

THE COLLECTIVE PROPERTIES IN LIQUID BISMUTH

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Abstract

The frequency spectra have been studied in liquid bismuth by cold neutron inelastic scattering technics, in wide energy interval, and in energy gain processes for the two angles and temperatures, respectively. The measured spectra, which are proportional to the double-differential cross section of the coherent scattering on the liquid bismuth, clearly indicated the existance of collective excitations.

I Introduction

As it is known, the solid bismuth has the layer structure, where each atom is surrounded by the three nearest neighbours. Such trigonal structure undergoes the significant change above the melting point. In the liquid phase one can get the static structure factor $S(q)$ using neutron¹⁾ or X-ray²⁾ scattering technics. The experimental static data show the subsidiary maximum on the high q side of the first $S(q_0)$ peak (a location of the first maximum lies at $q_0 = 2.12 \text{ \AA}^{-1}$) which slightly disappear with increasing temperature.³⁾ In the neutron inelastic scattering experiment one determines the double-differential cross section $\frac{d^2\sigma}{d\Omega dE}$ of a coherent scattering, i.e. the dynamic structure factor $S(q, E)$. In our experiment with incoming energy $E_0 = 5.2 \text{ meV}$, the $\frac{d^2\sigma}{d\Omega dE}$ shows the pronounced structure, as given in figure 1, for the two different temperatures.

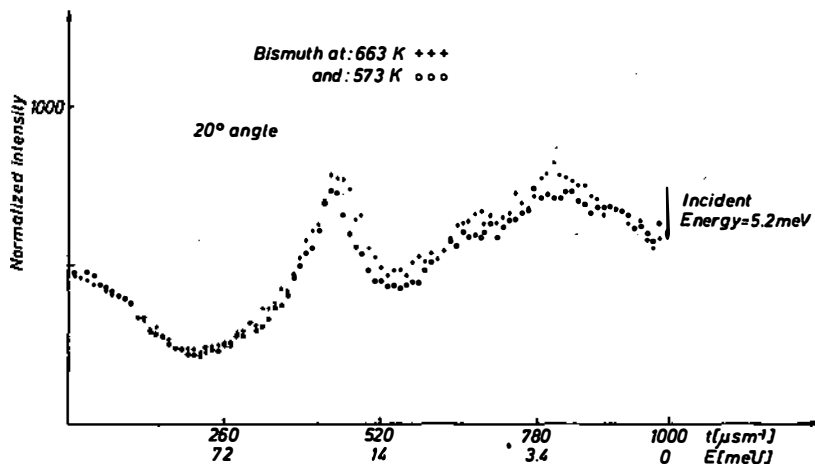


Figure 1.

II Experimental results

Using the time-of-flight spectrometer (TOFS) with Be-cut off neutrons a dynamic properties of liquid bismuth have been studied. The final scattering energy E' lies between 5 and 40 meV. The cold neutrons in the inelastic scattering process gain an energy E between 0 and 35 meV. The scattered neutron spectra were analyzed using TOFS. A sample of a rectangular slab type, with thickness of 5 mm, were measured at 20° and 60° angles of scattering. The measurements with and without sample were performed and the intensity normalized to the same time, as shown in figure 1. The (q, E) loci determined by these angles and by E_0 are illustrated in figure 2. Therefore these angles were chosen because they ensured approximately the same area that can be seen by neutrons. The mean free path of the cold neutrons in bismuth is of the order of 4.7 cm. The measured data were corrected for the background, the detector efficiency and chopper function. The corrected intensity, for the two tempera-

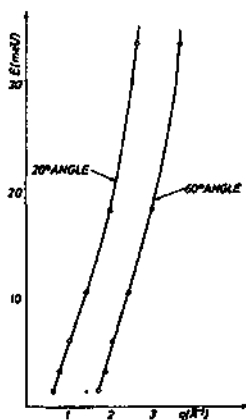


Figure 2.

tures and the two scattering angles, are shown in figure 3.

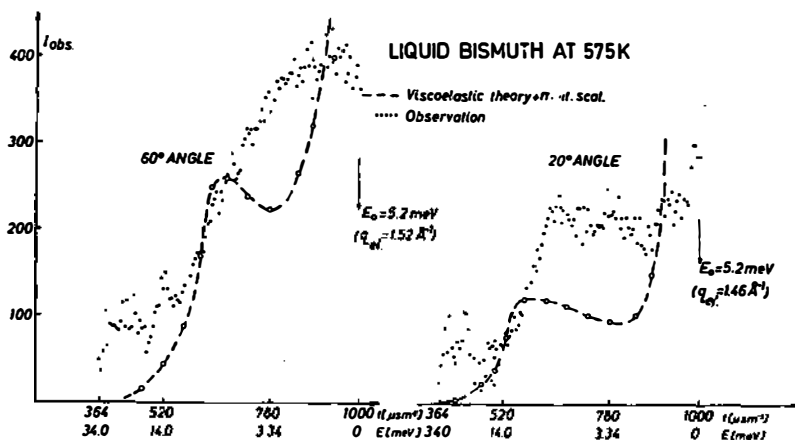


Figure 3.

