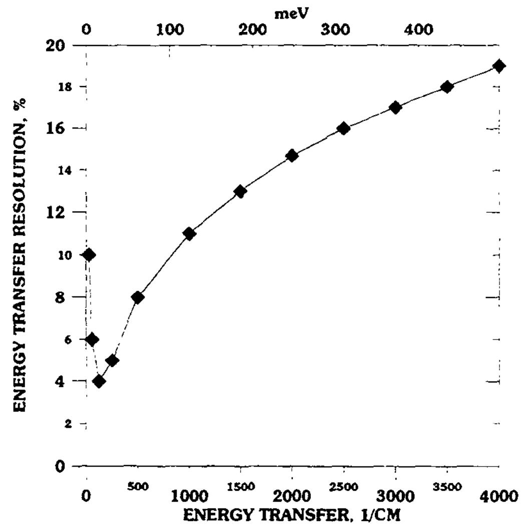


Fig. 4. Relative resolution of the KDSOG-M spectrometer.

investigate hydrogen vibrations in the lattices of metal hydrates due to the high luminosity of the device.

It is possible to conclude that the most straightforward directions for using the KDSOG-M spectrometer are the investigations of hydrogen containing crystals, molecular crystals and crystal field effects.

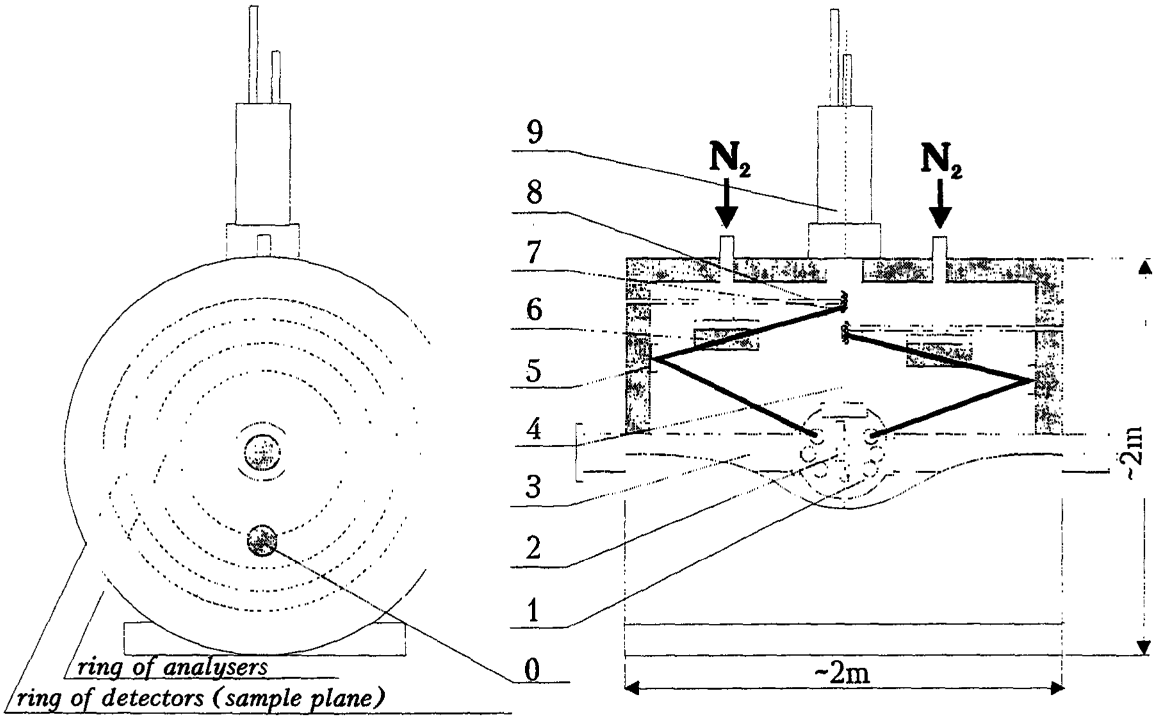
While discussing the possibilities of reconstruction of the spectrometer for use at the IN-06 neutron source of Moscow meson factory, it is necessary to take into account peculiarities of this neutron source. Such includes the considerably lower thermal neutron pulse width and several orders of magnitude lower background of fast neutrons in comparison with the IBR-2 reactor. Consequently, the creation of a spectrometer which would take into account these peculiarities of the source and at the same time include all the advantages of the KDSOG-M spectrometer (high luminosity, possibility of sample phase composition control) seems to be the most prospective.

