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by

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Resonance Enhancement of the Nickel d-Band Photoemission

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A detailed analysis of the Ni d-band photoemission near the 3p threshold is presented. The results demonstrate that the d-band emission is coupled to the 3p excitation. The coupling is shown to differ for different parts of the d-band.

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A strong resonance effect in photoemission from nickel was reported for the first time by Guillot et al. in 1977[1]. They showed that the intensity of a peak located at about 6 eV below the Fermi level increases dramatically when the photon energy passes through the 3p threshold at about 66 eV. They explained their result as a Fano type resonance[2] being due to the interaction between the discrete excitation $3p^6\ 3d^9\ 4s \rightarrow 3p^5\ 3d^{10}\ 4s$ and the continuum channel $3p^6\ 3d^9\ 4s \rightarrow 3p^6\ 3d^8\ 4s\ \varepsilon l$ coupled via the super-Coster-Kronig decay $3p^5\ 3d^{10}\ 4s \rightarrow 3p^6\ 3d^8\ 4s\ \varepsilon l$. This interaction had also been invoked for the explanation of the shape of the 3p absorption cross-section near the edge of solid and atomic Ni[3-6]. Since transitions from the s-p-band can explain only part of the emission at 6 eV binding energy (7, 8), several other origins for its interpretation have been suggested[9-13]. The atomic approach to the resonance phenomenon of this peak is supported by the result of Iwan and Koch[14] who found a similar resonance behavior in nickel-phthalocyanine 6 eV below the top of the valence band. While neither Guillot et al. nor Iwan and Koch found a resonant enhancement of the emission from the Ni d-states, photoemission measurements on rare earth compounds[15] showed an enhancement of all rare earth derived states above the 4d level when varying the photon energy through the giant resonance of the 4d cross section. Subsequently, Williams et al.[16] presented a "constant initial state (CIS)" spectrum of the topmost peak of the Ni d-band (initial energy: 0.5 eV below E_F) where a small intensity variation ($\sim$10%) could be seen around the 3p threshold.

In this letter, we present a detailed analysis of our resonant photoemission measurements of the Ni d-band region. The result is that different parts of the d-band photoemission show characteristically distinct variations in the region of the 3p onset. We shall point out that the processes involved appear to be even more complicated than previously assumed.

The measurements are performed on the (110) surface of a nickel single crystal prepared in ultrahigh vacuum (2×10^{-10} Torr) by ion bombardement and annealing. Synchrotron radiation of the storage ring DORIS is monochromatized by the Flipper monochromator[17, 18] and hits the sample in s-polarization. The photoelectrons are analyzed by a commercial double path cylindrical mirror analyzer. Details of the geometry are given in Ref. 19.

A series of energy distribution curves (EDC's) excited with photon energies near the 3p threshold (66 eV) is presented in Fig. 1. Two structures peaking at 0.5 eV (A) and 2 eV (B) below E_F are clearly resolved in the d-band. Of course, the dispersion of the d-bands observed by angular resolved photoemission is averaged out by the experimental arrangement used in our measurements. As can be seen qualitatively from this figure, the intensities of both structures show a different spectral dependence which is also markedly different from the behavior of the 6 eV-peak (C). It should also be noticed that the distribution of the $M_{2,3}$VV-Auger electrons appears to emerge from the 6 eV peak when the photon energy increases above the 3p onset which makes both structures undistinguishable over a certain energy range. Following these observations we analyzed the resonance enhancement of the

