ICANS XIX,
19th meeting on Collaboration of Advanced Neutron Sources
March 8 – 12, 2010
Grindelwald, Switzerland

PERSPECTIVES FOR ELECTRONVOLT NEUTRON SPECTROSCOPY AT LONG PULSE SPALLATION NEUTRON SOURCES

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ABSTRACT

Pulsed neutron sources open up new fields of investigation in condensed matter, as the intense fluxes of epithermal neutrons (above 500 meV) allow to achieve unique energy and wave vector transfers . The investigation of matter at small time and space scales is provides an insight into atomic momentum distribution $n(p)$ and mean kinetic energy $<E_K>$, through the deep inelastic neutron scattering (DINS) technique. On the other hand, epithermal neutrons allow to access the kinematical region space characterized by $\hbar\omega > 1$ eV and $q < 10$ Å^{-1}, i.e. the high energy inelastic neutron scattering (HINS) regime. HINS enables experimental studies on the dispersion relations of high energy excitations in metals, semiconductors and insulators, high lying molecular rotational– vibrational states, molecular electronic excitations, and the electronic level in solids. The neutron spectrum at Long (LPSS) and Short (SPSS)- Spallation Sources contains also a large amount of high energy neutrons (above 1 MeV). This special feature may be well exploited for electronic chips irradiation for the study of the so-called Single Event Effects (SEE). The measurement of SEEs is very important for the electronic industries to assess the robustness of their products, especially those featuring nanometric sizes that represent the new generation electronic components.

1. Introduction

A Long Pulse Spallation Source (LPSS) produces a high flux of epithermal neutrons that can in principle be exploited for unique investigations on condensed matter. However a short pulse source would appear to be more suitable for eV instruments and LPSS will need a dedicated development of instrumentation in order to make good use of the available epithermal neutron flux. In the last twenty years, intense instrumental and research activities have been carried on VESUVIO, the inverted geometry spectrometer installed at the ISIS spallation neutron source. The instrument currently operates routinely for Deep Inelastic Neutron Scattering (DINS) measurements, where the scattering process occurs at high energy and wave vector transfer, $\hbar\omega > 1\text{eV}$, $q > 20$ Å^{-1}, respectively [1]. This experimental technique is widely recognized as a unique tool to derive the single particle momentum distribution, $n(p)$, and its second moment, the mean kinetic energy $<E_k>$, physical quantities of great interest in those systems where the short time dynamics departs from the classical behavior. Indeed DINS demonstrated its potential in recognizing the line shape of $n(p)$ highlightening the presence of quantum phenomena in hydrogen containing systems such as water in both free and bulk geometry, water in its metastable phase or the hydration water surrounding biological systems, such as lysozyme [1]. .On the other hand, epithermal neutrons allow to access the kinematical region space characterized by $\hbar\omega > 1$ eV and $q < 10$ Å^{-1}, i.e. the high energy inelastic neutron scattering (HINS) regime. HINS enables experimental studies on the dispersion relations of high energy excitations in metals, semiconductors and insulators, high lying molecular rotational–vibrational states, molecular electronic excitations, and the electronic level in solids [2]. In order to carry out DINS measurements at LPSS, special kind of electronvolt spectrometers have to be conceived. In particular two possibilities may be considered: 1) A chopper spectrometer, with typical selection time significantly below the presently available 5 microseconds. The scattered neutron beam being analyzed using high rate capability neutron counters (direct geometry configuration); 2) An incident beam resonance filter selection for beam monochromation coupled to a multiple resonance filtering technique (e.g. the Resonance Filter or the Resonance Detector configuration) to select the final neutron energy (inverse geometry). These two configurations have to be fully investigated to find out actual benefits and drawbacks in order to build an optimal spectrometer.

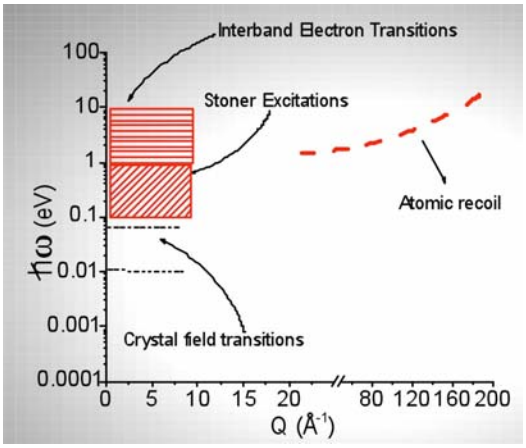

Fig. 1: Single particle properties probed by electronvolt neutron scattering.

