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AN ANOMALY OF THE X-RAY SPECTRUM OF GRAPHITE IN THE REGION OF THE RAMAN BAND

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In the spectrum of polycrystalline graphite, an anomaly has been found in the inelastic X-ray scattering. The anomaly occurs at a distance of about 311 eV from the primary line. The anomaly is ascribed to the transition of core electrons to the anti-bonding band of graphite.

1. INTRODUCTION

THE GRAPHITE is a semi-metal of hexagonal structure with high anisotropy [1]. The band in which the Fermi level belongs is constructed almost exclusively from a linear combination of the $2p_z$ orbitals. The results from calculations are based on the tight-binding approximation [2, 3]. Transitions of electrons above the Fermi level give the Raman band.

The linear combination of sp^2 orbitals gives on one hand the bonding band (occupied) below the Fermi level, and on the other hand the anti-bonding band (not occupied) above the Fermi level. The calculations yield a density of states which has a minimum, almost zero, on the Fermi level [1].

2. EXPERIMENT

In the present experiment, the Raman band was measured with X-rays (Cr$K\beta$, 34 kV, 24 mA) using a new type of spectrometer; its analysing crystal was a 0.5° mosaic graphite slab provided by Union Carbide. The reflecting plane was (0001) and was used in the sixth order. The spectrometer constructed without a collimator because of the weakness of the intensities. The specimens were polycrystalline and colloidal

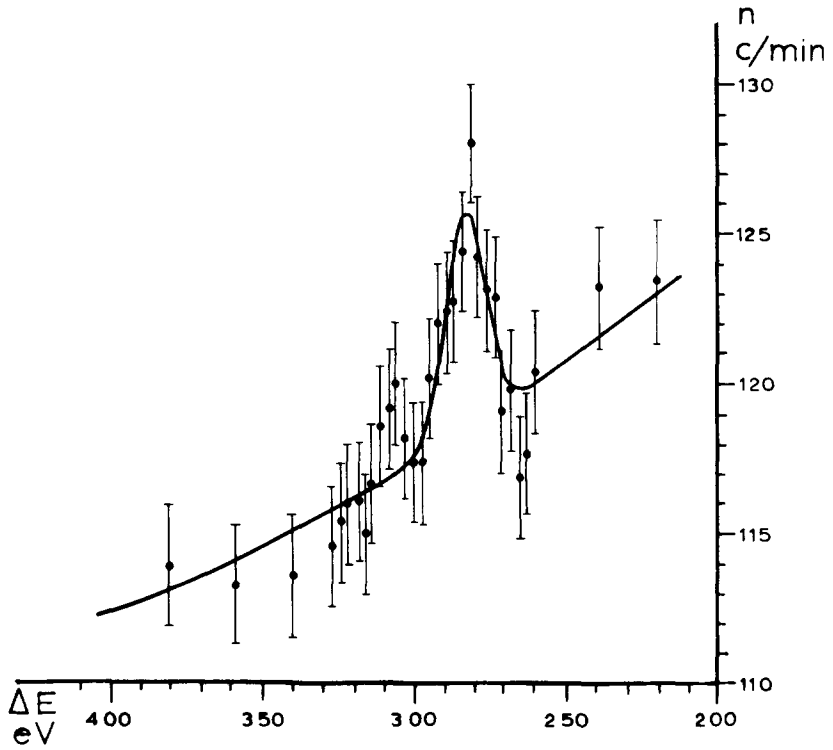

Fig. 1. The spectrum of polycrystalline graphite in the region of the Raman band, vs the energy loss from the primary line.

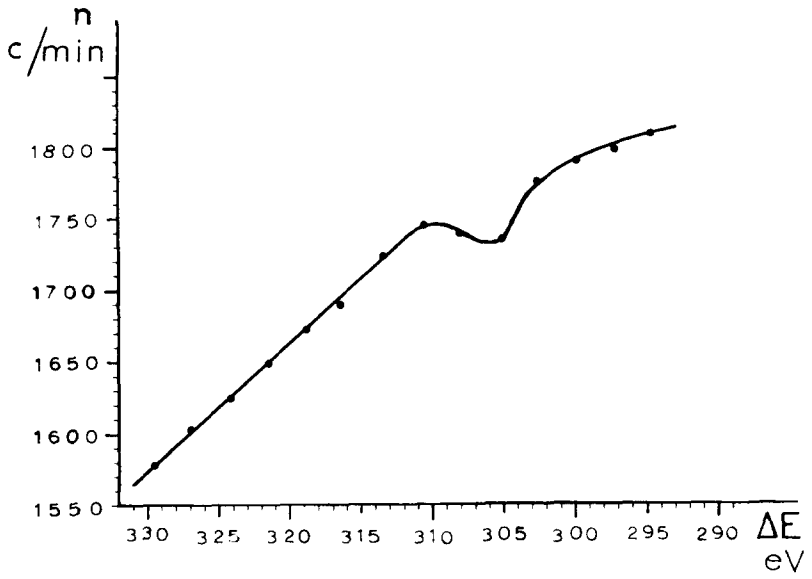

Fig. 2. The spectrum of polycrystalline graphite in the range 295–330 eV from the primary line. The statistical error is too small to be shown.

graphite slab, the last provided by Acheson Colloids Ltd. The scattering angle was 45° and the diffracted beam was detected by a Geiger–Müller counter. The spectrum was scanned point by point by rotating the analysing crystal in steps of 0.15° corresponding to 2.68 eV. The experimental data were fitted by a Control Data computer using a MINUIT program [4].

Figure 1 shows the spectrum of the polycrystalline graphite vs the energy loss with respect to the primary line, in the region of the Raman band with a statistical error 1.3%. One concludes that beyond the Raman band, i.e. towards lower energies, an additional line seems to exist. Such a line was not observed in colloidal graphite.

After improvement of the device, detailed measurements (error 0.1%) for polycrystalline graphite were carried out in this region. They are given in the Fig. 2. The band is centered at 311 eV from the primary line. Below, the possibility of attributing this second band to the anti-bonding band of graphite will be discussed.

3. DISCUSSION

Zunger [5] gives separately the density of states (see Fig. 5). The edge of the anti-bonding band lies about 10 eV above the Fermi level. If we assume that the width of the anti-bonding band is of the same order of magnitude as the width of the bonding band, which seems reasonable, then the observed anomaly fits within the limits of the position of the anti-bonding band.

Because of the low resolution of the spectrometer, details of the density of states could not be detected.

In conclusion, we attribute the observed additional peak to the shape of the density of states of graphite.

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REFERENCES

1. J.M. Ziman, *Electrons and Phonons*, p. 121. Cambridge University Press (1960).
2. P.R. Wallace, *Phys. Rev.* **71**, 622 (1947).
3. J.W. McClure, *Phys. Rev.* **108**, 612 (1957).
4. F. James & M. Roos, MINUIT, A System for Function Minimzation and Analysis of Parameter errors and Correlations. C.E.R.N. (1975).
5. A. Zunger, *Phys. Rev.* **B17**, 626 (1978).