3. The MAINS spectrometer

The inelastic scattering inverse geometry MAINS (Multy Analyser Inelastic Neutron Scattering spectrometer) spectrometer is being designed on the basis of the KDSOG-M spectrometer. It is intended for solid state dynamics investigations and is planned for use at the IN-06 neutron source.

3.1 The construction

The MAINS spectrometer is similar to the MODES spectrometer at ISIS, which is projected as an upgrade of the time focusing TFXA spectrometer. The MAINS spectrometer is different from that one in its neutron scattering analysis and detector systems. Due to the peculiarities of the IN-06 neutron source, the most reasonable construction of the spectrometer is the following (see Fig. 5):



0	*Diffraction detector*	*5*	*Single-crystal analyser*
1	*Vacuum bank*	*6*	*Beryllium filter*
2	*Sample*	*7*	*Inelastic scattering detector*
3	*Neutron guide*	*8*	*Detector holder*
4	*Well for sample insertion*	*9*	*Vacuum valve*

Fig. 5. The MAINS spectrometer

The inner vacuum volume of device is limited by the cylinder tank. Crystal-analysers 5 for inelastic scattering investigation are ring-shaped and are made of Zn- or PG-single crystals (see Fig. 6). Crystal-analysers are mounted on the side walls of the cylinder tank from inside. After being reflected from analysers 5, neutrons pass through beryllium filter 6 (the construction of which is shown in Fig. 7) and fall on detectors 7. The detector system consists of two detector rings of different radii which are located in the same plane with the sample. One of the

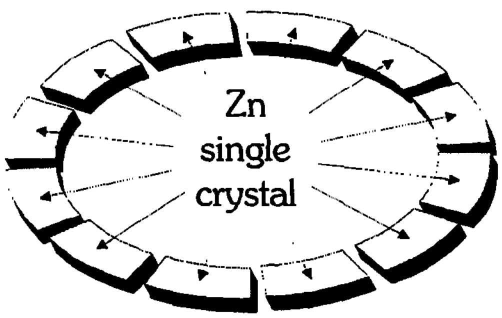


Fig. 6. Ring of analysers

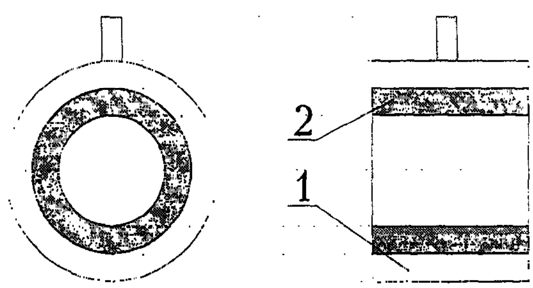


Fig. 7. Beryllium filter:
1. Liquid nitrogen bonjo
2. Polycrystal beryllium

detector rings is designed for registering neutrons scattered in the reflection geometry. Another is designed for the transmission geometry. Inelastic scattering sections are symmetrical relative to the neutron guide tube. The arrangement of the detectors in the same plane with the sample gives the possibility to use time focusing while collecting data.

The diffraction part of the spectrometer is the SNM-17 counter placed in the backscattering geometry and surrounded by a Cd-shield.

