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Resolution and Luminosity of Crystal Spectrometers for Neutron Diffraction

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Previously published theoretical results on resolution and luminosity of crystal spectrometers for neutron diffraction are extended in this study, also in view of useful applications to the programming of automatic collection of the data by means of spectrometers for single crystal analysis. Furthermore, experimental tests showing a satisfactory agreement with the theoretical results are presented and briefly discussed.

In previous papers[1)2)] a theory was published on resolution and luminosity of Bragg reflections obtained both from powder and single crystal samples with neutron diffraction spectrometers. General expressions were developed giving the full widths at half maximum of the Bragg reflections at any scattering angle and their luminosity in terms of the angular divergences of the Soller type collimators and of the mosaic spread of the crystal(s).

In this communication, we present some experimental proofs of our predictions; furthermore, we add some considerations to the previous treatment of the case[2)] of single crystal samples, leading to an operational definition of the mosaic spread of a single crystal, and to information which may eventually be useful for the programming of automatic collection of the data by means of modern crystal spectrometers.

The Bragg reflections under study were obtained with the neutron diffraction spectrometer previously described[3)], installed at a horizontal beam hole of the 5 MW Ispra-1 reactor.

The horizontal angular divergences of the Soller collimators were chosen as follows: $\alpha_1 = \pm 19$ min arc, $\alpha_2 = \pm 26$ min arc, $\alpha_3 = \pm 34$ min arc, the first, second and third collimator being located in the primary, monochromatic and diffracted beam respectively.

Powder samples as well as single crystal samples having very simple structure were alternately mounted on the spectrometer table.

The Bragg reflections of the diffraction patterns from nickel powder obtained using alternately quartz 10.1, aluminum 111 and lead 220 single crystal monochromators are found to have full widths at half maximum reasonably close to the one's computed by a formula given in ref. (1), the maximum discrepancy between experimental and calculated widths being approximately 12%.

Furthermore, the widths of the Bragg reflections obtained from single crystal samples with counter arm and crystal table coupled in the ratio two to one and using the same monochromators as above, turn out to be in satisfactory agreement with a formula given in ref. (2).

For the comparison between experimental and theoretical widths of the Bragg reflections obtained both from powder and single crystal samples, we utilized also an operational definition of the mosaic spread of a single crystal derived following the same lines indicated in references (1) and (2). Such a definition allows one to extract the mosaic spread of a single crystal sample from the width of a rocking curve at any Bragg angle, by eliminating any broadening due to experimental reasons.

Vice versa, the possibility of computing the widths of the rocking curves and their luminosities at any scattering angle as a function of the angular divergences of the collimators, the mosaic spread of monochromating crystal and crystal sample, and the Bragg angle of the monochromator, may offer a useful guide in the automatic collection of the data by means of modern neutron spectrometers for single crystal analysis.

References

1 G. Caglioti, A. Paoletti and F. P. Ricci: Nucl. Instr. **3** (1958) 223.
2 G. Caglioti, A. Paoletti and F. P. Ricci: Nucl. Instr. and Meth. **9** (1960) 195.
3 Caglioti, De Agostino, Marsili, Paoletti, Pellegrini and Ricci: To be published.

DISCUSSION

G. E. BACON: Have you any explanation why the observed line widths for nickel lay consistently above —10% or so— the calculated values for the 'parallel' position?

G. CAGLIOTI: The explanation for the small systematic difference between experimental and calculated widths of Bragg reflections for powder samples, appearing in some of the cases we considered, is not easy to be found. That difference seems not to be due to having neglected the vertical angular divergence of the collimators. Besides, in the present experimental conditions, the full width at half maximum vs. the dispersion parameter a does not depend on the mosaic spread of the monochromator.

It should be mentioned at this point that similar measurements, recently reported by Prof. Shull, seem to indicate a small systematic deviation of his results with respect to the theoretical predictions, but in a sense opposite to the one here presented. In fact Shull finds, at large Bragg angles, a better resolution than the one predicted by the theory, at least for large values of the scattering angle $2\theta_B$.

Finally, I would like to remark that any comparison of the predicted resolution with the experimental one should be made with the experimental conditions proposed by the theory, that is using Soller type collimators and standard powder samples.

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Neutron Diffraction Work at the Ispra Center

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In this communication we present results recently obtained with the neutron diffraction spectrometer installed at the Ispra-1 reactor on the structure of liquid bromine and cupric oxide.

The neutron diffraction analysis of liquid bromine near the melting point has been carried out up to a very large value of $4\pi \sin\theta/\lambda$. The radial distribution function shows clearly that in the liquid state, at room temperature, the molecules are not freely rotating. Moreover it seems that the main features of the structure of the parent solid, are preserved during the melting process.

The crystal and magnetic structures of copper oxide have been confirmed.

Liquid bromine

The structure of polyatomic liquids has not been so far widely investigated, as much as the structure of monoatomic liquids. While the latter is very important for an understanding of the general properties of a liquid, the structure of polyatomic liquids is worthwhile to be investigated because of the information one can get about particular aspects of the liquid state, such as, for instance, the