The neutron spectrum at LPSS contains also a large amount of high energy neutrons (above 1 MeV). This special feature may be well exploited for electronic chips irradiation for the study of the so-called Single Event Effects (SEE). The measurement of SEEs is very important for the electronic industries to assess the robustness of their products, especially those featuring nanometric sizes that represent the new generation electronic components.

2. Kinematic planes and energy resolution

An extended kinematic range can be accessed using electronvolt neutrons at LPSS and SPSS, using both inverse and direct geometry, which employ energy selection in the secondary or primary flight paths, respectively. Figure 2 and Figure 3 illustrate the energy and wave vector transfers accessed by both type of spectrometers for the DINS and HINS regime.

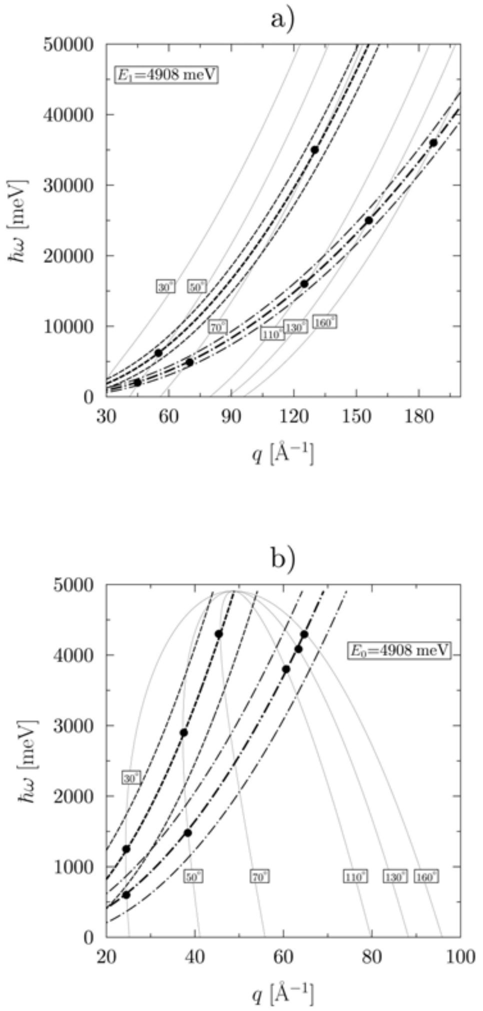

Fig. 2: Kinematical plane for atomic (H and D) recoil studies using: a) inverse geometry with E_1=4908 meV; b) direct geometry with E_0=4908 meV. Continuous and dashed lines mark the proton(deuteron) recoils with a recoil width of 5 Å^{-1}. Scattering angle contours are indicated.