3.2 Resolution

For estimation of the resolution ability of the inelastic scattering spectrometer we will use the general formula:

$$\frac{\Delta\varepsilon}{\varepsilon} = \frac{1}{\varepsilon}\sqrt{R_1^2 + R_2^2 + R_3^2 + R_4^2} \qquad (1),$$

where

$$R_1 = \frac{\partial\varepsilon}{\partial E_2}\Delta E_2 = \left(1 + \frac{L_2}{L_1}\left(\frac{E_1}{E_2}\right)^{3/2}\right) \times \Delta E_2 \qquad (2),$$

$$R_2 = \frac{\partial\varepsilon}{\partial L_2}\Delta L_2 = \frac{4E_1^{3/2}}{L_1 E_2^{1/2}} \times \Delta L_2 \qquad (3),$$

$$R_3 = \frac{\partial\varepsilon}{\partial t}\Delta t = \frac{2E_1^{3/2}}{AL_1} \times \Delta t \qquad (4),$$

$$R_4 = \frac{\partial\varepsilon}{\partial L_1}\Delta L_1 = \frac{2E_1}{L_1} \times \Delta L_1 \qquad (5).$$

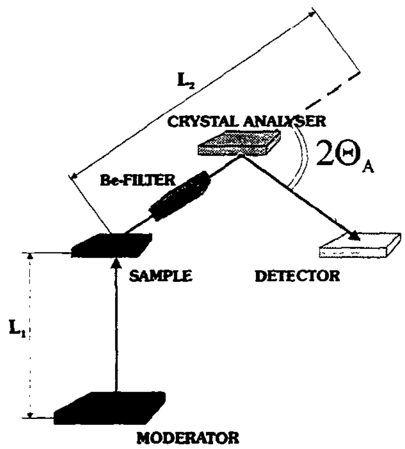


Fig. 8. Principle of the time focusing method.

Here

E_1, ΔE_1, E_2, ΔE_2	-	*the energies of neutrons before and after scattering and corresponding uncertainties;*
L_1, ΔL_1, L_2, ΔL_2	-	*first and second flight paths and corresponding uncertainties;*
$\varepsilon = E_1 - E_2$, $\Delta\varepsilon$	-	*energy transfer and uncertainty of energy transfer;*
$A = 2286.4$	-	*constant.*

The use of time focusing means (see Fig. 8) that all neutrons at the detector have one and the same secondary flight time. In the first order of approximation, mosaicity of the crystal analyser does not affect the focusing and the derivative (2) is reduced to $\partial\varepsilon / \partial E_2 = 1.0$ in this geometry. The uncertainty of the neutron energy after the scattering is defined by the expression $\Delta E_2 = 2E_2 \coth\Theta_A \times \Delta\Theta_A$. So we have:

$$R_1 = 2E_2 \coth\Theta_A \times \Delta\Theta_A \qquad (6).$$

Besides that, time focusing on the second flight path eliminates all the terms in the resolution connected with limitations of the beam collimation. Consequently, the term in resolution due to the uncertainty of the second flight path is connected only with the finite thickness of the sample, analyser and the detector. Let us define the effective uncertainty of thicknesses Δl as:

$$\Delta l = (\Delta s^2 + \Delta a^2 + \Delta d^2)^{\frac{1}{2}} \qquad (7),$$

where Δs, Δa, Δd are thicknesses of the sample, analyser and the detector. When $\Delta L_2 = \Delta l / \sin\Theta_A$ and:

$$R_2 = 4E_1^{3/2} \times \Delta l / L_1 E_2^{1/2} \sin\Theta_A \qquad (8).$$

In the third term of formula (1) we will define the time uncertainty as $\Delta t = \sqrt{\Delta t_{th} + \Delta t_{ch}}$, where Δt_s is the thermal neutron pulse width, Δt_{ch} is the time channel width.

