DEUTSCHES ELEKTRONEN-SYNCHROTRON DESY

Photo-Absorption Measurement of Li, Be, Na, Mg, Al in the XUV Range

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The absorption structure of five light metals has been measured from the onset of K respectively $L_{II,III}$ absorption up to photon energies of 140 eV (170 eV for Be). The edges at the threshold are followed by several broad peaks which are distributed over the total energy region covered by these measurements. There is a striking similarity between the $L_{II,III}$ absorption spectra of Na, Mg and Al; a similarity can also be seen between the K-absorption spectra of Li and Be.

Das optische Absorptionsverhalten von fünf Leichtmetallen wurde vom Einsatz der K- bzw. $L_{II,III}$-Absorption bis zu Photonenenergien von 140 eV (bei Be bis 170 eV) gemessen. Neben den Kanten beim Einsatz wurden im ganzen Spektralbereich mehrere breite Absorptionsmaxima beobachtet. Der allgemeine Verlauf der $L_{II,III}$-Absorptionsspektren von Na, Mg und Al stimmt gut überein, Ähnlichkeiten zeigen sich auch bei den K-Absorptionsspektren von Li und Be.

I. INTRODUCTION

Optical absorption in light metals associated with core state excitations has been investigated for many years. The aim is to get information about both the matrix elements and the density of empty states above the Fermi surface. However, many-body effects, Auger transitions and electron hole interactions complicate the interpretation of the results.

Furthermore, the experimental results do not agree with each other at all because of the inherent difficulties in the XUV region. As the experimental situation has improved since electron synchrotrons can now be used as intense continuous light sources in this region, it appeared desirable to repeat the absorption measurements. Recently, moreover, interest in the shape of absorption edges has been revived by theoretical calculations which predict a singularity of the absorption coefficient at the threshold. We have already reported in a short note[1] experimental proof of the existence of this structure in the Na $L_{II,III}$ absorption. The measurements of the $L_{II,III}$ edge in Na, Mg, and Al and the K edge in Li and Be will be published elsewhere.[2]

In the next section we are going to explain our experimental procedure, in particular the sample preparation. Section III gives the complete spectra from the onset of the respective core excitations to $\sim$ 140 eV (170 eV for Be).

II. EXPERIMENTAL PROCEDURE

A. Absorption measurements

Synchrotron radiation of the 7.5 GeV electron accelerator at DESY[3,4] served as light source. As the spectrum is continuous any structure found can, with a high degree of reliability, be attributed to the absorbing films. The samples were mounted in front of a Rowland spectrograph. Radiation damage to the films, caused by the intense irradiation, was not observed. Spectra were recorded without films and with films of different thicknesses. Higher orders for the different spectral regions were elliminated by the use of prefilters and different adjustments of the spectrograph: At the $L_{II,III}$ edge of Na a correction was made for a spectrally flat second-order background. This correction was possible since thorough investigations of the intensity distribution into the different diffraction orders had been performed. The instrument was used with a 3600 lines/mm grating (blaze angle $3^{o}8'$, grazing angle of incidence $3^{o}50'$) and a 2400 lines/mm grating (blaze angle $4^{o}16'$, grazing angle of incidence $12^{o}36'$). An open Bendix photomultiplier behind the exit slit served as detector. The position of the L_{III} edge in Al[5] and the positions of rare gas absorption lines as given by Madden and Codling[6] were used to calibrate our spectrograph. The resolution was of the order of 0.1 Å as determined from the slit width and from the width of the central image. The data were evaluated by a computer program. More details of the experimental procedure are given in References 3 and 4.

B. Sample preparation

The preparation technique varied for the different materials. Al and Mg films in the thickness range 500 to 2000 $\mathring{A}$ were evaporated onto microscope slides covered with a thick layer of zapon. This was dissolved in amyl acetate and the films were mounted on a copper mesh with 70 % transmissivity. The film thickness was determined with a calibrated oscillating quartz crystal and also with a Tolansky interferometer. Al and Mg films were also evaporated in situ onto bakelite films in order to be certain that none of the structures in the spectrum were due to oxide.