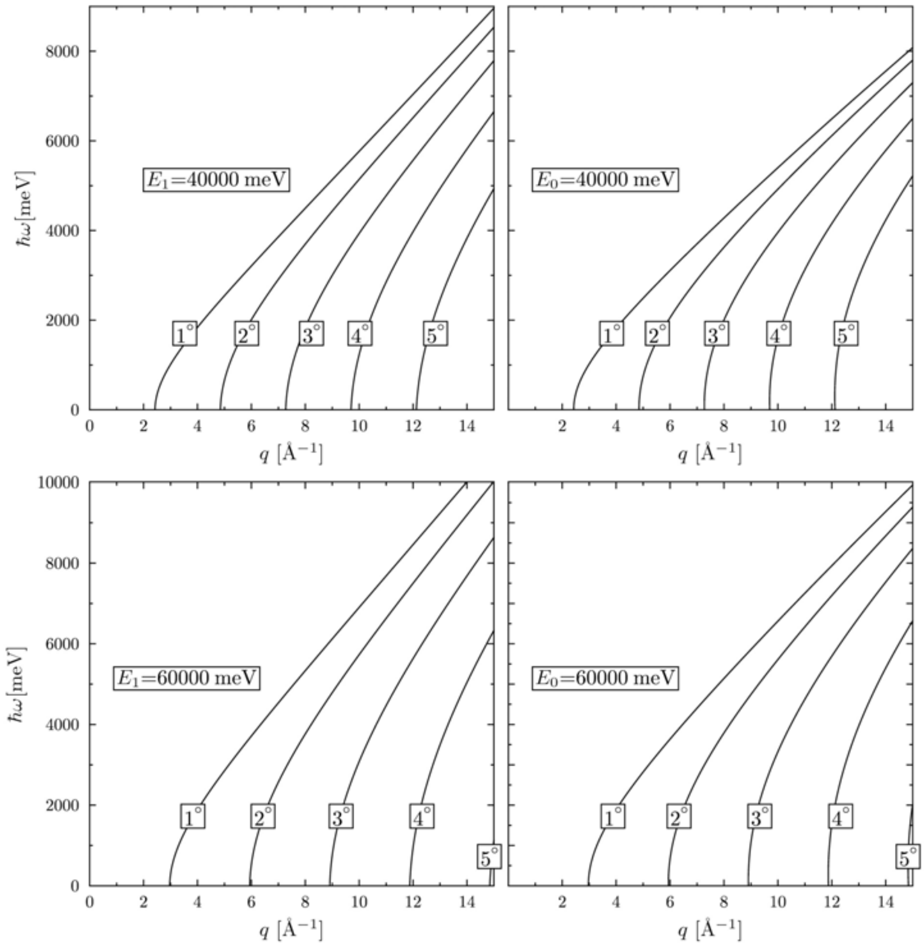

Fig. 3. Kinematical range for HINS studies using : a) inverse geometry with E_1=40000 meV and E_1=60000 meV; b) direct geometry with E_0=40000 meV and E_0=60000 meV. Low scattering angle contours are indicated .

Electronvolt neutron scattering can be achieved employing both direct (chopper) and inverse (resonance filter) geometry. In the latter case, at long pulse sources, a combination of resonance filters in both primary and secondary flight paths has to be employed to reduce the time resolution component of the long pulse source.

The current performances of spectrometers for electronvolt scattering are being tested at ISIS, where VESUVIO is currently operating as standard electronvolt spectrometer, and MARI is being investigated as eV chopper spectrometer. The maximum energies obtained are E_1(max)= 66 eV (VESUVIO), and E_0(max)= 100 eV (MARI), corresponding to maximum energy transfers $\hbar\omega_{max}$ =240 eV (VESUVIO) and $\hbar\omega_{max}$ =100 eV (MARI) [4,5].

The energy and wave vector transfer resolutions are determined by the energy selection devices (resonance filters, chopper) and by the geometrical uncertainties for flight paths, angles and time of flight. On VESUVIO the energy resolution is $\Delta\hbar\omega < 1$ eV and $\Delta\hbar\omega/\hbar\omega < 4$ % [1,6]. On MARI, the energy resolution is $\Delta\hbar\omega > 5$ eV [5] .

Table I reports the energy resolution calculations (full width at half maximum) for the inverse-geometry configuration [7], at selected values of energy transfers, for commonly employed energy analysers.

Table I. Energy analysis on inverse geometry eV instrumentation: resonance energy, E_1, and full widths at half maximum (FWHM), ΔE_1, for the selected energy analyser foils at room temperature, representing the energy (non-geometrical) contribution to the instrument resolution. The columns 4-8 report the calculated energy transfer resolution $\Delta\hbar\omega$, which include both energy and geometrical resolution components, for selected values of the energy transfer $\hbar\omega$ [7].

	E_1 [eV]	ΔE_1 [meV]	$\Delta\hbar\omega$ [meV]				
Filter			$\hbar\omega = 10$ meV	$\hbar\omega = 500$ meV	$\hbar\omega = 3$ eV	$\hbar\omega = 7$ eV	$\hbar\omega = 20$ eV
^{197}Au	4.91	182	216	221	252	313	581
^{238}U	6.67	103	125	128	144	174	307
^{238}U	20.9	177	243	246	262	290	404
^{238}U	36.6	242	387	391	411	446	578
^{238}U	66.0	320	701	707	736	784	952

It is instructive to compare the resolution performances of direct and inverse geometry instruments for multi-eV scattering. Figure 4 illustrates the energy width at the elastic peak for low angle scattering using incident (final) energies above 5 eV. From the above figure and Table I the energy resolution on VESUVIO is $\Delta\hbar\omega < 1$ eV and $\Delta\hbar\omega/\hbar\omega < 4$ % [6,7]. On the MARI direct geometry chopper spectrometer, the energy resolution is $\Delta\hbar\omega > 5$ eV [5].

