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Optical Absorption Measurements of the Transition Metals Ti, V, Cr, Mn, Fe, Co, Ni in the Region of 3p Electron Transitions

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Using the continuous spectrum of synchrotron radiation, the absolute absorption coefficient of seven transition metals has been determined in the spectral range 40 to 300 eV. The strong oscillations reported by previous investigators appear to have been spurious.

Interest in the contribution of the 3p electrons to optical absorption is justified by the hope of getting information about the empty 3d states in the transition metals titanium, vanadium, chromium, manganese, iron, cobalt, nickel. The results known until now[1-7] show rich structure above the onset of 3p transitions but are, in many cases, in contradiction with each other. These structures, if true, would have strong implications for theoretical interpretations.

We have made similar but more extensive measurements. The continuous spectrum of synchrotron light of the 7.5 GeV accelerator DESY was used between 40 and about 300 eV. The wavelength resolution was better than 1 Å (0.1 eV at 40 eV, 8 eV at 300 eV). The energy calibration was of the same order of accuracy. The optical absorption coefficient μ was determined with an absolute accuracy of ± 20 %, but the relative accuracy of adjacent regions was much better, about $1 \cdot 10^4$ cm^{-1}. The metals were evaporated, using an electron gun, onto substrates of zapon and aluminum films. In computing the absorption coefficient the influence of the substrate was eliminated. Most of the technical details are similar to those given in ref. 8.

Figure 1 shows our results in the region 40 eV to 200 eV. Above this region the absorption smoothly decreases to a value at 300 eV, given in Table I. The spectra show an appreciable rise at an energy where the onset of 3p transitions is expected according to values given by Bearden et al.[9] ($M_{II,III}$ in Fig. 1). The rise is rather slow, too slow to be caused by the finite width (∿ 0.2 eV) of the $M_{II,III}$ levels.[2] A measure of the width of the rise can be taken from E_{min} and E_{max} given in Table I. The expected separation of the M_{II} and M_{III} edges,[9] ∿ 1 to 2 eV, does not occur, despite adequate instrumental resolution. The M_I contributions, if at all, show up as a small hump only.

None of the prominent structures found previously is detectable here, though our means of detection were so sensitive that we were able to determine unambiguously small structures such as the double peak in chromium. We believe that the strong fine structure in all former measurements are due to the use of line sources. Also the absolute magnitude of μ in our measurements differs sometimes by an order of magnitude from the older results. We have checked our μ values by performing oscillator sums between the M and L onsets using the values of other authors, mainly Ershov,[10] in the adjacent region of higher energies. The values of N_{eff} given in Table I are near to the expected value of 8 electrons. The somewhat higher values for the heavier metals are probably due to 3d contributions which extend into this region, as indicated in Fig. 1.

The spectral behavior after the absorption maximum appears to be roughly intelligible along the lines of the atomic absorption theories given by Fano and Cooper.[11] The behavior at the first rise has to be interpreted by solid state theory,[12] perhaps by taking into account collective effects. Certainly the first maximum is too broad, in most cases, to enable one to attribute its width, in a one-electron approximation, to that of the empty part of the 3d band.

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Table I. Energy position in eV of E_{min} (the minimum before the strong rise) and E_{max} (the first maximum in absorption), $\mu_{300\ eV}$ (the absorption coefficient at 300 eV) and N_{eff} (the number of effective electrons contributing to the absorption between the M- and L-onset).

	E_{min}	E_{max}	$\mu_{300eV}(10^5\ cm^{-1})$	N_{eff} M to L
Ti	-	45.9	0.4	8.8
V	35.4	47.7	0.9	7.9
Cr	41.2	49.4	1.0	8.6
Mn	45.7	50.8	0.9	9.2
Fe	51.7	57.1	1.1	10.7
Co	57.7	62.3	0.8	9.1
Ni	63.9	68.5	1.4	12.4