Berillium was evaporated onto $\sim$ 1000 $\mathring{A}$ thick carbon substrates in a special vacuum system so as not to contaminate the standard equipment with this highly toxic material. The thickness was determined with a calibrated quartz oscillator. Most of the measurements were performed at room temperature; some of the Mg, Al, and Be films were also measured at 77° K.

Li and Na were evaporated in situ onto 500 $\mathring{A}$ thick Al and Mg substrate films. Li was also evaporated onto bakelite films. The substrates were mounted in a 77° K cold trap which served to reduce water vapor pressure[7] and thus decrease the rate of oxidation. The vacuum outside the trap was 10^{-6} Torr. The film temperature was also 77° K. In the case of Na it took about one hour before first indications of oxidation showed up in the spectrum; Li was less sensitive. After the measurements the films

were allowed to oxidize and the absorption spectra were measured again. Thus we could verify that the metal spectra had been free from oxide contributions. The spectra of the oxidation products are not shown since it is unclear which compounds are formed.

III. GENERAL SHAPE OF THE SPECTRA

Figures 1 to 5 give a survey of all five materials measured from the onset of either the 2p or the 1s electron excitation up to approximately 140 eV (170 eV for Be). Only in the cases of Be, where film thickness was known, and of Al, where curves were fitted to earlier results are absolute values for the absorption coefficient given. The data above 140 eV in Fig. 3 are taken from Ref. 8. The error in the absolute value of μ for Be was estimated to be $\pm$ 20 %. In all spectra the relative accuracy over the whole spectral region is better than $\pm$ 20 %. Differences in the absorption coefficient for a given sample of the order of 1 % are already detectable provided the photon energies are not more than some eV apart. The energy positions of the structures are given in Table I.

Na, Mg and Al. There is a striking similarity between the absorption spectra of Na, Mg and Al (Figs. 1, 2, and 3). In all of them the pronounced $L_{II,III}$ edge is followed by some very weak structures. At higher energies we find three broad peaks: E, F, G in Na; G (HIJ), K in Mg; F, (GHI), J in Al. Going from Na to Al the distance from the $L_{II,III}$ edge for corresponding peaks increases systematically. The available band calculations for these metals do not give any information on states lying so high above the Fermi level. Calculations for free atoms[9] (Cooper's[10] results for Al are indicated in Fig. 3) show only a flat hump for these three materials.

To the best of our knowledge these are the first observations of the L_I edges for Mg and Al in absorption. The structure is only about 2 % of the total μ and much weaker than expected from atomic calculations[10], for instance, indicated in Fig. 3. The edge positions are in excellent agreement with the ESCA results[11]. Near the peak some more unexplained weak structures can be observed.

Earlier measurements on Na were performed by O'Bryan[12]. These measurements disagree with ours expect in the vicinity of the edge. For Mg we find best agreement with the results obtained by Skinner and Johnston[13] who give results up to 110 eV. They give part of the structure around 55 eV but none in the vicinity of 85 eV. For Al our results agree only with those of Fomichev[14], who, however, did not observe the finer details around 75 and 120 eV.

Li: At the onset of the K-absorption of Li we find a prominent peak A followed by a broad absorption maximum C. The agreement with older measurements[13,15] is poor and leads to the suggestion that the Li-films used in the older measurements were not free from contamination.

Be: The K-absorption of Be is very similar to the K-absorption of Li. At the onset the K-absorption of Be has a prominent peak B and a broad structured hump (C, D, E) extending from 115 to 130 eV. The gross structure of the absorption spectrum agrees with the structure of the transmission curves given by Sagawa et al.[16] and by Swanson and Codling[17]. The positions of the absorption peaks as tabulated by Swanson and Codling[17] are in good agreement with our results.

Sagawa et al.[16] have compared their results with Loucks' unpublished density of states curve. We have included this curve in our Fig. 5 and obtained good agreement with the positions of the maxima.