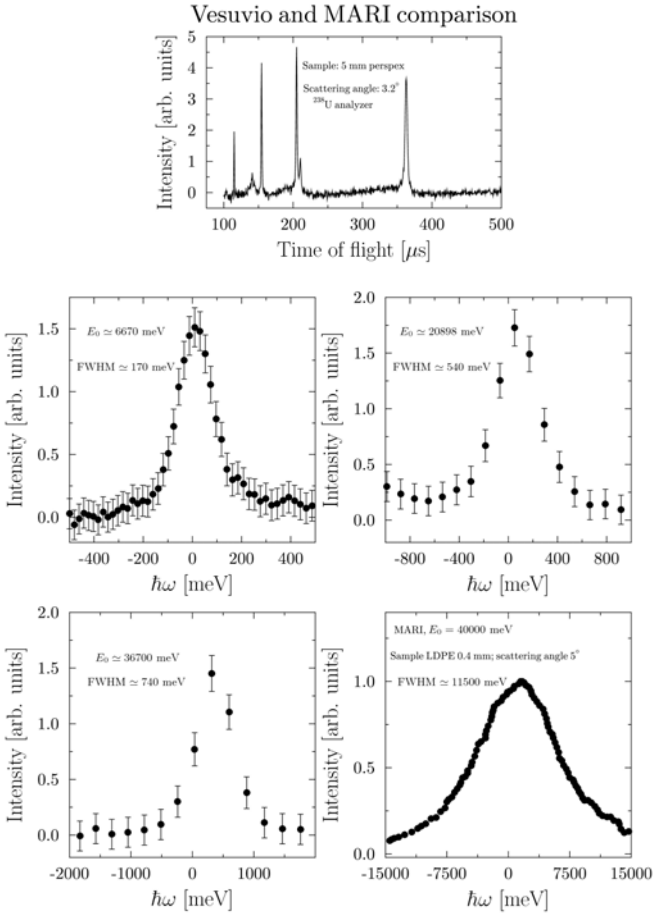

Fig. 4: Comparison of VESUVIO [6] (inverse geometry) and MARI [5] (direct geometry) resolution at the hydrogen elastic peaks for low angle multi eV scattering .

Both inverse and direct geometry spectrometers can be employed for eV spectroscopy at long and short pulse sources. At long pulse sources, the time resolution broadening can be reduced by employing either resonance filters in both primary and secondary flight paths, or use a primary chopper to modulate and shape the pulse structure, then applying energy selection on the final flight path. At the current state of the art on short-pulse sources such as ISIS, inverse geometry offer superior performance in terms of resolution, at both low angle (HINS) and high angle (DINS) scattering.

3. Chip Irradiation studies

The large flux of high energy neutrons (above 1 MeV) [8], present at eV instruments at both SPSS and LPSS, may be exploited for electronic chips irradiation for the study of the so-called Single Event Effects (SEE). Figure 5 reports the recently measured neutron spectrum at sample position on VESUVIO, in the energy range 1 meV < E < 600 MeV [8]. The measurement of SEEs is of primary importance for the electronic industries to assess the robustness of their products, especially those featuring nanometric sizes, and a dedicated beamline is under construction at the ISIS second target station [9].

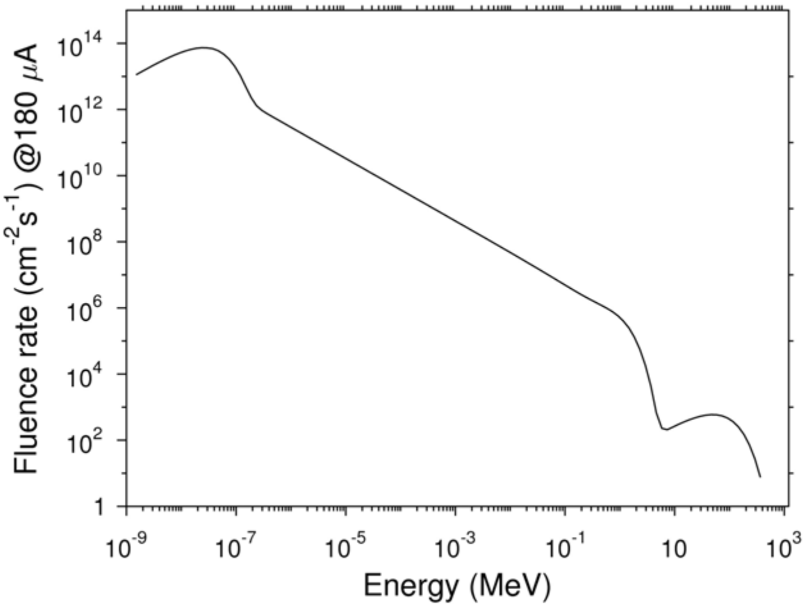

Fig. 5: Energy distribution measurement of the neutron fluence rate on VESUVIO normalized to 180 μA proton current [8].

4. Acknowledgements

This work was supported within the CNR-STFC Agreement No. 01/9001 concerning collaboration in scientific research at the spallation neutron source ISIS. The financial support of the Consiglio Nazionale delle Ricerche in this research is hereby acknowledged.

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