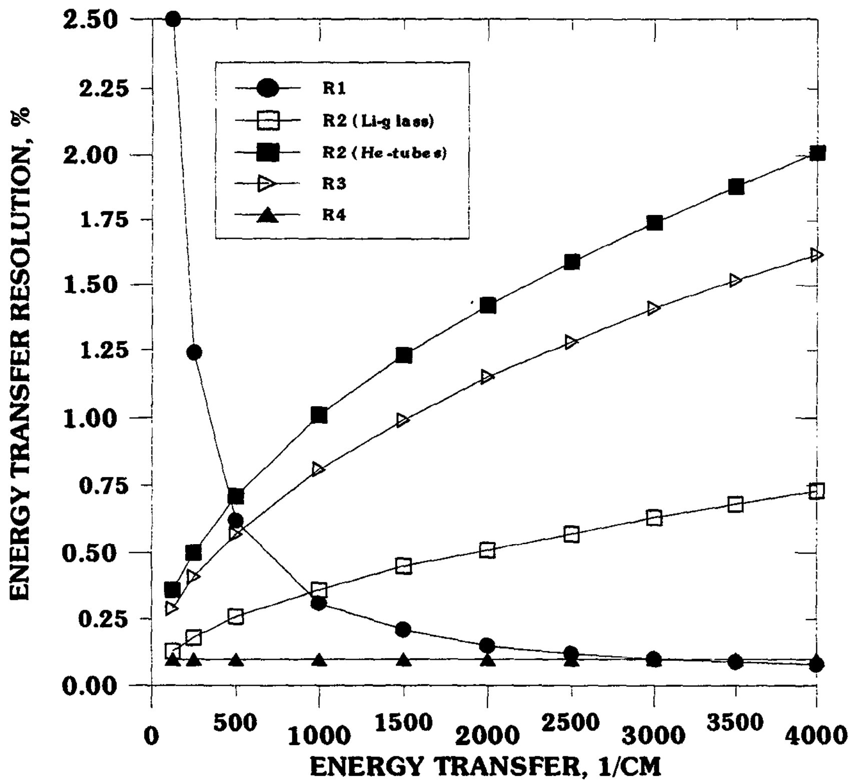


Fig. 9. Contributions to the resolution of the MAINS spectrometer from different terms of formula (1).

In the fourth term of formula (1) the uncertainty of the first flight path ΔL_1 is low (see Fig. 9) and the contribution of R_4 is also low. Neglecting these we obtain the final expression for the resolution of the spectrometer:

$$\frac{\Delta\varepsilon}{\varepsilon} = \frac{1}{E_1 - E_2}\sqrt{(2E_2\coth\Theta_A \times \Delta\Theta_A)^2 + \left(\frac{4E_1^{3/2} \times \Delta l}{L_1 E_2^{1/2}\sin\Theta_A}\right)^2 + \left(\frac{2E_1^{3/2}\Delta t}{AL_1}\right)^2} \qquad (9).$$

From Fig. 9 it is obvious that the $\boldsymbol{R_2}$ term is most valuable, after the $\boldsymbol{R_3}$ term, which depends on the thermal neutron pulse width or even exceeds it. So the question about the type of detectors for the detector system of the spectrometer seems to be the most interesting. The use of scintillation detectors made of Li-glass (of 2 mm thickness) gives sufficient improvement in resolution compared to the He^3-detectors (of 8 mm thickness) and allows MAINS to reach the level of the TFXA and MODES (ISIS) devices.