Table I: Position of absorption maxima in the absorption spectra of
Li, Be, Na, Mg, and Al. The third column gives the temperature
at which the tabulated energy positions were measured.
(RT = room temperature, LNT = liquid nitrogen temperature)

Metal	Maximum	Energy (eV)		Temperature
Li	K-Edge	54.7	± 0.1	LNT
	A	55.3	± 0.2	"
	B	58	± 0.5	"
	C	64	± 0.5	"
Be	K-Edge	112.1	± 0.2	RT
	A	112.3	± 0.2	"
	B	113.65	± 0.4	"
	C	119	± 0.5	"
	D	122	± 0.5	"
	E	126	± 0.5	"
Na	L_{III}	30.68	± 0.1	LNT
	A	30.74	± 0.1	"
	L_{II}	30.84	± 0.1	"
	B	30.88	± 0.1	"
	C	32.5	± 0.4	"
	D	35	± 1	"
	E	48.5	± 1	"
	F	65.5	± 1	"
Mg	L_{III}	49.60	± 0.1	LNT
	A	49.66	± 0.1	"
	L_{II}	49.87	± 0.1	"
	B	49.9	± 0.1	"
	C	51.7	± 0.2	RT
	D	52.9	± 0.3	"
	E	55.5	± 0.3	"
	F	58	± 0.5	"
	G	72	± 0.5	"
	H	82	± 0.5	"
	I	85	± 0.5	"
	J	89.5	± 1	"
Al	L_{III}	72.72		Calibration from Ref. 5
	A	72.8	± 0.1	LNT
	L_{II}	73.15	± 0.1	"
	B	73.25	± 0.1	"
	C	74.9	± 0.2	RT
	D	77.3	± 0.2	"
	E	84.3	± 0.3	"
	F	97	± 1	"
	G	113.5	± 1	"
	H	118	± 0.5	"
	I	124	1	"

References

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1. R. Haensel, G. Keitel, P. Schreiber, B. Sonntag, and C. Kunz,
   Phys.Rev. Letters 23, 528 (1969)

2. Proceedings of the NBS-Symposium "Electronic Density of States"
   Nov. 3. - 6. 1969, Washington, D.C.

3. R. Haensel and C. Kunz, Z. Angew. Phys. 37, 3449 (1966)

4. R.P. Godwin in Springer Tracts in Modern Physics,
   Vol. 51; ed G. Höhler (Springer-Verlag) 1969, p. 1

5. K. Codling and R.P. Madden, Phys.Rev. 167, 587 (1968)

6. R.P. Madden and K. Codling, Phys.Rev. 10, 516 (1963)
   K. Codling and R.P. Madden, Phys.Rev. Letters 12, 106 (1964)
   R.P. Madden and K. Codling, Astroph. J. 141, 364 (1965)
   K. Codling and R.P. Madden, J.Chem.Phys. 42, 3935 (1965)

7. C. Kunz, Z. Physik 196, 311 (1966)

8. R. Haensel, C. Kunz, T. Sasaki, and B. Sonntag,
   J.Appl.Phys. 40, 3046 (1969)

9. E.J. McGuire, Phys.Rev. 175, 20 (1968)

10. J.W. Cooper (private Comm.)

11. K. Siegbahn et al.: ESCA, Atomic molecular and solid
    state structure studied by means of electron spectroscopy,
    Uppsala: Almqvist and Wiksell 1967

12. H.M. O'Bryan, Phys.Rev. 57, 995 (1940)

13. H.W.B. Skinner and J.E. Johnston, Proc.Roy.Soc. A 161, 420 (1937)

14. V.A. Fomichev, Sov.Phys. - Solid State 8, 2312 (1967)

15. D.J. Baker Jr. and D.H. Tomboulian, Phys.Rev. 128, 677 (1962)

16. T. Sagawa et al., J.Phys.Soc. Japan 21, 2602 (1966)

17. N. Swanson and K. Codling, JOSA 58, 1192 (1968)

Figure Captions

Fig. 1   Photoabsorption of Na from the onset of the $L_{II,III}$ absorption up to 140 eV. The values for the energy levels are taken from Ref. 11.

Fig. 2   Photoabsorption of Mg from the onset of the $L_{II,III}$ absorption up to 140 eV. The values for the energy levels are taken from Ref. 11.