The next step in treatment of the observed neutron intensity is the correction for multiple scattering ⁴⁾. Recently published results on liquid aluminium ⁵⁾ stimulated us to make similar analysis of our liquid bismuth data. This correction is important for interpretation of the measured data, especially for cold neutrons, where a single-scattering intensity depends on neutron incident energy. To avoid the effect of high order scattered neutrons on $S(q, E)$, the input kernel was chosen so that it provides a near true value ⁵⁾. To calculate the second order scattered S_2 component, the programme developed by Cocking was used ⁴⁾ and compared with single scattered S_1 component. The ratio $\frac{S_1 + S_2}{S_1}$ is about 1-1,5 at 60° and 2-9 at 20° scattered angles, within energy transfer 0-35 meV. In figure 3 the observed neutron intensity and the calculated scattering intensity are compared with the second order contribution are compared.

III Dynamic properties

Several years ago, when the dynamic properties of the liquid metals were poorly understood, the liquid bismuth was already studied ^{6,7)}. There are a few theoretical approaches ⁸⁾ which can describe the atomic motion in the monatomic liquids. One of the first is the convolution approxima-

tion ⁹⁾ where dynamic properties are provided studying a simple particle motion. This type of motion can be described by the generalized Langevin equation which is based on the theory of fluctuations. The kernel in this equation is the memory function which is terminated by three-pole approximation ¹⁰⁾. By this approximation and convolution method, $S(q, \omega)$ can be derived by following expression ^{8, 11)}

$$S(q, \omega) = \frac{S(q) \omega_{\text{coh}}^2(q) [\omega_1^2(q) - \omega_{\text{coh}}^2(q)] \mathcal{T}(q)}{\mathcal{H} [\omega \cdot \mathcal{T}(q) (\omega^2 - \omega_1^2)]^2 + [\omega^2 - \omega_{\text{coh}}^2(q)]^2} \quad (1)$$

where the second $[\omega_{\text{coh}}^2(q)]$ and the fourth $[\omega_{\text{coh}}^4(q)]$ moment $\left[\omega_1^2 = \frac{\omega_{\text{coh}}^4(q)}{\omega_{\text{coh}}^2(q)} \right]$ are quantities which depend, for the coherent scatterer (bismuth is 99.8% coherent scatterer), on the static structure and the interaction potential. The crucial problem in calculation of the multiple scattering according to the kernel (eq. 1) is the choice of the parameter $\mathcal{T}(q)$.

Since q interval ($q_{\text{inel}} = 1.46$ and 1.52 \AA^{-1}) covered by cold neutrons, lies between hydrodynamic and viscoelastic theory, the parameter $\mathcal{T}(q)$ can be defined by simple approximation ⁸⁾

$$\mathcal{T}(q) = \frac{0,886}{\sqrt{\omega_1^2(q) - \omega_{\text{coh}}^2(q)}} \quad (2)$$

This can be applied only for high energy transfer, where liquid show elastic behaviour and existence of collective excitations which is predicted by condition $3\omega_{\text{coh}}^2 > \omega_1^2$ ⁸⁾ (for Bi at $q_{\text{inel}} = 1.8 \text{ \AA}^{-1}$; $3\omega_{\text{coh}}^2 = 1.8 \omega_1^2$).

The second approach starts from the first principle of the kinetic theory ¹²⁾ and makes an ansatz for a memory function. The description of $S(q, \omega)$ by this approach bases on the coupling of the thermal fluctuation and the self-part of the correlation function. Our knowledge from the previous work ¹³⁾ tells us that there exists a very small difference between the above mentioned approach and the viscoelastic theory, except for the small q . Generally speaking the kernel $S(q, \omega)$ in the multiple scattering correction depends on the in-

coming energy.

In the figure 3, the calculated spectra $S(q, E)$, (eq. 1) together with the multiple scattering contribution are compared with the experimental intensity.

As a conclusion it comes out that correction for the multiple scattering changes significantly the shape of the observed intensity, although the mean free path of neutron is large. Disagreement shown in figure 3 comes out mainly because of the inappropriate correction of the background⁵⁾ which appears as very important for the type spectrometry we applied.

The peak which remains on the energy gained part of the spectra, figure 3, indicates the collective excitation corresponding to the longitudinal acoustic phonon in solid bismuth. This phonon peak is rather overdumped in the liquid compared with the solid phase.

IV References

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