area under the two d-band maxima and the 6 eV peak separately. After subtraction of reasonable background of inelastically scattered electrons, we divided the valence band region into three portions with binding energies $E_B \leq 1$ eV (A), 1 eV $\leq E_B \leq 4$ eV (B) and $E_B \geq 4$ eV (C) so choosing the minima of the EDC at 65.9 eV photon energy (Fig. 1) as the boarderlines. The obtained peak areas have been corrected for the photon flux and the transmission of the electron analyzer. The results are presented in Fig. 2. Curve A agrees qualitatively with the CIS-spectrum of Williams et al. (E_i = 0.5 eV) yet showing an intensity variation within 10 eV above the 3p onset which is 2.5 times larger (~25%). The line shape in this energy range shows a typical Fano type resonance with a minimum at 66 eV and a maximum at 71 eV photon energy. A Fano type resonance with similar intensity variation can also be seen at curve B, but this is nearly 3 times broader having the minimum at 61 eV and the maximum at 73 eV. The additional sharp maximum at 67 eV might be due to the overlap with states that are responsible for the huge resonance of the 6 eV peak (curve C), since it has the maximum just at the same energy. Curve C is in agreement with the result of Guillot et al. for the resonance of the 6 eV peak at the (100) surface of Ni under the restriction that we did not obtain data points between 68 eV and 74 eV photon energy because of the impossible subtraction of the $M_{2,3}$VV-Auger signal. For higher photon energies the area of the $M_{2,3}$VV-Auger distribution is also drawn in Fig. 2. For comparison we included the absorption curve of Brown et al.[20] .

The results clearly demonstrate that not only the 6 eV peak but also the Ni d-band photoemission is coupled to the 3p excitation at threshold.

The interaction, however, appears to be weaker since the intensity variation is much smaller than for the 6 eV peak. In particular, it could be shown that the valence band emission is enhanced over a remarkably large photon energy range of at least 30 eV. Furthermore, we want to stress that the 3p - 3d interaction is not the same for the whole d-band but rather differs from the top to the bottom part of the band.

References

1) C. Guillot, Y. Ballu, J. Paigné, J. Lecante, K.P. Jain, P. Thiry, R. Pinchaux, Y. Petroff and L.M. Falicov, Phys. Rev. Lett. 25, 1632 (1977)

2) U. Fano, Phys. Rev. 124, 1866 (1961)

3) B. Sonntag, R. Haensel and C. Kunz, Solid State Comm. 7, 597 (1969)

4) R. Bruhn, B. Sonntag and H.W. Wolff, J. Phys. B12, 203 (1979)

5) L.C. Davis and L.A. Feldkamp, Solid State Comm. 19, 413 (1976)

6) L.C. Davis and L.A. Feldkamp, Phys. Rev. A17, 2012 (1978)

7) R.J. Smith, J. Anderson, J. Hermanson and G.J. Lapeyre, Solid State Comm. 21, 459 (1977)

8) W. Eberhardt and E.W. Plummer, to be published

9) G.G. Tibbetts and W.F. Egelhoff, Jr., Phys. Rev. Lett. 41, 188 (1978)

10) D.R. Penn, Phys. Rev. Lett. 42, 921 (1979)

11) L.A. Feldkamp and L.C. Davis, Phys. Rev. Lett. 43, 151 (1979)

12) H.-W. Wolff, thesis University of Hamburg (1979) and to be published

13) M. Iwan, F.J. Himpsel and D.E. Eastman, to be published

14) M. Iwan and E.E. Koch, Solid State Comm. 31, 261 (1979)

15) W. Lenth, F. Lutz, J. Barth, G. Kalkoffen and C. Kunz, Phys. Rev. Lett. 41, 1185 (1978)

16) G.P. Williams, G.J. Lapeyre, I. Anderson, F. Cerrina, R.E. Dietz and Y. Yafet, Proceedings of the ECOSS Conference, Surface Science

17) W. Eberhardt, G. Kalkoffen and C. Kunz, Nucl. Instr. and Methods 152, 81 (1978)

18) W. Eberhardt, thesis University of Hamburg (1978)

19) G. Kalkoffen, thesis University of Hamburg (1978)

20) F.C. Brown, C. Gähwiller and A.B. Kunz, Solid State Comm. 9, 487 (1971)

Figure Captions

Fig. 1 Energy distribution curves for the d-band region of a Ni (110) surface excited by s-polarized photons with energies close to the 3p threshold. The EDC's are normalized to equal intensity at peak A. MMM marks the maximum of the $M_{2,3}$VV-Auger distribution. Binding energies are referred to the Fermi level. The overall resolution is 0.35 eV.