Fig. 3   Absolute value of the photoabsorption coefficient of Al from the onset of the $L_{II,III}$ absorption up to 210 eV. The region around the onset of the L_I absorption is shown in an enlarged scale. The values for the energy levels are taken from Ref. 11. Included are Cooper's[10] results of atomic calculations.

Fig. 4   Photoabsorption of Li from the onset of K-absorption up to 140 eV. The energy value for the K-level is taken from Ref. 11.

Fig. 5   Absolute absorption coefficient of Be from the onset of K-absorption up to 170 eV. Included are the results of Loucks' unpublished density of states calculations taken from Ref. 16. The value for the energy of the K-level is taken from Ref. 11.
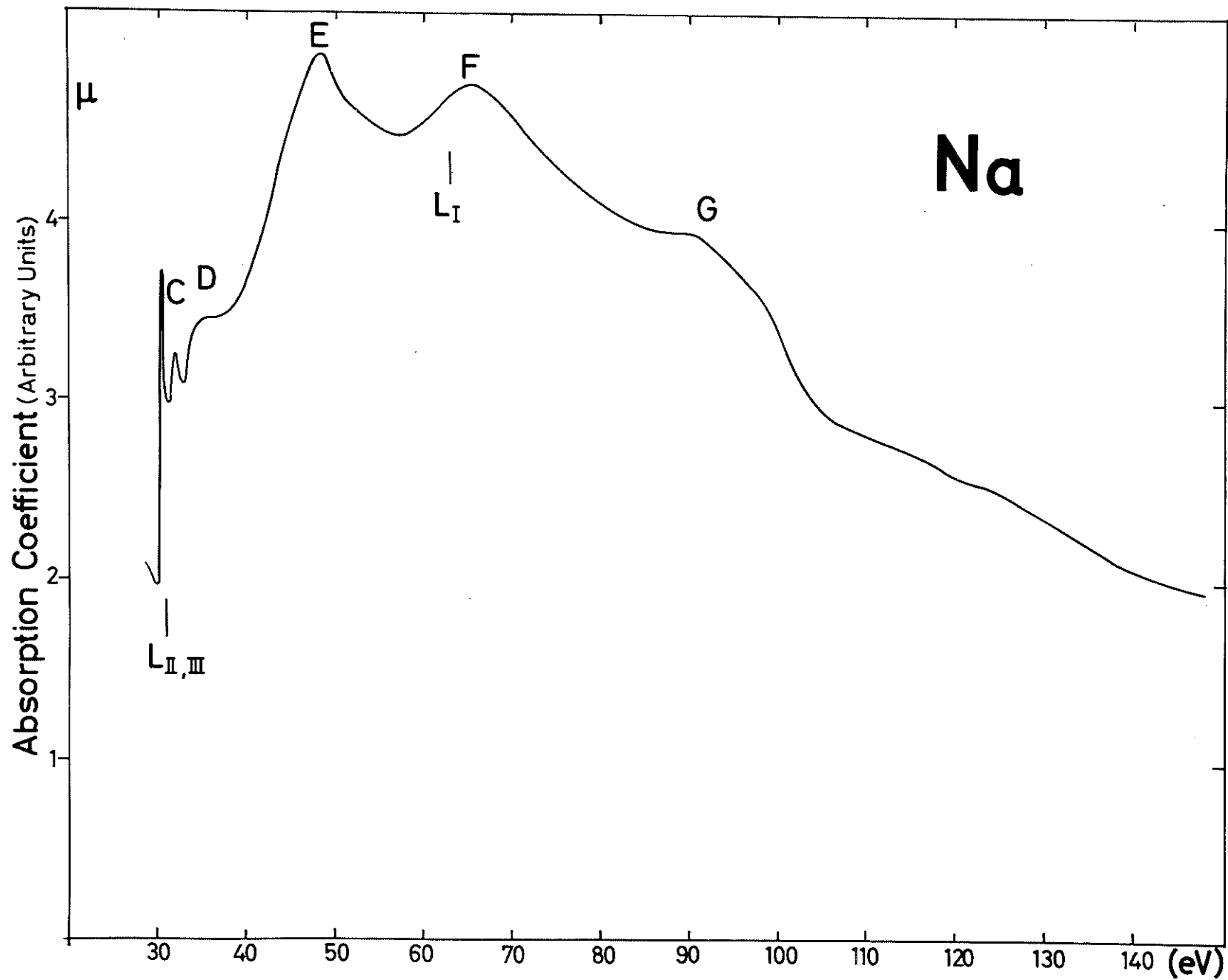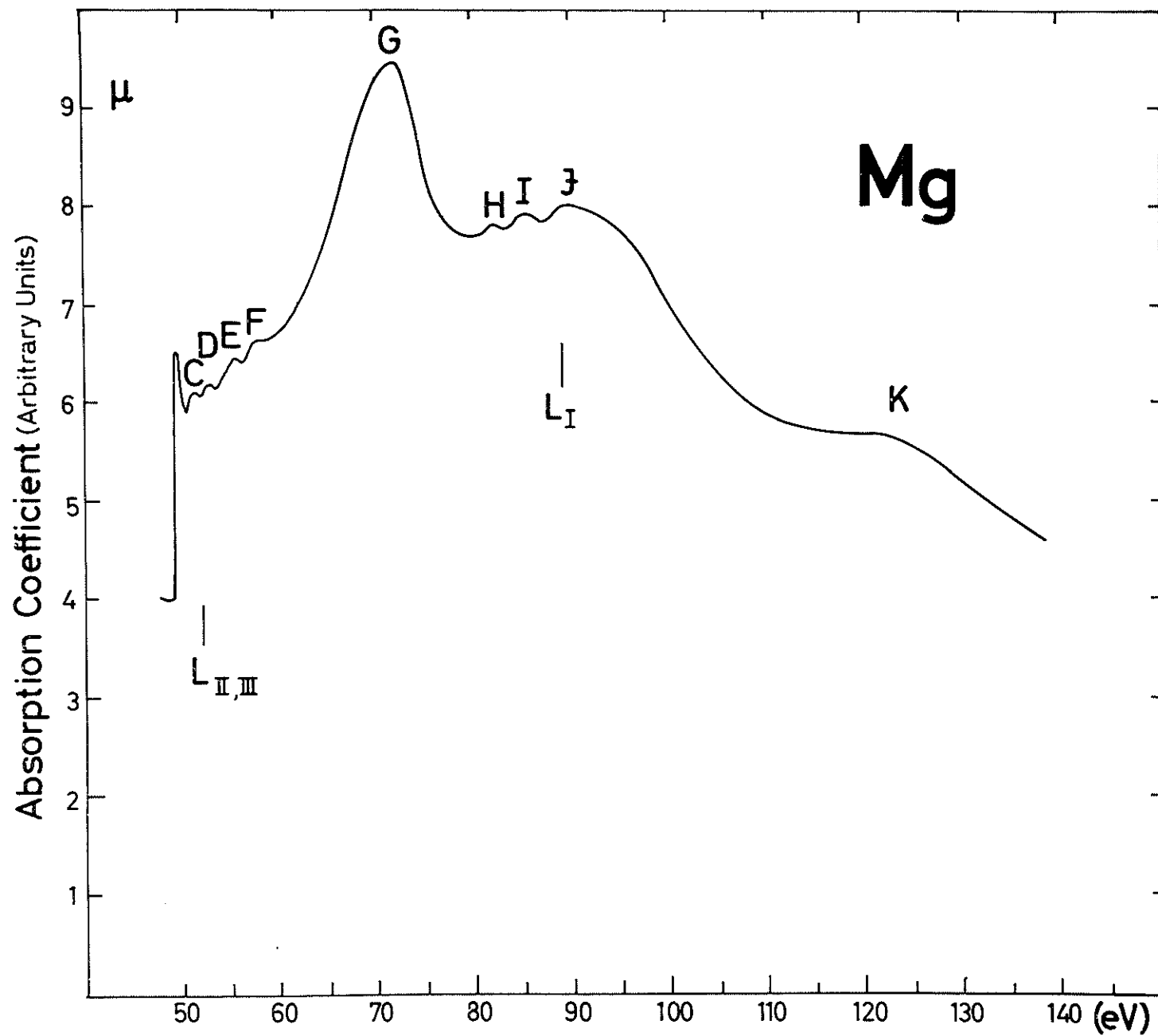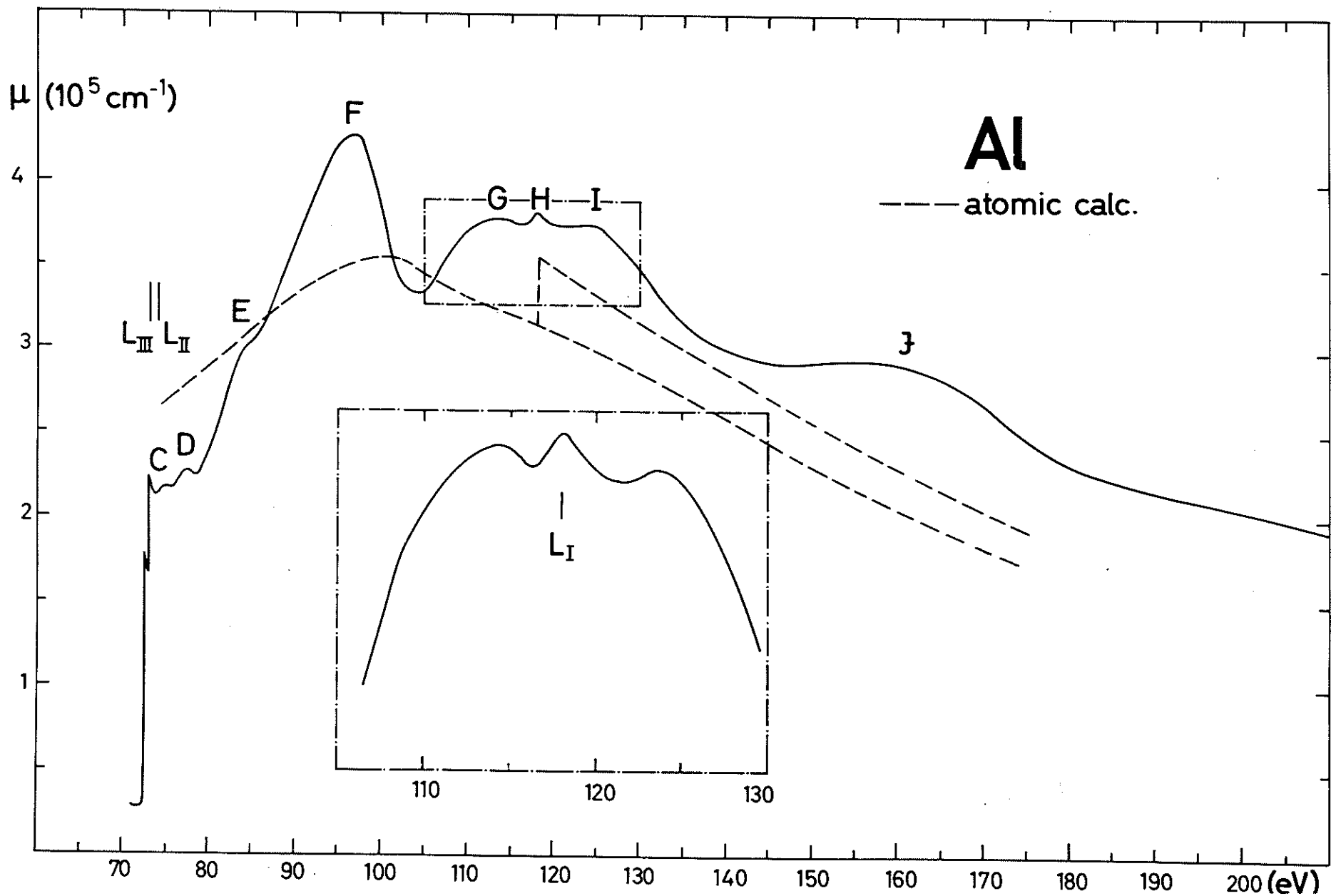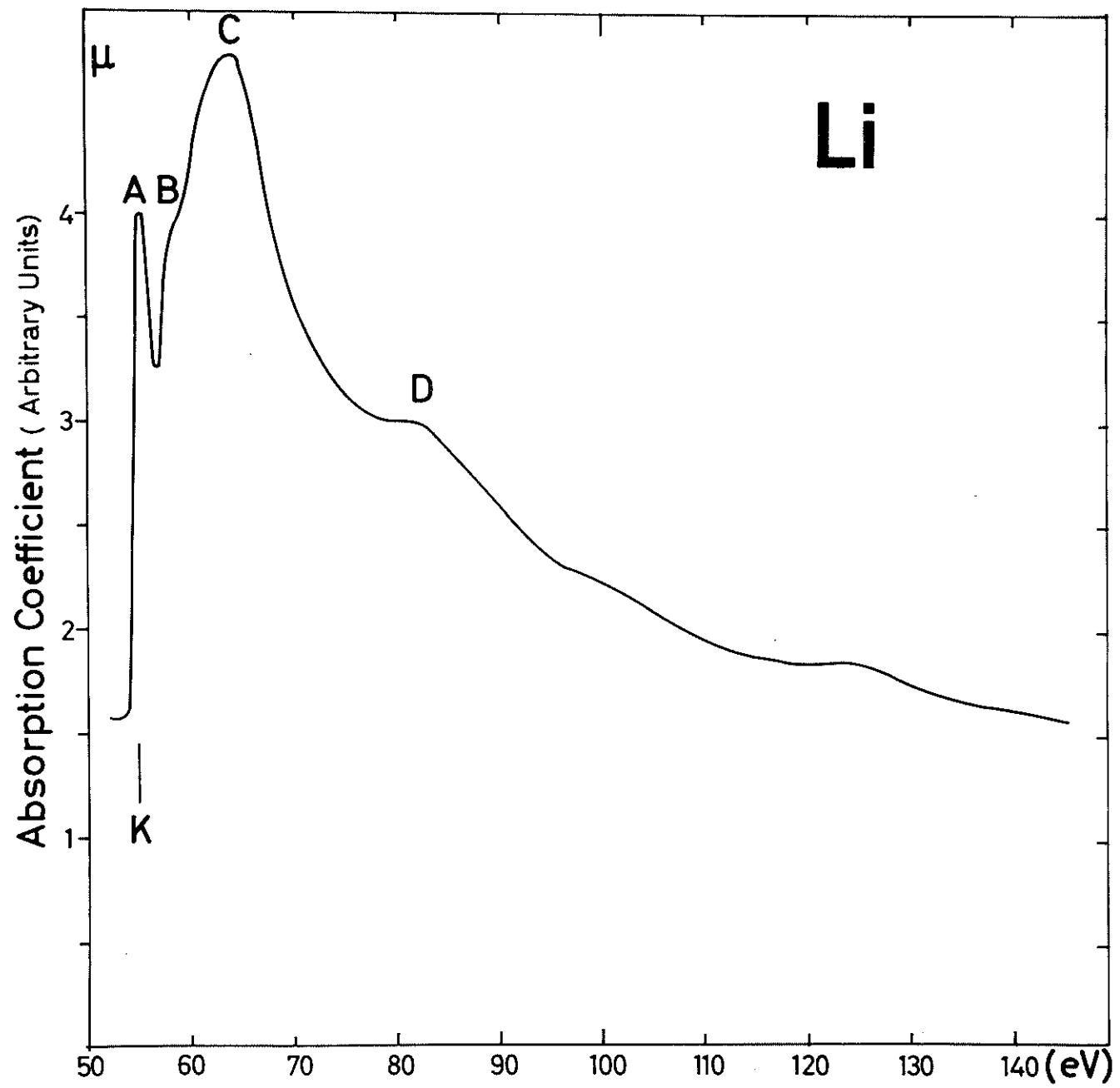
Fig.1

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