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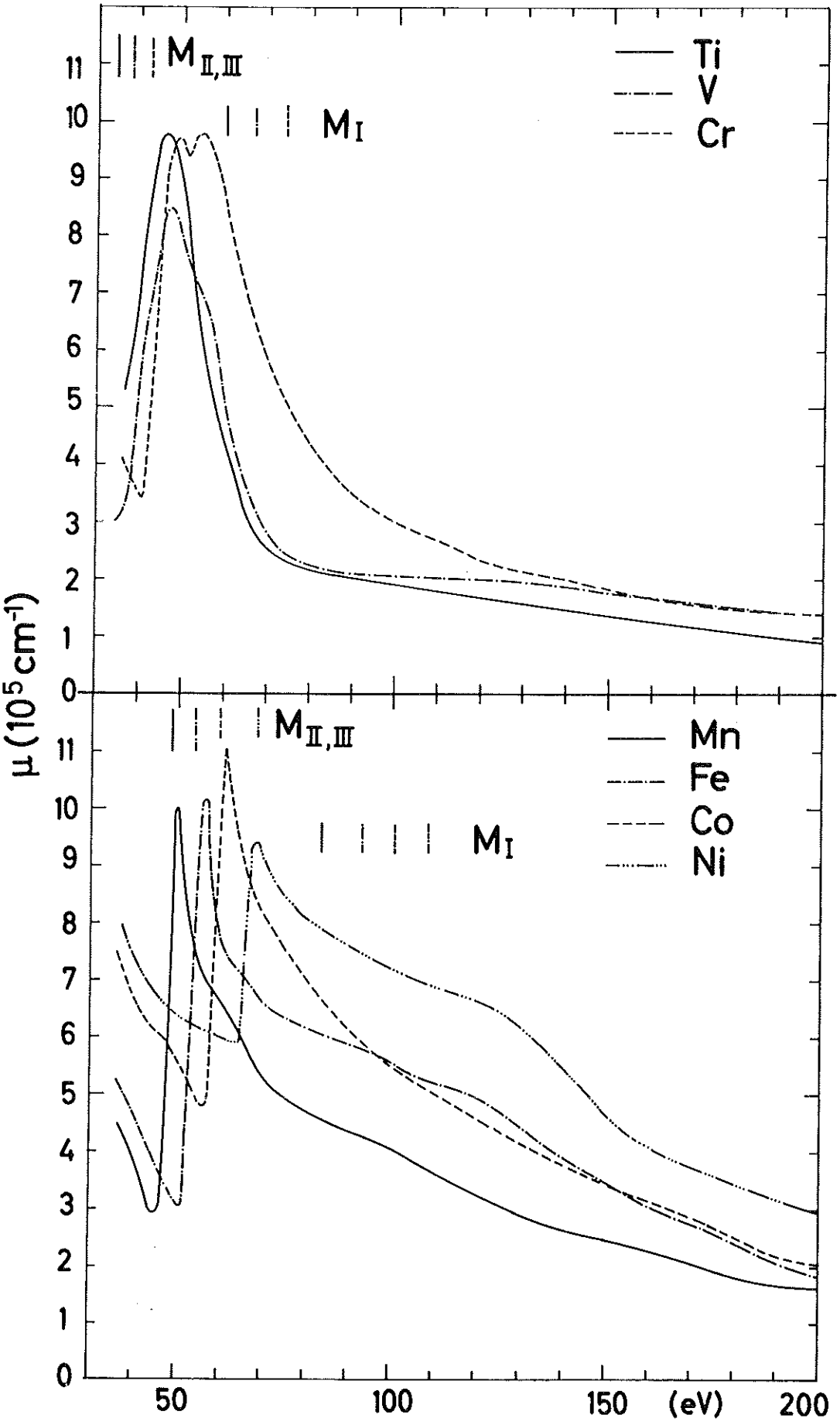
Figure caption

Fig. 1 Absorption coefficient μ of the transition metals Ti, V, Cr, Mn, Fe, Co and Ni.


$M_{II,III}$
M_I
Ti
V
Cr
$M_{II,III}$
M_I
Mn
Fe
Co
Ni
$\mu(10^5 cm^{-1})$
0
1
2
3
4
5
6
7
8
9
10
11
50
100
150
(eV)
200