Fig. 2 Areas under the EDC structures vs. photon energy: Curve A gives the contribution for $E_B \leq 1$ eV (o), curve B for 1 eV $\leq E_B \leq$ 4 eV (◇) and curve C for $E_B \geq 4$ eV (●); curve MMM shows the area under the $M_{2,3}$VV-Auger distribution (□). The scales of the abscissa of these curves are comparable. For comparison, the absorption spectrum of Brown et al. [20] is included.

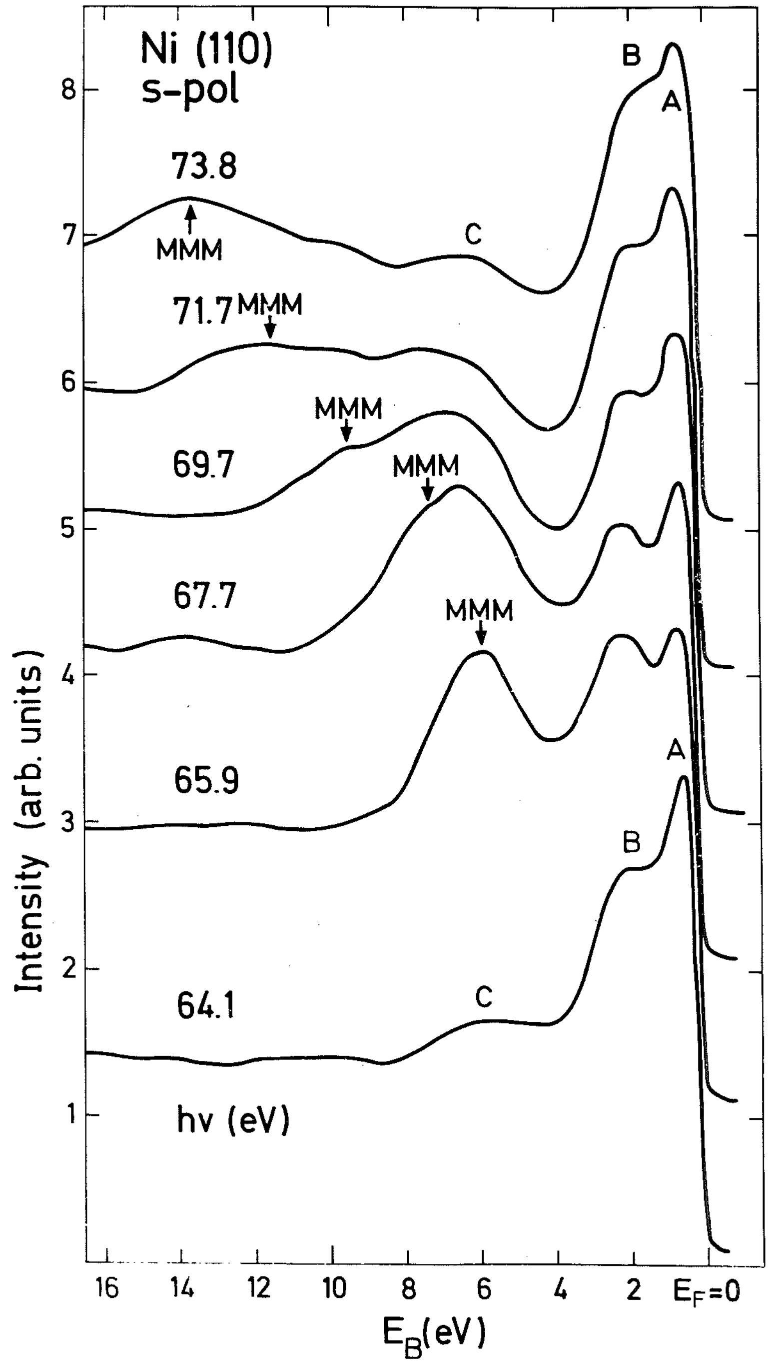

Fig. 1

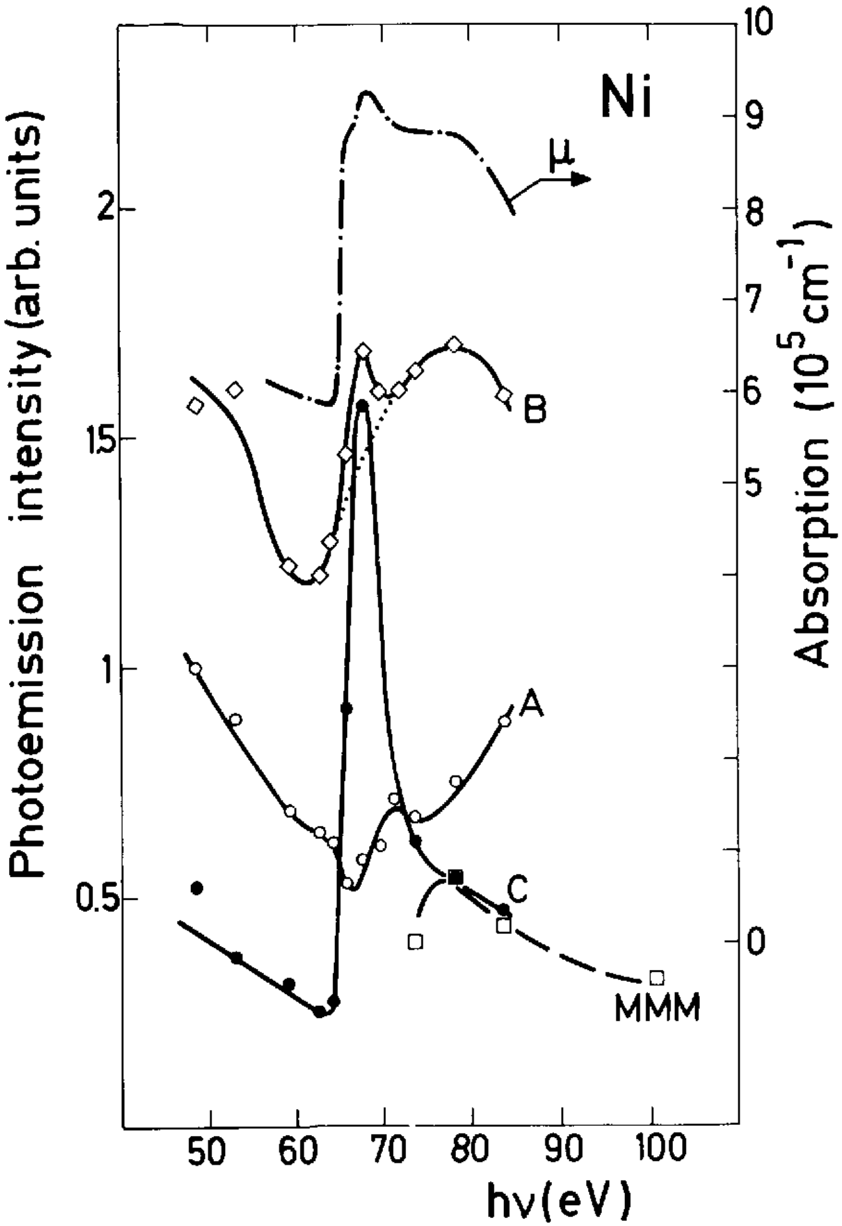
Ni
μ
B
A
C
MMM
Photoemission intensity (arb. units)
Absorption ($10^5 cm^{-1}$)
2
1.5
1
0.5
10
9
8
7
6
5
0
50
60
70
80
90
100
hν(eV)

Fig. 2