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Report:

Determination of molecular structures in the liquid phase

Introduction: A high real space resolution is often necessary for an unambiguous determination of the molecular structure in a liquid. This is equivalent to saying that the structure function $i(Q)$ has to be known in a large momentum transfer range Q = $4\pi/\lambda \sin(\theta)$, where λ is the wave length and θ is the half of the full scattering angle 26. The structure function $i(Q)$ is related to the normalized intensity by:

$$i(Q) = \frac{I(Q) - \sum^{uc} f_i^2 - \sum^{uc} C_i(Q)}{(\sum^{uc} f_i)^2}, \qquad (1)$$

where I(Q) is the normalized intensity, f_i are the form factors, C_i the Compton intensities and the sums are extending over the unit composition of the sample. At large momentum transfers especially when light elements are present, Compton scattering is by far dominating. The relative energy shift of Compton scattered photons at a given momentum transfer is largest for back scattering:

$$\Delta E/E = 1 - \frac{1}{1 + \frac{E}{511keV}[1 - \cos(2\theta)]} = 1 - \frac{1}{1 + 3.81110 \cdot 10^{-3} keV \text{Å}^2 \frac{Q^2}{E}} \qquad (2)$$

The experiment was aiming to determine i(Q) at momentum transfer values $30\text{Å}^{-1} < Q < 50\text{Å}^{-1}$.

Experiment: The experiment has been carried out at the High Energy beam line ID15, BL.5. The geometry of the experiment is illustrated in Fig. 1. The detector position is fixed at a large scattering angle. The energy is tuned continuously in the range from 30-50 keV with the monochromator, corresponding to the desired momentum transfer range. The analyzer selects the elastically scattered photons. Both monochromator and analyzer crystal were flat $Si/TaSi_2$ crystals reflecting at the (311) plane in Laue geometry. The sample was liquid formamide $OHC\text{-}NH_2$. The MCA spectra of Ge- solid state detector at an incident energy of 50 keV are shown in Fig. 2.

Discussion: Fig. 2 demonstrates, that the energy resolution obtained is clearly sufficient to separate the elastic part of the scattered intensity in the proposed geometry. The total count rate without analyzer is at the count rate limit of the Ge-detector. In the set-up with analyzer the detector is not saturated with the (unwanted) Compton scattered photons. The count rates in the present set-up (20-50 s^{-1}) are, however, still to low to obtain a structure function a with sufficient statistical accuracy. The main problem to be surmounted are the incompatible requirements on momentum transfer and energy resolution. The first can be quite low the second has to be quite good. In order to improve the reported experiment, an analyzer (based e. g. on a bent Bragg crystal) is needed which allows to diminish the distance sample/ detector - and, hence, diminish the Q-resolution in order to gain intensity - without degrading the energy resolution.

Fig. 1 Schema of the experimental geometry
M: Monochromator, S: Sample, A: Analyzer, D: Detector. See text for further description

Fig. 2: MCA spectrum of the scattered intensity at an incident energy of 50 keV
A: Set-up without analyzer, B: Set-up with analyzer

Fig.1

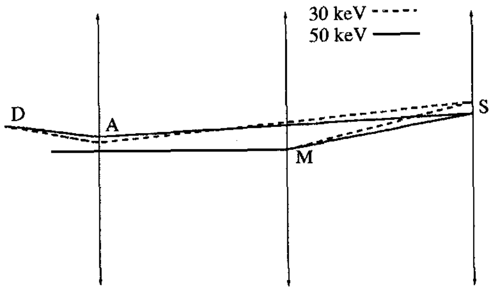

Fig. 2