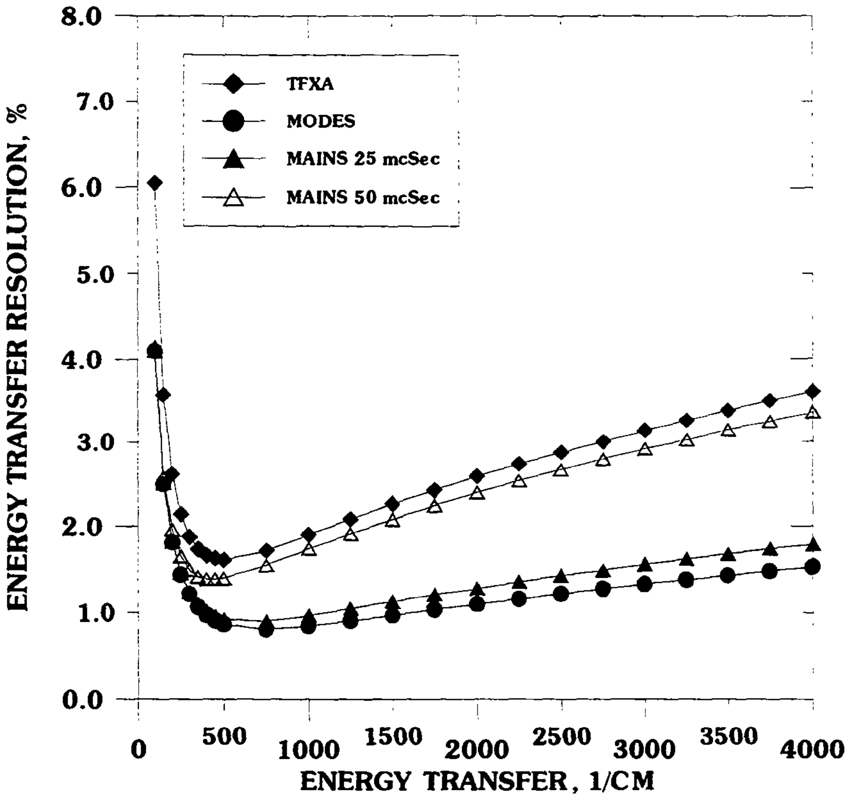


Fig. 10. Resolution of the MAINS spectrometer

Assuming the spectrometer parameters are equal to the following:

Primary flight path	L_1	30 m
Secondary flight path	L_2	0.7 m
Initial neutron energy	E_1	0-4000 cm^{-1}
Scattering neutron energy	E_2	3 meV
Angle of incidence	θ	45^o
Beam divergence	$\Delta\theta$	0.064 rad
Sample thickness	Δs	1 mm
Analyser thickness	Δa	2 mm
Detector thickness	Δd	2 mm
Pulse width	Δt	25, 50 μs

we obtain estimations of resolution at different energy transfer (see Fig. 10).

Comparing the resolution of the MAINS spectrometer with the resolutions of the TFXA spectrometer [3] operating at ISIS and designed on its base MODES spectrometer [4] shows that the use of Li-glass detectors compensates for the differences in the widths of the thermal neutron pulses. The creation of a storage ring will allow a decrease in the thermal neutron pulse width. The substitution of the non-multiplying target by the multiplying one gives the possibility for a sufficient increase in the peak flux and consequently for enlargement of the first flight path without any intensity loss.

3.3 Sample environment

The sample environment of the MAINS spectrometer must contain the standard set of systems including "ORANGE" He-cryostats, a high pressure cell, closed cycle refrigerator. Thus will provide a wide range of possibilities for investigations of the crystal lattice dynamics of different substances, including high temperature superconductors, molecular crystals, non-ideal crystals and alloys.

4. Conclusion

The described MAINS spectrometer is designed for carring out investigations in condensed matter physics and gives possibilities to study the structure and dynamics of substances. Due to specific features of the device and of the IN-06 neutron source, the most straightforward directions of investigations with this spectrometer are the following:

◊ investigations of the vibration spectra of hydrogen containing materials;
◊ investigations of catalysis process;
◊ investigations of molecular crystals;
◊ investigations of the lattice dynamics of novel materials.

Improvement of the experimental data quality and widening the range of scientific problems demands the development of neutron source, precise inspection of the detector system of the spectrometer and the creation of an advanced software for treatment of experimental results.

5. Aknowledgements

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6. References

[1] Proceedings of the ICANS-XII, RAL94-025, vol.2, T71, 1994.
[2] G.Baluka et al. Preprint of JINR, R13-84-242, 1984.
[3] J.Penfold and J.Tomkinson: Report RAL-86-019, Rutherford Appleton Laboratory, Chilton, UK, 1986.
[4] R.E.Hester, P.C.H.Mitchell, K.Prassides. Research proposal for MODES, EPSRC, Polaris House, November 1994.